ASYMPTOTIC RESULTS FOR THE MINIMUM ENERGY AND BEST PACKING PROBLEMS ON RECTIFIABLE SETS

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CHAPTER I

INTRODUCTION

The problem of determining N points on a d-dimensional manifold that are in some sense uniformly distributed over its surface (or have a prescribed non-uniform distribution) has applications to such diverse fields as crystallography, electrostatics, nanomanufacture, viral morphology, molecular modelling, global positioning and others. There also are a variety of mathematical needs for the discretization of manifolds such as statistical sampling, quadrature rules, starting points for Newton's method, computer-aided geometric design, interpolation schemes, and finite element tesselations.

Various criteria used for generation of such points include best-packing, minimization of energy (e.g. Coulomb potential), and, in particular, for the sphere, t-designs (cubature) and maximization of volume of convex polyhedra with N vertices on the sphere.

In this work we consider two related problems - minimization of energy and best-packing. They are connected to potential theory, real analysis, measure theory, discrete geometry, coding theory.

The minimum energy problem studied in this thesis concerns the generalization of the *Thomson problem* of finding ground state configurations of N classical electrons that can move freely along the surface of a sphere, but cannot leave it (see [46]). Research into this problem has revived during the last decade in connection with the discovery of the third stable state of carbon (after diamond and graphite), fullerenes, molecules C_{60}, C_{70} and others. The study of these large carbon molecules is expected to find applications such areas as nanomanufacture and self-assembling materials.

It is known that the potential energy of a system of two classical electrons in the space is proportional to the reciprocal of the distance between them. The potential energy of a system of N electrons $e_1, \ldots, e_N$ is proportional to the quantity

$$\sum_{1\leq i\neq j\leq N} \frac{1}{\operatorname{dist}(e_i, e_j)}. \tag{1}$$

The Thomson problem asks for configurations of N electrons on a sphere that attain the absolute minimum in (1).

In our considerations the Coulomb potential is replaced by the Riesz potential which is proportional to the reciprocal of the power $s > 0$ of the distance, and the particles are restricted to a rectifiable compact set in Euclidean space $\mathbb{R}^{d'}$ (we reserve the symbol d for the dimension of the conductor).

The rigorous setting of the discrete minimal s-energy problem is as follows. For a collection $\omega_N := \{x_1, \ldots, x_N\}$ of points in $\mathbb{R}^{d'}$ and $s > 0$ we let

$$E_s(\omega_N) := \sum_{1 \le i \ne j \le N} \frac{1}{|x_i - x_j|^s} = \sum_{j=1}^{N} \sum_{\substack{i=1 \\ i \ne j}}^{N} \frac{1}{|x_i - x_j|^s},$$

where $|\cdot|$ stands for the Euclidean distance. The *minimal discrete N-point Riesz s-energy* of a compact set $A \subset \mathbb{R}^{d'}$ is defined as

$$\mathcal{E}_s(A, N) := \min\{E_s(\omega_N) : \omega_N \subset A,\ \#\omega_N = N\}, \tag{2}$$

where $\#W$ denotes the cardinality of W. Our considerations are restricted to compact sets A since the quantity (2) vanishes for unbounded sets and is the same for A and its closure (in the general case we would need to replace "min" with "inf").

For the case $s = 0$ which is known as the logarithmic case, the Riesz potential $|x - y|^{-s}$ is replaced with $\ln(|x - y|^{-1})$. When $A = S^2$ (unit sphere in $\mathbb{R}^3$), the polynomial time generation of "nearly optimal" points for the logarithmic energy is the focus of one of S. Smale's "problems for the next century"; see [45].

The other problem considered in the thesis is the best-packing problem. Given a positive integer N, it is required to find the largest radius $r(N)$ such that there exist N non-overlapping balls with this radius centered at points of the set A. This problem can also be stated in the following way. For a collection $\omega_N = \{x_1, \ldots, x_N\}$ of points in $\mathbb{R}^{d'}$, let

$$\delta(\omega_N) := \min_{1 \le i \ne j \le N} |x_i - x_j|.$$

The *best-packing distance* of N point collections on a compact set A is defined as

$$\delta_N(A) := \max\{\delta(\omega_N) : \omega_N \subset A,\ \#\omega_N = N\}.$$

When $A = S^2$, this problem is called the *Tammes problem.* In the limit as s gets large, the minimum s-energy problem tends to the best-packing problem; namely, for a fixed N and any compact set A

$$\mathcal{E}_s(A, N)^{1/s} \to \frac{1}{\delta_N(A)}, \quad s \to \infty,$$

and if ω_N^s is an s-energy minimizing N point collection on A, $s > 0$, then

$$\delta(\omega_N^s) \to \delta_N(A), \quad s \to \infty.$$

In view of this connection, the best-packing problem is referred to as the case $s = \infty$ of the minimal energy problem. It is known [3] that best-packing configurations on Jordan measurable planar sets and sphere S^2 (as N gets large) give nodes for asymptotically optimal cubature formulas on classes of functions with a given majorant for the modulus of continuity.

We also show in Chapter III that if one raises asymptotic results on the minimal s-energy problem to the power $1/s$ and lets $s \to \infty$, reciprocals of asymptotic results on best-packing will be obtained. This allows to both obtain asymptotics for best-packing from the asymptotics for minimal energy, and having some information on best-packing problem, get immediately information on minimal s-energy problem for sufficiently large values of s.

The exact solution to the best-packing and minimal energy problems are known only in some special cases. When $A = S^1$ (unit circumference), N equally spaced points will provide an optimal configuration for every $s \in [0, \infty]$. On S^2 optimal configurations are known for $s = 0, 1$ and $N = 2 - 4,\ 6,\ 12$ (cf. [50, 31, 1]) and for $s = 0$ and $N = 5$ [15]; when $s = \infty$ the solution is known for $N = 2 - 12$ and $N = 24$ (see [6] for references). The solution is also known in three concrete cases on the sphere in higher dimensions [32, 2].

Obtaining a precise solution to the problems mentioned above for every N is an intractable problem even when A is a sphere. Moreover, numerical computations become very complicated, since the number of local minima appears to increase exponentially, at least for subsequences of cardinalities of configurations.

However, it is possible to find out the asymptotic behavior of both problems on certain classes of compact sets as N gets large. This case is sometimes referred to as "$N = \infty$". The asymptotic behavior of the minimal s-energy depends on the value of s. If s is less than $\dim_H A$ (the Hausdorff dimension of the set A), then $\mathcal{E}_s(A, N) \sim C(s)N^2$, $N \to \infty$, where $C(s)$ is the minimum of the continuous s-energy

$$\int_A \int_A \frac{1}{|x-y|^s} d\mu(x) d\mu(y) \tag{3}$$

taken over all Borel probability measures μ supported on A (see e.g. [36]). In the limit as N gets large the optimal configurations will be distributed according to the probability measure that delivers the minimum in (3), namely the so-called *equlibrium measure.*

Our dissertation will concern the case $s \geq \dim_H A$. In this case, the following results are known.

Theorem A (Martinez-Finkelshtein et al. [39]). *Let $\Gamma \subset \mathbb{R}^{d'}$ be a finite union of rectifiable Jordan arcs such that the total arclength measure of their pairwise intersections is zero. Then for $s > 1$*

$$\mathcal{E}_s(\Gamma, N) \sim 2\zeta(s)\, |\Gamma|^{-s}\, N^{s+1}, \quad N \to \infty,$$

where $\zeta(s) = \sum_{k=1}^{\infty} k^{-s}$ is the classical Riemann zeta-function and $|\Gamma|$ is the total length of the arcs constituting Γ. When $s = 1$ we also have

$$\mathcal{E}_1(\Gamma, N) \sim 2\, |\Gamma|^{-1}\, N^2 \ln N, \quad N \to \infty.$$

Moreover, for any $s \geq 1$, every sequence $\{\omega_N^*\}_{N=2}^{\infty}$ of s-energy minimizing configurations on Γ such that $\#\omega_N^* = N$, $N \geq 2$, is asymptotically uniformly distributed on Γ with respect to the arclength measure.

Remark. Here and below the limit distribution of optimal configurations is understood in the sense of the weak* convergence of the normalized counting measure supported at points of optimal configurations (see Chapter II for the precise definition).

Consider a set in $\mathbb{R}^{d'}$ which is a bi-Lipschitz homotopy of an open set from $\mathbb{R}^d$. We say that a compact set A is a d-dimensional rectifiable manifold if it is contained in a finite union of such sets. By $\mathcal{H}_d(A)$ we will denote the d-dimensional Hausdorff measure in $\mathbb{R}^{d'}$ normalized so that the isometric copy of the cube $[0,1]^d$ has measure 1. The following result was obtained earlier by Hardin and Saff [28, 27].

Theorem B. *Let $s > d \geq 1$ and A be a compact set in $\mathbb{R}^d$ or a d-dimensional rectifiable manifold in $\mathbb{R}^{d'}$. Then*

$$\lim_{N\to\infty} \frac{\mathcal{E}_s(A,N)}{N^{1+s/d}} = \frac{C_{s,d}}{\mathcal{H}_d(A)^{s/d}}, \tag{4}$$

where $C_{s,d} > 0$ is a constant independent of A. If A is a compact set in $\mathbb{R}^d$ or a compact subset of a d-dimensional C^1 manifold in $\mathbb{R}^{d'}$, then

$$\lim_{N\to\infty} \frac{\mathcal{E}_d(A,N)}{N^2 \ln N} = \frac{\beta_d}{\mathcal{H}_d(A)}, \tag{5}$$

where β_d is the Lebesgue measure of the unit ball in $\mathbb{R}^d$.

Moreover, if $\mathcal{H}_d(A) > 0$, any sequence $\{\omega_N^*\}_{N=2}^{\infty}$ of s-energy minimizing configurations on A ($s \geq d$) such that $\#\omega_N^* = N$, $N \geq 2$, is asymptotically uniformly distributed on A with respect to $\mathcal{H}_d$.

It follows from Theorem A that $C_{s,1} = 2\zeta(s)$, $s > 1$. However, for $s > d > 1$, the fundamental energy constant $C_{s,d}$ is unknown. Finding $C_{s,d}$ is, in fact, a very difficult problem. Even the value of the limit as s gets large of $C_{s,d}^{1/s}$ is still unknown for $d > 3$, because it is expressed through the largest sphere packing density in $\mathbb{R}^d$, which has been found only for $d \leq 3$.

For a ball in 3D, it is shown in [37] that N particles repelling each other via the Riesz potential with $0 < s \leq 1$ will be forced to go to the surface of the ball, while for $s > 1$ and N sufficiently large, it will be more energy efficient for at least some of them to go inside the ball. The results from potential theory mentioned above and Theorem B imply that for $s \geq 2$ and large N the particles will uniformly distribute themselves along the ball to achieve the ground state configuration. According to Theorem B, this will also happen for a 3D conductor of any shape, as long as it has a finite and positive volume and its surface has a finite area.

Paper [29] considers the Riesz energy problem on the surface of a torus. It proves that the ground state configurations of a large number of particles interacting via the logarithmic potential ($s = 0$) will be forced out of a certain stripe on the inner part of the torus' surface. This phenomenon is also predicted by computations (by R. Womersley and in [29]) for $0 < s < 1$ with the stripe vanishing as s approaches 1. For $1 < s < 2$ the particles are predicted to distribute (non-uniformly) along the whole surface. Theorem B guarantees for $s \geq 2$ that large ground state configurations will have a uniform distribution.

In Chapter II (see Theorem II.1.1) we extend Theorem B to the case when $A \subset \mathbb{R}^{d'}$ is an image of a compact set from $\mathbb{R}^d$ with respect to a Lipschitz mapping (or which is the same, a finite union of such sets). Sets A constructed in this way are called *d-rectifiable sets*. Thus, we replace the "bi-Lipschitz" with "Lipshitz" in the assumption about the set A in Theorem B. This result also extends Theorem A to the case of an arbitrary finite union of rectifiable curves in $\mathbb{R}^{d'}$, since every rectifiable curve is known to be a Lipschitz image of $[0,1]$ (cf. e.g. [18]). A crucial property for the proof of this theorem is the equality between $\mathcal{H}_d(A)$ and the d-dimensional Minkowski content $\mathcal{M}_d(A)$ (see (13) for the precise definition) on every closed d-rectifiable set [19, Theorem 3.2.29].

For the case when compact set A is a countable but not a finite union of d-rectifiable sets, we prove the following. If $\mathcal{M}_d(A) = \mathcal{H}_d(A)$, then (4) still holds. When $\mathcal{M}_d(A) \neq \mathcal{H}_d(A)$ or $\mathcal{M}_d(A)$ is undefined, for sufficiently large values of s relation (4) fails (for an example of a countable union of d-rectifiable sets with $\mathcal{M}_d(A) \neq \mathcal{H}_d(A)$ see [19, p. 276]).

For the whole Euclidean space $\mathbb{R}^d$, the best-packing problem is stated as the problem of finding the largest density Δ_d of packing equal non-overlapping balls in $\mathbb{R}^d$ (see (37) for the definition). It follows from the definiton of Δ_d that

$$C_{\infty,d} := \lim_{N\to\infty} \delta_N([0,1]^d)\cdot N^{1/d} = 2\left(\frac{\Delta_d}{\beta_d}\right)^{1/d}.$$

The constant Δ_d, and hence, the constant $C_{\infty,d}$, is not known for $d > 3$ (it was shown in [47], [21] that $\Delta_2 = \pi/\sqrt{12}$ and it was recently proved in [26] that $\Delta_3 = \pi/\sqrt{18}$. See [11] for more references). We show in this dissertation that $\lim_{s\to\infty} C_{s,d}^{1/s} = 1/C_{\infty,d}$ for any integer $d \geq 1$ (see Theorem III.1.2).

Concerning the case when $A = S^2$, the papers [25], [48] prove that $\lim_{N\to\infty}\delta_N(S^2)N^{1/2} = \left(8\pi/\sqrt{3}\right)^{1/2}$. Furthermore, the results of [26] imply that for the unit sphere $S^3 \subset \mathbb{R}^4$ we have $\lim_{N\to\infty}\delta_N(S^3)N^{1/3} = \sqrt{2}\pi^{2/3}$.

If A is a d-dimensional compact smooth manifold in $\mathbb{R}^{d'}$, it can be approximated by a tangent plane in the neighborhood of every point, and it is not difficult to see that

$$\lim_{N\to\infty} \delta_N(A)\cdot N^{1/d} = C_{\infty,d}\cdot \mathcal{H}_d(A)^{1/d}. \tag{6}$$

In Chapter III, for compact sets $A \subset \mathbb{R}^{d'}$ representable as at most countable unions of d-rectifiable sets, we show that relation (6) still holds if $\mathcal{M}_d(A) = \mathcal{H}_d(A)$, and fails if $\mathcal{M}_d(A) \neq \mathcal{H}_d(A)$ or $\mathcal{M}_d(A)$ is undefined. In particular, we show that for every closed d-rectifiable set, relation (6) holds and every sequence of best-packing configurations $\{\overline{\omega}_N\}_{N=2}^{\infty}$ such that $\#\overline{\omega}_N = N$, $N \geq 2$, will be asymptotically uniformly distributed on A with respect to $\mathcal{H}_d$. Results similar to (6) for compact sets in $\mathbb{R}^d$ (with $d' = d$) that concern the covering radius, were obtained in [24].

The condition of countable rectifiability in our results is crucial, since in Section III.3 we provide examples of unrectifiable compact sets of integer Hausdorff dimension d with $0 < \mathcal{H}_d(A) < \infty$ such that the limit

$$\lim_{N\to\infty} \delta_N(A) \cdot N^{1/d}$$

and the limit

$$\lim_{N\to\infty} \frac{\mathcal{E}_s(A,N)}{N^{1+s/d}}$$

for s sufficiently large *do not exist*.

If we fix any $s > d'$, using the highest and the lowest order of minimal s-energy among all subsequences of cardinalities of configurations on an arbitrary set in $\mathbb{R}^{d'}$, we can define its upper and lower dimension. We prove that the upper and the lower dimension of any set $A \subset \mathbb{R}^{d'}$ defined in this way coincides with the upper and the lower Minkowski dimension of A, respectively. We also prove that the upper and the lower Minkowski dimensions coincide with the upper and the lower dimensions of a set defined via the asymptotics of the best-packing distance (see Proposition III.2.1).

Minimum s-energy configurations do not, in general, coincide with best-packing configurations. However, on certain classes of sets they turn out to have the same order of the separation distance. Since minimal energy points are easier to compute than best-packing ones, they are suitable for the applications requiring uniform distribution of points on a surface with a "good" separation.

The following estimates of the separation distance of minimal energy points are known. When A is the unit sphere S^d in $\mathbb{R}^{d+1}$, for every $s > d-2$, $s \neq d$, there is a constant $C = C(s,A) > 0$ such that for any sequence $\{\omega_N^*\}_{N=2}^{\infty}$ of s-energy minimizing collections on A with $\#\omega_N^* = N$, $N \geq 2$, there holds

$$\delta(\omega_N^*) \geq \frac{C}{\sqrt[d]{N}}, \quad N \geq 2, \tag{7}$$

(see [12, 41, 17, 22, 14, 35, 16] for the proof of (7) for different ranges of values of s). The estimate (7) is also proved in [28] for $s > d$ and A being a bi-Lipschitz homotopy in $\mathbb{R}^{d'}$ of a compact set from $\mathbb{R}^d$. Earlier, the estimate (7) for $d = 1$ was proved for $s > 1$ on Carleson's curves (cf. [39]). In Section II.3 (the proof is given in Section IV.5 for the more general weighted case) we extend estimate (7) for any $s > d > 0$ to an arbitrary compact set A with $\mathcal{H}_d(A) > 0$ (not requiring d to be an integer). Independently, in [13] estimate (7) was obtained for d-dimensional rectifiable manifolds.

Papers mentioned above, which prove (7) for $s > d$, also show on the corresponding classes of sets that for $s = d$ we have

$$\delta(\omega_N^*) \geq \frac{C}{\sqrt[d]{N \ln N}}, \quad N \geq 2.$$

Better separation estimates for $s = d$ are not known on compact sets $A \neq S^1$. In Section II.3, we also extend this estimate to any compact set with $\mathcal{H}_d(A) > 0$.

Some applications may require placing a large number of points on a surface according to a prescribed non-uniform distribution. For example, for modelling a surface in computer aided geometric design more points are generally required on regions with higher curvature. In Chapter IV we consider the problem of minimizng the *weighted s-energy* for s greater than or equal to the dimension of the surface, as a method for generating non-uniformly distributed points.

Let $w : A \times A \to [0, \infty)$ be a bounded function such that $w(x, y)$ is continuous and strictly positive at every point $(x, y) \in A \times A$ with $x = y$. For $s > 0$ and a collection of points $\omega_N = \{x_1, \ldots, x_N\} \subset A$, let

$$E_s^w(\omega_N) := \sum_{1 \leq i \neq j \leq N} \frac{w(x_i, x_j)}{|x_i - x_j|^s}$$

and define the *weighted N-point s-energy* of a compact set A to be

$$\mathcal{E}_s^w(A, N) := \inf\{E_s^w(\omega_N) : \omega_N \subset A, \ \#\omega_N = N\}.$$

When $w(x, y) \equiv 1$, we get the non-weighted minimal energy problem described above. If $w(x, y) \not\equiv 1$, the particles are still assumed to have the same charge, but the potential through which they interact depends on the positions of the particles on the set A. This problem is different from another generalization of the Thomson problem where particles are allowed to have different charges. In general, instead of a sequence of energy minimizing collections, we study asymptotically energy minimizing sequences of configurations, that is sequences $\{\widetilde{\omega}_N\}_{N=2}^{\infty}$ with $\#\widetilde{\omega}_N = N$, $N \geq 2$, such that

$$\lim_{N \to \infty} \frac{E_s^w(\widetilde{\omega}_N)}{\mathcal{E}_s^w(A, N)} = 1. \tag{8}$$

Theorem IV.1.1 in Chapter IV establishes relation (4) with $\mathcal{H}_d(A)$ replaced by

$$\mathcal{H}_d^{s,w}(A) := \int_A w(x,x)^{-d/s} d\mathcal{H}_d(x)$$

for $s > d$ and any closed d-rectifiable set $A \subset \mathbb{R}^{d'}$. Analogous modifications of relation (5) for the case when $s = d$ and A is a compact subset of a d-dimensional C^1 manifold are proved in Theorem IV.1.2. Moreover, in these cases the limit distribution of any asymptotically energy minimizing sequence of configurations on A will have density

$$\frac{1}{\mathcal{H}_d^{s,w}(A)} \cdot w(x,x)^{-d/s} d\mathcal{H}_d, \quad x \in A.$$

Thus, if we set for example $w(x,y) = (\rho(x)\rho(y))^{-\frac{s}{2d}}$, where the continuous function $\rho(x)$ is the density of the prescribed distribution on A, then the limit distribution of optimal points will have density $\rho(x)$, $x \in A$.

In Chapter V, we investigate the next order term of the minimal s-energy on curves. As Theorem A shows, the main term of $\mathcal{E}_s(\Gamma, N)$ on a Jordan curve Γ is determined by its length for every $s \geq 1$. For a closed, simple and regular C^3 curve in $\mathbb{R}^d$ we show that the next order term of minimal s-energy as $N \to \infty$ has the form $C_s N^{s-1}$, $s > 3$, or $C_3 N^2 \ln N$ for $s = 3$, where the constant C_s is positive and depends on the length of Γ and on the mean square of its curvature. For $1 \leq s < 3$ the next order term has the form $C_s N^2$.

For non-closed simple regular rectifiable C^2 curves $\Gamma \subset \mathbb{R}^d$ we show that the next order term is negative and has order N^s for $s > 2$ and $N^2 \ln N$ for $s = 2$.

Known separation estimates provide only the order of the separation distance in ground state configurations. For the closed curves described above and $s > 2$, we show that the separation distance between N minimal s-energy points asymptotically equals $|\Gamma|/N$ as $N \to \infty$.

CHAPTER II

ASYMPTOTIC RESULTS FOR MINIMUM ENERGY

In this chapter we study the behavior of the discrete minimal Riesz s-energy and optimal configurations as N gets large on rectifiable compact sets and give remarks for other classes of sets. We also extend known lower estimates for the minimal pairwise distance between points in optimal configurations to quite general classes of sets which include sets of arbitrary Hausdorff dimension.

II.1 Minimum energy problem on rectifiable sets.

Notation and definitions. Let d and d' be positive integers with $d \leq d'$. In this section we obtain the main term as $N \to \infty$ of the minimum s-energy on compact d-rectifiable sets in $\mathbb{R}^{d'}$ for $s > d$. We also find the limit distribution of optimal configurations on such sets.

For a collection $\omega_N := \{x_1, \ldots, x_N\}$ of points in $\mathbb{R}^{d'}$ and $s > 0$ we let

$$E_s(\omega_N) := \sum_{1 \leq i \neq j \leq N} \frac{1}{|x_i - x_j|^s},$$

where $|\cdot|$ stands for the Euclidean distance. The *minimal discrete N-point Riesz s-energy* of a compact set $A \subset \mathbb{R}^{d'}$ is defined as

$$\mathcal{E}_s(A, N) := \min_{\substack{\omega_N \subset A \\ \#\omega_N = N}} E_s(\omega_N), \tag{9}$$

where $\#W$ denotes the cardinality of a set W.

Recall that a mapping $\phi : T \to \mathbb{R}^{d'}$, $T \subset \mathbb{R}^d$, is said to be a *Lipschitz mapping on T* if there is some constant $\lambda > 0$ such that

$$|\phi(x) - \phi(y)| \leq \lambda |x - y| \qquad \text{for } x, y \in T, \tag{10}$$

and that ϕ is said to be a *bi-Lipschitz mapping on T (with constant λ)* if

$$(1/\lambda)|x - y| \leq |\phi(x) - \phi(y)| \leq \lambda |x - y| \qquad \text{for } x, y \in T. \tag{11}$$

Following [19] we give the following definitions.

Definition II.1.1. *We say that a set $A \subset \mathbb{R}^{d'}$ is d-rectifiable, if it is the image of a bounded set in $\mathbb{R}^d$ under a Lipschitz mapping.*

Denote by $\mathcal{H}_d$ the d-dimensional Hausdorff measure in $\mathbb{R}^{d'}$ normalized so that an isometric image of $[0,1]^d$ has measure 1.

Definition II.1.2. *A set $A \subset \mathbb{R}^{d'}$ is called $(\mathcal{H}_d, d)$-rectifiable, if $\mathcal{H}_d(A) < \infty$ and A is a union of at most a countable collection of d-rectifiable sets and a set of $\mathcal{H}_d$-measure zero.*

Let β_d be the Lebesgue measure of the unit ball in $\mathbb{R}^d$ and $\beta_0 = 1$. Then,

$$\beta_d = \frac{\pi^{d/2}}{\Gamma\left(1 + d/2\right)}, \quad d \in \mathbb{N}. \tag{12}$$

Denote by $\mathcal{L}_{d'}$ the Lebesgue measure in $\mathbb{R}^{d'}$ and let

$$A(\epsilon) := \{x \in \mathbb{R}^{d'} : \operatorname{dist}(x, A) < \epsilon\}, \quad \epsilon > 0,$$

be the ϵ-neighborhood of the set $A \subset \mathbb{R}^{d'}$.

Definition II.1.3. *The lower and the upper d-dimensional Minkowski content of A are defined by*

$$\underline{\mathcal{M}}_d(A) := \liminf_{\rho \to 0^+} \frac{\mathcal{L}_{d'}(A(\rho))}{\beta_{d'-d}\rho^{d'-d}} \quad \text{and} \quad \overline{\mathcal{M}}_d(A) := \limsup_{\rho \to 0^+} \frac{\mathcal{L}_{d'}(A(\rho))}{\beta_{d'-d}\rho^{d'-d}}, \tag{13}$$

respectively. If they coincide, then the quantity $\mathcal{M}_d(A) := \underline{\mathcal{M}}_d(A) = \overline{\mathcal{M}}_d(A)$ is called the d-dimensional Minkowski content of the set A.

Noting that $\beta_{d'-d}\rho^{d'-d}$ is the Lebesgue measure of a ball of radius ρ in $\mathbb{R}^{d'-d}$, it is not difficult to see that, say, one-dimensional Minkowski content of a rectifiable arc equals its length. In fact, the following statement holds.

Lemma II.1.1. *(see* [19, Theorem 3.2.39]*). If $W \subset \mathbb{R}^{d'}$ is a closed d-rectifiable set, then*

$$\mathcal{M}_d(W) = \mathcal{H}_d(W). \tag{14}$$

We shall also need the following fundamental lemma from geometric measure theory.

Lemma II.1.2. *(see [19, Lemma 3.2.18]). A set $W \subset \mathbb{R}^{d'}$ is $(\mathcal{H}_d, d)$-rectifiable, if and only if for every $\epsilon > 0$ there exist compact sets $K_1,\ K_2,\ K_3, \ldots \subset \mathbb{R}^d$ and bi-Lipschitz mappings $\psi_i : K_i \to \mathbb{R}^{d'}$ with constant $1+\epsilon$, $i = 1, 2, 3, \ldots$, such that $\psi_1(K_1),\ \psi_2(K_2),\ \psi_3(K_3), \ldots$ are disjoint subsets of W with*

$$\mathcal{H}_d\left(W \setminus \bigcup_i \psi_i(K_i)\right) = 0.$$

Another way to characterize $(\mathcal{H}_d, d)$-rectifiable sets is as follows. A set $A \subset \mathbb{R}^{d'}$ with $\mathcal{H}_d(A) < \infty$ is $(\mathcal{H}_d, d)$-rectifiable if and only if A is a union of at most a countable family of d-dimensional C^1 manifolds and a set of $\mathcal{H}_d$-measure zero (cf. [38, p. 214]).

Definition II.1.4. *Let A be compact with $\mathcal{H}_d(A) > 0$ and $\{\omega_N\}_{N=2}^{\infty}$ be a sequence of point configurations on A such that $\#\omega_N = N$, $N \geq 2$. We say that $\{\omega_N\}_{N=2}^{\infty}$ is asymptotically distributed on A according to Borel probability measure μ supported on A, if, for every subset $B \subset A$ whose boundary relative to A has μ-measure zero, we have*

$$\frac{\#(\omega_N \cap B)}{N} \to \mu(B), \quad N \to \infty. \tag{15}$$

Equivalently (cf. [36, p. 9]), this definition can be stated in terms of the weak* convergence of normalized counting measures.

If μ and μ_N, $N \in \mathbb{N}$, are Borel probability measures on A, then the sequence $\{\mu_N\}_{N=1}^{\infty}$ is said to converge *weak** to μ (and we write $\mu_N \xrightarrow{*} \mu$, $N \to \infty$), if for any function f continuous on A, we have

$$\lim_{N\to\infty} \int_A f d\mu_N = \int_A f d\mu.$$

Denote by δ_x the atomic probability measure in $\mathbb{R}^{d'}$ centered at the point $x \in \mathbb{R}^{d'}$. Sequence $\{\omega_N\}_{N=2}^{\infty}$, $\omega_N := \{x_1^N, \ldots, x_N^N\}$, is said to be *asymptotically distributed on A according to Borel probability measure μ*, if

$$\nu(\omega_N) := \frac{1}{N}\sum_{k=1}^{N} \delta_{x_k^N} \xrightarrow{*} \mu, \quad N \to \infty.$$

Main result. In this chapter we prove the following statement.

Theorem II.1.1. *Let $s > d$ and $d' \geq d$, where d and d' are positive integers. For every compact*

$(\mathcal{H}_d, d)$-rectifiable set A in $\mathbb{R}^{d'}$ with $\mathcal{M}_d(A) = \mathcal{H}_d(A)$ we have

$$\lim_{N\to\infty} \frac{\mathcal{E}_s(A,N)}{N^{1+s/d}} = \frac{C_{s,d}}{\mathcal{H}_d(A)^{s/d}}. \tag{16}$$

Moreover, if A is d-rectifiable with $\mathcal{H}_d(A) > 0$, then any sequence $\{\omega_N^*\}_{N=2}^\infty$ of s-energy minimizing collections on A such that $\#\omega_N^* = N$, $N \geq 2$, is asymptotically uniformly distributed on A with respect to $\mathcal{H}_d$, that is

$$\nu(\omega_N^*) \overset{*}{\longrightarrow} \frac{\mathcal{H}_d|_A}{\mathcal{H}_d(A)}, \quad N \to \infty. \tag{17}$$

Remark. In view of (14), equality (16) holds for any closed d-rectifiable set in $\mathbb{R}^{d'}$.

All other results of this chapter will be proved later, since they are either a partial case of the results for the weighted energy from Chapter IV or follow from the best-packing results in Chapter III.

As we prove in Proposition III.1.3 in Chapter III, relation (16) fails for sufficiently large values of s if A is a compact $(\mathcal{H}_d, d)$-rectifiable set for which equality $\mathcal{M}_d(A) = \mathcal{H}_d(A)$ does not hold.

As an example of a rectifiable set not satisfying equality $\mathcal{M}_d(A) = \mathcal{H}_d(A)$, we mention a compact $(\mathcal{H}_2, 2)$-rectifiable set $B \subset \mathbf{R}^3$ with $0 < \mathcal{H}_2(B) < \infty = \mathcal{M}_2(B)$ given in [19, p. 276]. Proposition III.2.1 will imply that $\mathcal{E}_s(B,N) = o(N^{1+s/d})$, $N \to \infty$, for $s > 3$.

We also show in Proposition III.3.1 of Chapter III that the condition of $(\mathcal{H}_d, d)$-rectifiability in Theorem II.1.1 is crucial in the sense that there are non-rectifiable compact sets with $0 < \mathcal{H}_d(A) < \infty$ such that

$$0 < \liminf_{N\to\infty} \frac{\mathcal{E}_s(A,N)}{N^{1+s/d}} < \limsup_{N\to\infty} \frac{\mathcal{E}_s(A,N)}{N^{1+s/d}} < \infty$$

for sufficiently large s. Indeed, we show that this is true for a class of Cantor-type sets described in Section III.3.

II.2 Remarks for general sets.

Next, we state results on the order of the minimal s-energy for compact sets of arbitrary Hausdorff dimension without proof. Proposition II.2.1 is a partial case of Corollary IV.5.1 proved in chapter IV and Proposition II.2.2 is a part of the Proposition III.2.1 proved in Chapter III. Let

$$\mathcal{H}_\alpha^\infty(A) := \inf\{\sum_i (\text{diam } G_i)^\alpha : A \subset \bigcup_i G_i\}.$$

Note that the condition of positivity of the α-dimensional Hausdorff measure $\mathcal{H}_\alpha(A)$ is equivalent to the condition $\mathcal{H}_\alpha^\infty(A) > 0$.

Proposition II.2.1. *Suppose that $\alpha > 0$ and $s > \alpha$. There is a constant $M_{s,\alpha} > 0$ such that for every compact set $A \subset \mathbb{R}^{d'}$ with $\mathcal{H}_\alpha(A) > 0$*

$$\mathcal{E}_s(A, N) \leq \frac{M_{s,\alpha}}{\mathcal{H}_\alpha^\infty(A)^{s/\alpha}} N^{1+s/\alpha}, \quad N \geq 2.$$

For every compact set A with $\mathcal{H}_d(A) > 0$, there also exists a constant $M_\alpha > 0$ such that

$$\mathcal{E}_\alpha(A, N) \leq M_\alpha N^2 \log N, \quad N \geq 2.$$

For a non-integer $\alpha > 0$ let

$$\underline{\mathcal{M}}_\alpha(A) := \liminf_{\rho\to 0^+} \frac{\mathcal{L}_{d'}(A(\rho))}{\rho^{d'-\alpha}} \quad \text{and} \quad \overline{\mathcal{M}}_\alpha(A) := \limsup_{\rho\to 0^+} \frac{\mathcal{L}_{d'}(A(\rho))}{\rho^{d'-\alpha}}$$

denote the lower and the upper α-dimensional Minkowski content of a set $A \subset \mathbb{R}^{d'}$, respectively (when our considerations include sets of non-integer dimension we do not look for numerical values of the constants and therefore, remove in this definition any additional constant factors in the denominator).

Proposition II.2.2. *If $0 < \alpha \leq d' < s$, there are positive constants $c_1 = c_1(s, \alpha)$ and $c_2 = c_2(s, \alpha)$ such that for any infinite set $A \subset \mathbb{R}^{d'}$ we have*

$$c_1 \underline{\mathcal{M}}_\alpha(A)^{-s/\alpha} \leq \limsup_{N\to\infty} \frac{\mathcal{E}_s(A, N)}{N^{1+s/\alpha}} \leq c_2 \underline{\mathcal{M}}_\alpha(A)^{-s/\alpha},$$

$$c_1 \overline{\mathcal{M}}_\alpha(A)^{-s/\alpha} \leq \liminf_{N\to\infty} \frac{\mathcal{E}_s(A, N)}{N^{1+s/\alpha}} \leq c_2 \overline{\mathcal{M}}_\alpha(A)^{-s/\alpha}.$$

Proposition II.2.2 in particular implies that if for some $\alpha > 0$ we have $0 < \underline{\mathcal{M}}_\alpha(A) < \overline{\mathcal{M}}_\alpha(A) < \infty$, then for every $s > d'$ there holds

$$\mathcal{E}_s(A, N) \asymp N^{1+s/\alpha}, \quad N \to \infty.$$

Note that the assertion of Proposition II.2.2 is restricted to $s > d'$ while Proposition II.2.1 gives some information for $s \in [\alpha, d']$.

Using $\underline{\mathcal{M}}_\alpha$ and $\overline{\mathcal{M}}_\alpha$ one can define the lower and the upper Minkowski dimension, respectively, in the same way as the Hausdorff dimension. For certain compact sets A, the upper and the lower Minkowski dimensions do not coincide (cf. [38, p. 77]), which combined with Proposition II.2.2 means that $\mathcal{E}_s(A, N)$ will have different order as $N \to \infty$ for different subsequences of cardinalities of configurations.

II.3 Separation results

The theorem below is a partial case of results obtained in Section IV.5 for the weighted energy problem and its proof will be given there. For a configuration $\omega_N = \{x_1, \ldots, x_N\} \subset A$ let

$$\delta(\omega_N) := \min_{1 \le i \ne j \le N} |x_i - x_j| \tag{18}$$

be its separation distance (or separation radius). We obtain estimates for the separation radius of optimal configurations on sets of arbitrary Hausdorff dimension α. We remark that the normalization for the Hausdorff measure $\mathcal{H}_\alpha$ plays no essential role here.

Theorem II.3.1. *Let $0 < \alpha \le d'$ and $s > \alpha$. There is a constant $c_{s,\alpha} > 0$ such that for every compact set $A \subset \mathbb{R}^{d'}$ with $\mathcal{H}_\alpha(A) > 0$ and any s-energy minimizing configuration $\omega_N^* \subset A$ with $N \ge 2$ points, there holds*

$$\delta(\omega_N^*) \ge \frac{c_{s,\alpha}}{(\mathcal{H}_\alpha^\infty(A) \cdot N)^{1/\alpha}}.$$

For every compact set $A \subset \mathbb{R}^{d'}$ with $\mathcal{H}_\alpha(A) > 0$ there also exists a constant $c_\alpha > 0$ such that for any α-energy minimizing N-point configuration $\omega_N^* \subset A$

$$\delta(\omega_N^*) \ge c_\alpha (N \log N)^{-1/\alpha}, \quad N \ge 2.$$

Remark. There exist compact sets with $0 < \mathcal{H}_\alpha(A) < \infty$ for which best-packing distance $\delta_N(A)$ will go to zero slower than $N^{-1/\alpha}$ as $N \to \infty$ (see comments to Proposition III.2.1). However, taking into account this proposition, for any compact set with $0 < \mathcal{H}_\alpha(A), \overline{M}_\alpha(A) < \infty$ and $s > d'$, we will have

$$\delta(\omega_N^*) \asymp \delta_N(A) \asymp N^{-1/\alpha}, \quad N \to \infty.$$

II.4 Proof of the results on rectifiable sets.

In this section we prove Theorem II.1.1. First, show (16). To describe the precise rate of growth of $\mathcal{E}_s(A,N)$, for $s>d$ define

$$\underline{g}_{s,d}(A) := \liminf_{N\to\infty} \frac{\mathcal{E}_s(A,N)}{N^{1+s/d}}, \qquad \overline{g}_{s,d}(A) := \limsup_{N\to\infty} \frac{\mathcal{E}_s(A,N)}{N^{1+s/d}} \tag{19}$$

and

$$g_{s,d}(A) := \lim_{N\to\infty} \frac{\mathcal{E}_s(A,N)}{N^{1+s/d}}, \tag{20}$$

if this limit exists. We will need the following statements (see Lemmas 3.2 and 3.3 in [28]). Recall that $\operatorname{dist}(B,D) := \inf\{|x-y| : x\in B,\ y\in D\}$ denote the distance between sets $B, D\subset \mathbb{R}^{d'}$.

Lemma II.4.1. *Let $s\geq d$ and suppose that B and D are bounded sets in $\mathbb{R}^{d'}$ such that* $\operatorname{dist}(B,D)>0$*. Then*

$$\overline{g}_{s,d}(B\cup D)^{-d/s} \geq \overline{g}_{s,d}(B)^{-d/s} + \overline{g}_{s,d}(D)^{-d/s}.$$

Lemma II.4.2. *Let $s\geq d$ and $B, D\subset\mathbb{R}^{d'}$ be bounded sets. Then*

$$\underline{g}_{s,d}(B\cup D)^{-d/s} \leq \underline{g}_{s,d}(B)^{-d/s} + \underline{g}_{s,d}(D)^{-d/s}.$$

Furthermore, if $\underline{g}_{s,d}(B), \underline{g}_{s,d}(D)>0$ and at least one of these quantities is finite, then

$$\lim_{\mathcal{N}\ni N\to\infty} \frac{\#(\widetilde{\omega}_N\cap B)}{N} = \frac{\underline{g}_{s,d}(D)^{d/s}}{\underline{g}_{s,d}(B)^{d/s} + \underline{g}_{s,d}(D)^{d/s}} \tag{21}$$

holds for any subsequence $\{\widetilde{\omega}_N\}_{N\in\mathcal{N}}$ of N-point configurations in $B\cup D$ such that

$$\lim_{\mathcal{N}\ni N\to\infty} \frac{E_s(\widetilde{\omega}_N)}{N^{1+s/d}} = \left(\underline{g}_{s,d}(B)^{-d/s} + \underline{g}_{s,d}(D)^{-d/s}\right)^{-s/d},$$

where $\mathcal{N}$ is some infinite subset of $\mathbb{N}$.

This statement in particular shows sub-additivity of $\underline{g}_{s,d}(\cdot)^{-d/s}$. We also remark that these lemmas hold when quantities are 0 or infinite using $0^{-d/s} = 0^{-s/d} = \infty$ and $\infty^{-d/s} = \infty^{-s/d} = 0$.

Regularity lemma. To get an estimate from below for $\underline{g}_{s,d}(A)$ we will also need the following result.

Lemma II.4.3. *Let $s > d$ and suppose that $A \subset \mathbb{R}^{d'}$ is a compact set such that $\mathcal{M}_d(A)$ exists and is finite. Then for every $\epsilon \in (0,1)$ there is some $\delta > 0$ such that for any compact set $K \subset A$ with $\underline{\mathcal{M}}_d(K) > \mathcal{M}_d(A) - \delta$ we have*

$$\underline{g}_{s,d}(A) \geq (1-\epsilon)\underline{g}_{s,d}(K). \tag{22}$$

Proof. The assertion of the lemma holds trivially if $\underline{g}_{s,d}(A) = \infty$. Hence, we assume $\underline{g}_{s,d}(A) < \infty$. Let $\mathcal{N} \subset \mathbb{N}$ be an infinite subset such that

$$\lim_{\mathcal{N}\ni N\to\infty} \frac{\mathcal{E}_s(A,N)}{N^{1+s/d}} = \underline{g}_{s,d}(A).$$

Choose $\delta \in \left(0, 1/2^{4d}\right)$ and set

$$\rho := \delta^{1/(4d)} \quad \text{and} \quad h_N := \frac{1}{3}\rho^2 N^{-1/d}, \qquad N \in \mathcal{N}. \tag{23}$$

Suppose K is a compact subset of A such that $\underline{\mathcal{M}}_d(K) > \mathcal{M}_d(A) - \delta$. Then there is some $N_\delta \in \mathbb{N}$ such that for any $N > N_\delta$, $N \in \mathcal{N}$, we have

$$\frac{\mathcal{L}_{d'}[A(h_N)]}{\beta_{d'-d} h_N^{d'-d}} \leq \mathcal{M}_d(A) + \delta \quad \text{and} \quad \frac{\mathcal{L}_{d'}[K(h_N)]}{\beta_{d'-d} h_N^{d'-d}} \geq \mathcal{M}_d(A) - \delta. \tag{24}$$

For $N \in \mathcal{N}$ with $N > N_\delta$, let $\omega_N^* := \{x_{1,N}, \ldots, x_{N,N}\}$ be an s-energy minimizing N-point configuration on A. For $i = 1, \ldots, N$, let $r_i^N := \min_{j:j\neq i} |x_{j,N} - x_{i,N}|$ denote the distance from $x_{i,N}$ to its nearest neighbor in ω_N^*. Further, we partition ω_N^* into a "well-separated" subset

$$\omega_N^1 := \{x_{i,N} \in \omega_N^* : r_i^N \geq \rho N^{-1/d}\},$$

and its complement $\widetilde{\omega}_N^1 := \omega_N^* \setminus \omega_N^1$. We next show that ω_N^1 has sufficiently many points. For $N \in \mathcal{N}$, we obtain

$$\begin{aligned}\mathcal{E}_s(A,N) = E_s(\omega_N^*) &= \sum_{i=1}^{N}\sum_{\substack{j=1\\ j\neq i}}^{N} \frac{1}{|x_{i,N} - x_{j,N}|^s} \geq \sum_{i=1}^{N} \frac{1}{(r_i^N)^s} \\ &\geq \sum_{x_{i,N}\in\widetilde{\omega}_N^1} \frac{1}{(r_i^N)^s} \geq \sum_{x_{i,N}\in\widetilde{\omega}_N^1} \frac{1}{\left(\rho N^{-1/d}\right)^s} = \#\widetilde{\omega}_N^1 \rho^{-s} N^{s/d}.\end{aligned}$$

Let $k_0 := \underline{g}_{s,d}(A) + 1$. There is $N_1 \in \mathbb{N}$ such that for any $N > N_1$, $N \in \mathcal{N}$,

$$\frac{\mathcal{E}_s(A,N)}{N^{1+s/d}} < k_0.$$

For the rest of the proof of this lemma, let $N \in \mathcal{N}$ be greater than $N_2 := \max\{N_1, N_\delta\}$. Then,

$$\frac{\#\widetilde{\omega}_N^1}{\rho^s N} \le \frac{\mathcal{E}_s(A,N)}{N^{1+s/d}} < k_0,$$

and, hence, we have

$$\#\widetilde{\omega}_N^1 < k_0\rho^s N \text{ and } \#\omega_N^1 > (1 - k_0\rho^s)N. \tag{25}$$

Next we consider

$$\omega_N^2 := \omega_N^1 \bigcap K(3h_N), \quad \widetilde{\omega}_N^2 := \omega_N^1 \setminus K(3h_N),$$

and show that the cardinality of ω_N^2 is sufficiently large. From (24) we get

$$\begin{aligned} \mathcal{L}_{d'}[A(h_N)\backslash K(h_N)] &= \mathcal{L}_{d'}[A(h_N)] - \mathcal{L}_{d'}[K(h_N)] \\ &\le (\mathcal{M}_d(A)+\delta)\beta_{d'-d}h_N^{d'-d} - (\mathcal{M}_d(A)-\delta)\beta_{d'-d}h_N^{d'-d} \\ &= 2\beta_{d'-d}\delta h_N^{d'-d}. \end{aligned} \tag{26}$$

Note, that

$$F_N := \bigcup_{x\in\widetilde{\omega}_N^2} B(x,h_N) \subset A(h_N) \setminus K(h_N), \tag{27}$$

where $B(a,r)$ is the open ball in $\mathbb{R}^{d'}$ centered at a point a with radius $r > 0$.

For any distinct points $x_{i,N}, x_{j,N} \in \widetilde{\omega}_N^2$ we have

$$|x_{i,N} - x_{j,N}| \ge r_i^N \ge \rho N^{-1/d} > \rho^2 N^{-1/d} = 3h_N.$$

Hence, $B(x_{i,N}, h_N) \bigcap B(x_{j,N}, h_N) = \emptyset$. Then, using (26) and (27), we get

$$\begin{aligned} \#\widetilde{\omega}_N^2 &= \left(\beta_{d'}h_N^{d'}\right)^{-1} \sum_{x\in\widetilde{\omega}_N^2} \mathcal{L}_{d'}[B(x,h_N)] = \left(\beta_{d'}h_N^{d'}\right)^{-1} \mathcal{L}_{d'}(F_N) \\ &\le \left(\beta_{d'}h_N^{d'}\right)^{-1} \mathcal{L}_{d'}[A(h_N) \setminus K(h_N)] \le 2\beta_{d'-d}\beta_{d'}^{-1}\delta h_N^{-d}. \end{aligned}$$

Hence, recalling (23), we have

$$\#\widetilde{\omega}_N^2 \le 2 \cdot 3^d \beta_{d'-d} \beta_{d'}^{-1} \delta^{1/2} N. \tag{28}$$

Let $\chi_0 := 2 \cdot 3^d \beta_{d'-d} \beta_{d'}^{-1}$. Then, using (25) and (28), we have

$$\#\omega_N^2 = \#\omega_N^1 - \#\widetilde{\omega}_N^2 \ge \left(1 - k_0 \rho^s - \chi_0 \delta^{1/2}\right) N.$$

Next, we choose a configuration ω_N^K of points in K which is close to ω_N^2 and has the same number of points and order of the minimal s-energy as ω_N^2. For every $x_{i,N} \in \omega_N^2$ pick a point $y_{i,N} \in K$ such that $|x_{i,N} - y_{i,N}| < 3h_N = \rho^2 N^{-1/d}$ and let $\omega_N^K := \{y_{i,N} : x_{i,N} \in \omega_N^2\}$. Since every point $x_{i,N} \in \omega_N^2$ lies in ω_N^1, we have

$$|x_{i,N} - y_{i,N}| < \rho^2 N^{-1/d} \le \rho r_i^N \le \rho \, |x_{i,N} - x_{j,N}| \, , \quad j \ne i.$$

Then, if $x_{i,N} \ne x_{j,N}$ are points from ω_N^2, we have

$$\begin{aligned} |y_{i,N} - y_{j,N}| &= |y_{i,N} - x_{i,N} + x_{i,N} - x_{j,N} + x_{j,N} - y_{j,N}| \\ &\ge |x_{i,N} - x_{j,N}| - |x_{i,N} - y_{i,N}| - |x_{j,N} - y_{j,N}| \\ &\ge |x_{i,N} - x_{j,N}| - 2\rho \, |x_{i,N} - x_{j,N}| = (1 - 2\rho) \, |x_{i,N} - x_{j,N}| \, . \end{aligned}$$

Since $\rho \in (0, 1/2)$, it follows that $\#\omega_N^K = \#\omega_N^2$ and for $N \in \mathcal{N}$,

$$\begin{aligned} E_s(\omega_N^*) &= \sum_{x \ne y \in \omega_N^*} \frac{1}{|x-y|^s} \ge \sum_{x \ne y \in \omega_N^2} \frac{1}{|x-y|^s} \\ &\ge (1-2\rho)^s \sum_{x \ne y \in \omega_N^K} \frac{1}{|x-y|^s} = (1-2\rho)^s E_s(\omega_N^K). \end{aligned}$$

Now suppose $\epsilon \in (0,1)$. We may choose $\delta > 0$ sufficiently small (recall $\rho = \delta^{1/(4d)}$) so that

$(1-2\rho)^s(1-k_0\rho^s-\chi_0\delta^{1/2})^{1+s/d} \geq (1-\epsilon)$. Hence,

$$\begin{aligned}
\underline{g}_{s,d}(A) &= \lim_{\mathcal{N}\ni N\to\infty} \frac{E_s(\omega_N^*)}{N^{1+s/d}} \geq (1-2\rho)^s \liminf_{\mathcal{N}\ni N\to\infty} \frac{E_s(\omega_N^K)}{N^{1+s/d}} \\
&\geq (1-2\rho)^s \liminf_{\mathcal{N}\ni N\to\infty} \frac{\mathcal{E}_s(K,\#\omega_N^2)}{(\#\omega_N^2)^{1+s/d}} \cdot \left(\frac{\#\omega_N^2}{N}\right)^{1+s/d} \\
&\geq (1-2\rho)^s \left(1-k_0\rho^s-\chi_0\delta^{1/2}\right)^{1+s/d} \liminf_{N\to\infty} \frac{\mathcal{E}_s(K,N)}{N^{1+s/d}} \\
&\geq (1-\epsilon)\underline{g}_{s,d}(K)
\end{aligned}$$

holds for any compact subset $K \subset A$ such that $\underline{\mathcal{M}}_d(K) > \mathcal{M}_d(A) - \delta$. Lemma II.4.3 is proved.

Final part of the proof of (16). We remark that if $K \subset \mathbb{R}^d$ is compact, then by Theorem B, for $s > d$,

$$g_{s,d}(K) = \frac{C_{s,d}}{\mathcal{L}_d(K)^{s/d}}. \tag{29}$$

Suppose $0 < \epsilon < 1$. Since $A \subset \mathbb{R}^{d'}$ is a compact $(\mathcal{H}_d, d)$-rectifiable set, Lemma II.1.2 implies the existence of compact sets $K_1,\ K_2,\ K_3,\ \ldots \subset \mathbb{R}^d$ and bi-Lipschitz mappings $\psi_i : K_i \to \mathbb{R}^{d'}$, $i = 1, 2, 3, \ldots$, with constant $1+\epsilon$ such that $\psi_1(K_1)$, $\psi_2(K_2)$, $\psi_3(K_3), \ldots$ are disjoint subsets of A whose union covers $\mathcal{H}_d$-almost all of A.

Let n be large enough so that

$$\mathcal{H}_d\left(\bigcup_{i=1}^n \psi_i(K_i)\right) = \sum_{i=1}^n \mathcal{H}_d(\psi_i(K_i)) \geq (1+\epsilon)^{-d}\,\mathcal{H}_d(A).$$

Since each ψ_i is bi-Lipschitz with constant $(1+\epsilon)$, we have

$$\begin{aligned}
\overline{g}_{s,d}(\psi_i(K_i)) &\leq (1+\epsilon)^s g_{s,d}(K_i) = C_{s,d}(1+\epsilon)^s \mathcal{L}_d(K_i)^{-s/d} \\
&\leq C_{s,d}(1+\epsilon)^{2s}\mathcal{H}_d(\psi_i(K_i))^{-s/d}.
\end{aligned} \tag{30}$$

Applying Lemma II.4.1 and (30) we obtain

$$\begin{aligned}
\overline{g}_{s,d}(A) &\leq \overline{g}_{s,d}\left(\bigcup_{i=1}^n \psi_i(K_i)\right) \leq \left(\sum_{i=1}^n \overline{g}_{s,d}(\psi_i(K_i))^{-d/s}\right)^{-s/d} \\
&\leq C_{s,d}(1+\epsilon)^{2s}\left(\sum_{i=1}^n \mathcal{H}_d(\psi_i(K_i))\right)^{-s/d} \leq C_{s,d}(1+\epsilon)^{3s}\mathcal{H}_d(A)^{-s/d}.
\end{aligned} \tag{31}$$

We next provide a lower bound for $\underline{g}_{s,d}(A)$. By assumptions, $\mathcal{M}_d(A) = \mathcal{H}_d(A) < \infty$. Let $\delta > 0$ be as in Lemma II.4.3, i.e., inequality (22) holds for every compact set $K \subset A$ such that $\mathcal{M}_d(K) > \mathcal{M}_d(A) - \delta$. Since all sets $\psi_i(K_i)$ ate d-rectifiable, Lemma II.1.1 holds for each of them. Let n' be large enough so that

$$\mathcal{M}_d\left(\bigcup_{i=1}^{n'} \psi_i(K_i)\right) = \sum_{i=1}^{n'} \mathcal{H}_d[\psi_i(K_i)] > \mathcal{H}_d(A) - \delta = \mathcal{M}_d(A) - \delta.$$

As in (30) we have

$$\begin{aligned}\underline{g}_{s,d}(\psi_i(K_i)) &\geq (1+\epsilon)^{-s} g_{s,d}(K_i) = C_{s,d}(1+\epsilon)^{-s}\mathcal{L}_d(K_i)^{-s/d} \\ &\geq C_{s,d}(1+\epsilon)^{-2s}\mathcal{H}_d(\psi_i(K_i))^{-s/d}.\end{aligned} \tag{32}$$

Then Lemmas II.4.2 and II.4.3, and relation (32) give

$$\begin{aligned}\underline{g}_{s,d}(A) &\geq (1-\epsilon)\underline{g}_{s,d}\left(\bigcup_{i=1}^{n'} \psi_i(K_i)\right) \geq (1-\epsilon)\left(\sum_{i=1}^{n'} \underline{g}_{s,d}[\psi_i(K_i)]^{-d/s}\right)^{-s/d} \\ &\geq \frac{(1-\epsilon)C_{s,d}}{(1+\epsilon)^{2s}}\left(\sum_{i=1}^{n'} \mathcal{H}_d[\psi_i(K_i)]\right)^{-s/d} \geq \frac{(1-\epsilon)C_{s,d}}{(1+\epsilon)^{2s}}\mathcal{H}_d(A)^{-s/d}.\end{aligned} \tag{33}$$

Letting ϵ go to zero in (31) and (33), we obtain (16).

Proof of (17). Now suppose that A is d-rectifiable, $\mathcal{H}_d(A) > 0$ and $\omega_N^* = \{x_1^N, \ldots, x_N^N\}$, $N \in \mathbb{N}$, is a sequence of s-energy minimizing N-point configurations on A. To show (17), it is sufficient to prove that $\{\omega_N^*\}_{N=2}^\infty$ satisfies (15) with $\mu = \frac{\mathcal{H}_d|_A}{\mathcal{H}_d(A)}$. Let $B \subset A$ be such that its boundary relative to A has $\mathcal{H}_d$-measure zero.

Let $\overline{B}$ be the closure of the set B. Since $\overline{B}$ and $\overline{A \setminus B}$, as subsets of A, are also d-rectifiable, in view of Lemma II.1.1 they satisfy relaton (16). Hence,

$$\begin{aligned}\lim_{N\to\infty} \frac{E_s(\omega_N^*)}{N^{1+s/d}} &= C_{s,d}\left(\mathcal{H}_d(A)\right)^{-s/d} \\ &= C_{s,d}\left(\mathcal{H}_d(\overline{B}) + \mathcal{H}_d(\overline{A \setminus B})\right)^{-s/d} \\ &= \left(g_{s,d}(\overline{B})^{-d/s} + g_{s,d}(\overline{A \setminus B})^{-d/s}\right)^{-s/d}.\end{aligned}$$

Since $\mathcal{H}_d(\overline{B}) < \infty$, and $\mathcal{H}_d(\overline{A \setminus B}) < \infty$ as for d-rectifiable sets, relation (16) implies that

$\underline{g}_{s,d}(\overline{B}), \underline{g}_{s,d}(\overline{A \setminus B}) > 0$. One of the quantities $\underline{g}_{s,d}(\overline{B})$ or $\underline{g}_{s,d}(\overline{A \setminus B})$ will be finite, since $\mathcal{H}_d(\overline{B})$ or $\mathcal{H}_d(\overline{A \setminus B})$ has to be positive. Then using relation (21) in Lemma II.4.2 and relation (16), we get

$$\lim_{N \to \infty} \frac{\#\left(\omega_N^* \bigcap B\right)}{N} = \frac{g_{s,d}(\overline{A \setminus B})^{d/s}}{g_{s,d}(\overline{B})^{d/s} + g_{s,d}(\overline{A \setminus B})^{d/s}} = \frac{\mathcal{H}_d(B)}{\mathcal{H}_d(A)}.$$

showing that (17) holds.

CHAPTER III

ASYMPTOTIC RESULTS FOR BEST-PACKING

As usually, we will denote by $\mathbf{R}^{d'}$ the embedding space, reserving the symbol d for the dimension of the set being considered. As before, for a collection of N distinct points $\omega_N = \{y_1, \ldots, y_N\} \subset \mathbf{R}^{d'}$ we set

$$\delta(\omega_N) := \min_{1 \le i \ne j \le N} |y_i - y_j|,$$

and for an infinite set $A \subset \mathbb{R}^{d'}$, we let

$$\delta_N(A) := \sup\{\delta(\omega_N) \ : \ \omega_N \subset A, \ \#\omega_N = N\} \tag{34}$$

be the *best-packing distance* of N-point configurations on A, where $\#X$ denotes the cardinality of the set X. Let $0 < \alpha \le d'$ and set

$$\underline{g}_{\infty,\alpha}(A) := \liminf_{N\to\infty} \ \delta_N(A) \cdot N^{1/\alpha}, \qquad \overline{g}_{\infty,\alpha}(A) := \limsup_{N\to\infty} \ \delta_N(A) \cdot N^{1/\alpha}. \tag{35}$$

We further put

$$g_{\infty,\alpha}(A) := \lim_{N\to\infty} \delta_N(A) \cdot N^{1/\alpha},$$

if this limit exists. On relating these quantities to the *largest sphere packing density* in $\mathbb{R}^d$, which we denote by Δ_d (see (37) below), it can be shown that $g_{\infty,d}([0,1]^d)$ exists and is given by

$$C_{\infty,d} := g_{\infty,d}([0,1]^d) = 2\left(\frac{\Delta_d}{\beta_d}\right)^{1/d}, \tag{36}$$

where, as before, β_d is the Lebesgue measure (volume) of the unit ball in $\mathbb{R}^d$. It is not difficult to show that $g_{\infty,d}(A)$ exists for d-dimensional smooth manifolds and domains. In this chapter we shall establish the existence of $g_{\infty,d}(A)$ for a class of rectifiable sets and provide a formula for it in terms of the largest sphere packing density in $\mathbb{R}^d$; we also describe the limiting distribution of best-packing points (see Theorem III.1.1).

Recall that the definition of Δ_d is as follows (cf. [20, Chapter 3] or [42, Chapter 1]). Let $\mathcal{L}_d$

stand for the Lebesgue measure in $\mathbb{R}^d$. Denote by Λ_d the set of collections $\mathcal{P}$ of non-overlapping unit balls in $\mathbb{R}^d$ for which the density

$$\rho(\mathcal{P}) := \lim_{r\to\infty} (2r)^{-d} \cdot \mathcal{L}_d \left(\bigcup_{B\in\mathcal{P}} B \cap [-r,r]^d \right)$$

exists. Then

$$\Delta_d := \sup_{\mathcal{P}\in\Lambda_d} \rho(\mathcal{P}). \tag{37}$$

Recall that $\Delta_2 = \pi/\sqrt{12}$ (cf. [47] or [20]), $\Delta_3 = \pi/\sqrt{18}$ [26], and Δ_d is unknown for $d > 3$. On the plane the highest density is achieved by the hexagonal packing of circles, where each circle touches six others. In 3D the maximum of the density is attained by packing of balls whose centers form the face center cubic lattice and by the canonball packing.

For non-integer $\alpha \geq 0$ we set $\beta_\alpha = 1$. Recall that $A(\epsilon)$, $\epsilon > 0$, is the ϵ-neighborhood of the set $A \subset \mathbb{R}^{d'}$, and the lower and the upper α-dimensional Minkowski content of A are defined by

$$\underline{\mathcal{M}}_\alpha(A) := \liminf_{\rho\to 0^+} \frac{\mathcal{L}_{d'}(A(\rho))}{\beta_{d'-\alpha}\rho^{d'-\alpha}} \quad \text{and} \quad \overline{\mathcal{M}}_\alpha(A) := \limsup_{\rho\to 0^+} \frac{\mathcal{L}_{d'}(A(\rho))}{\beta_{d'-\alpha}\rho^{d'-\alpha}}, \tag{38}$$

respectively. If they coincide, then the quantity $\mathcal{M}_\alpha(A) := \underline{\mathcal{M}}_\alpha(A) = \overline{\mathcal{M}}_\alpha(A)$ is called the α-dimensional Minkowski content of the set A.

III.1 Best-packing on rectifiable sets

The main result of this chapter is an analogue of Theorem II.1.1 for best-packing configurations stated below.

Theorem III.1.1. *Let $d \leq d'$, where d, d' are positive integers, and $A \subset \mathbf{R}^{d'}$ be an infinite compact $(\mathcal{H}_d, d)$-rectifiable set. If $\mathcal{M}_d(A) = \mathcal{H}_d(A)$, then $g_{\infty,d}(A)$ exists and is given by*

$$g_{\infty,d}(A) = C_{\infty,d} \cdot \mathcal{H}_d(A)^{1/d} = 2\left(\frac{\Delta_d}{\beta_d}\right)^{1/d} \cdot \mathcal{H}_d(A)^{1/d}. \tag{39}$$

Moreover, if $\overline{\mathcal{M}}_d(A) > \mathcal{H}_d(A)$, then

$$\overline{g}_{\infty,d}(A) > C_{\infty,d} \cdot \mathcal{H}_d(A)^{1/d}. \tag{40}$$

If A is d-rectifiable with $\mathcal{H}_d(A) > 0$, then every sequence $\{\overline{\omega}_N\}_{N=2}^{\infty}$ of best-packing configurations on A such that $\#\overline{\omega}_N = N$, $N \geq 2$, is asymptotically uniformly distributed on A with respect to $\mathcal{H}_d$, that is

$$\nu(\overline{\omega}_N) \xrightarrow{*} \frac{\mathcal{H}_d|_A}{\mathcal{H}_d(A)}, \quad N \to \infty. \tag{41}$$

In view of relation (14), and the fact that any $(\mathcal{H}_d, d)$-rectifiable set can be approximated by its closed d-rectifiable subsets (cf. Lemma II.1.2), we either have $\mathcal{M}_d(A) = \mathcal{H}_d(A)$ or $\overline{\mathcal{M}}_d(A) > \mathcal{H}_d(A)$, so that either (39) or (40) must hold.

As the definition of the minimal energy constant $C_{s,d}$ which appears in Theorem B and Theorem II.1.1, one can take equality

$$C_{s,d} := \lim_{N\to\infty} \frac{\mathcal{E}_s\left([0,1]^d, N\right)}{N^{1+s/d}}, \quad s > d, \tag{42}$$

where quantity $\mathcal{E}_s(A, N)$ is defined in (9). It follows from Theorem A that $C_{s,1} = 2\zeta(s)$, $s > 1$. However, constants $C_{s,d}$ are still not known for $d > 1$.

Below, we relate the constants $C_{s,d}$ and $C_{\infty,d}$.

Theorem III.1.2. *The limit $\lim_{s\to\infty} C_{s,d}^{1/s}$ exists for each integer $d \geq 1$ and*

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

In particular, results on packing density mentioned above, imply that

$$\lim_{s\to\infty} C_{s,2}^{1/s} = \frac{\sqrt[4]{3}}{\sqrt{2}}$$

and

$$\lim_{s\to\infty} C_{s,3}^{1/s} = \frac{1}{\sqrt[6]{2}}.$$

We next show that asymptotic behavior of the minimal energy obtained in Chapter II, relation (16), can fail for certain $(\mathcal{H}_d, d)$-rectifiable sets.

Proposition III.1.3. *Let $A \subset \mathbb{R}^{d'}$ be a compact $(\mathcal{H}_d, d)$-rectifiable set with $\overline{\mathcal{M}}_d(A) > \mathcal{H}_d(A)$. Then for s sufficiently large*

$$\underline{g}_{s,d}(A) = \liminf_{N\to\infty} \frac{\mathcal{E}_s(A, N)}{N^{1+s/d}} < C_{s,d}\mathcal{H}_d(A)^{-s/d}. \tag{43}$$

III.2 Remarks for general sets.

For a set $A \subset \mathbb{R}^{d'}$, let $\dim_H A$ be the Hausdorff dimension and

$$\underline{\dim}_M A := \inf(\{\alpha > 0 : \underline{\mathcal{M}}_\alpha(A) = 0\} \cup \{d'\}) =$$

$$= \sup(\{\alpha \in (0, d'] : \underline{\mathcal{M}}_\alpha(A) = \infty\} \cup \{0\})$$

and

$$\overline{\dim}_M A := \inf(\{\alpha > 0 : \overline{\mathcal{M}}_\alpha(A) = 0\} \cup \{d'\}) =$$

$$= \sup(\{\alpha \in (0, d'] : \overline{\mathcal{M}}_\alpha(A) = \infty\} \cup \{0\})$$

denote the lower and the upper Minkowski dimension of A, respectively. One can also introduce the lower and the upper dimension of a set using s-energy or best-packing.

For any $0 < \alpha \le d'$ and $s > \alpha$ denote

$$\underline{g}_{s,\alpha}(A) := \liminf_{N\to\infty} \frac{\mathcal{E}_s(A, N)}{N^{1+s/\alpha}}, \qquad \overline{g}_{s,\alpha}(A) := \limsup_{N\to\infty} \frac{\mathcal{E}_s(A, N)}{N^{1+s/\alpha}}$$

and

$$g_{s,\alpha}(A) := \lim_{N\to\infty} \frac{\mathcal{E}_s(A, N)}{N^{1+s/\alpha}},$$

if this limit exists. Let

$$\underline{\dim}_\infty A := \inf(\{\alpha > 0 : \underline{g}_{\infty,\alpha}(A) = 0\} \cup \{d'\}) =$$

$$= \sup(\{\alpha \in (0, d'] : \underline{g}_{\infty,\alpha}(A) = \infty\} \cup \{0\})$$

and for a fixed $s > d'$ denote

$$\underline{\dim}_s A := \inf(\{\alpha > 0 : \overline{g}_{s,\alpha}(A) = \infty\} \cup \{d'\}) =$$

$$= \sup(\{\alpha \in (0, d'] : \overline{g}_{s,\alpha}(A) = 0\} \cup \{0\})$$

with $\overline{\dim}_\infty A$ and $\overline{\dim}_s A$ being defined in an analogous way through $\overline{g}_{\infty,\alpha}$ or $\underline{g}_{s,\alpha}$. The following proposition implies that for any set $A \subset \mathbf{R}^{d'}$ we have

$$\underline{\dim}_s A = \underline{\dim}_\infty A = \underline{\dim}_M A$$

and

$$\overline{\dim}_s A = \overline{\dim}_\infty A = \overline{\dim}_M A,$$

provided $s > d'$.

Proposition III.2.1. *If* $0 < \alpha \le d' < s$, *there are positive constants* $c_1 = c_1(s, \alpha)$ *and* $c_2 = c_2(s, \alpha)$ *such that for any infinite set* $A \subset \mathbb{R}^{d'}$ *we have*

$$c_1 \underline{\mathcal{M}}_\alpha(A)^{-s/\alpha} \le \overline{g}_{s,\alpha}(A) \le c_2 \underline{\mathcal{M}}_\alpha(A)^{-s/\alpha}, \tag{44}$$

$$c_1 \overline{\mathcal{M}}_\alpha(A)^{-s/\alpha} \le \underline{g}_{s,\alpha}(A) \le c_2 \overline{\mathcal{M}}_\alpha(A)^{-s/\alpha}. \tag{45}$$

There are also positive constants $c_3 = c_3(\alpha)$ *and* $c_4 = c_4(\alpha)$ *such that for every infinite set* $A \subset \mathbb{R}^{d'}$

$$c_3 \underline{\mathcal{M}}_\alpha(A)^{1/\alpha} \le \underline{g}_{\infty,\alpha}(A) \le c_4 \underline{\mathcal{M}}_\alpha(A)^{1/\alpha}, \tag{46}$$

$$c_3 \overline{\mathcal{M}}_\alpha(A)^{1/\alpha} \le \overline{g}_{\infty,\alpha}(A) \le c_4 \overline{\mathcal{M}}_\alpha(A)^{1/\alpha}. \tag{47}$$

It is known that $\underline{\dim}_M A \ge \dim_H A$ with a strict inequality possible for some compact sets (cf. e.g. [38, p. 77]). Hence, for such sets A and any numbers $\alpha \le \alpha_1$ strictly between $\dim_H A$ and $\underline{\dim}_M A$, we have $\mathcal{H}_\alpha(A) = 0$, but $g_{s,\alpha_1}(A) = 0$, $s > d'$, and $g_{\infty,\alpha_1}(A) = \infty$. That is $\delta_N(A)$ will go to zero slower than $N^{-1/\dim_H A}$, as $N \to \infty$, and $\mathcal{E}_s(A, N)$ will have order of growth less than $N^{1+s/\dim_H A}$.

For every $s \in (d', \infty]$ and compact sets with sufficiently large gap between $\underline{\mathcal{M}}_\alpha(A)$ and $\overline{\mathcal{M}}_\alpha(A)$ for some $\alpha > 0$, we will have $\underline{g}_{s,\alpha}(A) < \overline{g}_{s,\alpha}(A)$. Moreover, if $\underline{\dim}_M A < \overline{\dim}_M A$ (cf. e.g. [38, p. 77] for examples), the order of the best-packing radius and the minimal s-energy for $s > d'$ will vary depending on the subsequence of cardinalities of configurations.

III.3 Divergence results for best-packing distance and minimal energy on certain Cantor-type sets

We show that the condition of $(\mathcal{H}_d, d)$-rectifiability in Theorems II.1.1 and III.1.1 is crucial in the sense that there are non-rectifiable compact sets with $\dim_H A = d$ and $0 < \mathcal{H}_d(A) < \infty$ such that $g_{\infty,d}(A)$ and $g_{s,d}(A)$ (for sufficiently large s) do not exist. Indeed, we show that this is true for a class of Cantor-type sets which we will denote by $\mathcal{K}$.

We say that a non-empty compact set $K \subset \mathbb{R}^{d'}$ belongs to the class $\mathcal{K}$, if there are a finite number of distinct similitudes $S_1, \dots, S_p : \mathbb{R}^{d'} \to \mathbb{R}^{d'}$ with the same contraction coefficient $\sigma \in (0,1)$ (that is $|S_i(x) - S_i(y)| = \sigma\,|x-y|\,, \quad x, y \in \mathbb{R}^{d'}, \quad i = 1, \dots, p$) such that

$$\bigcup_{i=1}^{p} S_i(K) = K, \quad \text{and} \quad S_i(K) \cap S_j(K) = \emptyset, \quad i \neq j. \tag{48}$$

According to [30], we have $\lambda := \dim_H K = -\log_\sigma p$ and $0 < \mathcal{H}_\lambda(K) < \infty$. This is a subclass of the class of self-similar sets constructed in [30] (this construction is also cited in [38, Section 4.13]). We remark that from a fixed point argument for the Hausdorff metric, for every finite collection of similitudes $S_1, \dots, S_p$ in $\mathbb{R}^{d'}$ with arbitrary contraction coefficients, there is a unique non-empty compact set K such that

$$\bigcup_{i=1}^{p} S_i(K) = K.$$

For our results, we have required additional restrictions on K.

Class $\mathcal{K}$ contains the classical Cantor subset of $[0,1]$. Parameters p and σ can also be chosen so that $\dim_H K$ is any number (in particular, any integer) between 0 and d'. For example, if a_1, a_2 and a_3 are vertices of an equilateral triangle on the plane and S_i, $i = 1, 2, 3$, is the homothety of the plane with respect to a_i and the contraction coefficient 1/3, then K will be a set of Hausdorff dimension one, known as the Sierpinski gasket [38, p. 75].

Proposition III.3.1. *Let K be a compact set from the class $\mathcal{K}$ with $\lambda = \dim_H K$. Then, for $s < \infty$ sufficiently large and for $s = \infty$ we have*

$$0 < \underline{g}_{s,\lambda}(K) < \overline{g}_{s,\lambda}(K) < \infty.$$

In this statement, we cannot replace condition $S_i(K) \cap S_j(K) = \emptyset, \quad i \neq j$, with a less restrictive condition $\mathcal{H}_\lambda(S_i(K)\cap S_j(K))=0$, $i\neq j$, from the definition of a self-similar set, since for example, if S_i, $i=1,2,3,4$, are homotheties of the plane with respect to the vertices of some square K_0 and the same $\sigma=1/2$, then $\lambda=2$ and K will coincide with K_0. But by Theorem B, $g_{s,2}(K_0)$ exists for any $s>2$.

III.4 Relation between asymptotic behavior of minimal s-energy and best-packing distance.

To prove relation (39) we will need Theorem II.1.1 and the following statement. (With regard to the extended real number limits in $[0,\infty]$, we agree that $1/0=0^{-s}=\infty^s=\infty$, $1/\infty=\infty^{-s}=0$, $s>0$.)

Proposition III.4.1. *For every infinite set $A\subset\mathbb{R}^{d'}$ and $0<\alpha\leq d'$ we have*

$$\lim_{s\to\infty}\left(\overline{g}_{s,\alpha}(A)\right)^{1/s}=\frac{1}{\underline{g}_{\infty,\alpha}(A)}\quad\text{and}\quad\lim_{s\to\infty}\left(\underline{g}_{s,\alpha}(A)\right)^{1/s}=\frac{1}{\overline{g}_{\infty,\alpha}(A)}.\tag{49}$$

Proposition III.4.1 immediately yields the following statements.

Proposition III.4.2. *Let $A\subset\mathbb{R}^{d'}$ be an infinite set and $0<\alpha\leq d'$. If for every s sufficiently large $\underline{g}_{s,\alpha}(A)=\overline{g}_{s,\alpha}(A)$, then $g_{\infty,\alpha}(A)$ exists and*

$$\lim_{s\to\infty}\left(g_{s,\alpha}(A)\right)^{1/s}=\frac{1}{g_{\infty,\alpha}(A)}.$$

Proposition III.4.3. *Let $A\subset\mathbb{R}^{d'}$ be an infinite set such that $\underline{g}_{\infty,\alpha}(A)<\overline{g}_{\infty,\alpha}(A)$ for some $0<\alpha\leq d'$. Then for sufficiently large s we have $\underline{g}_{s,\alpha}(A)<\overline{g}_{s,\alpha}(A)$.*

Proof of Proposition III.4.1. Lower estimates. We can assume $A\subset\mathbb{R}^{d'}$ to be compact, since on unbounded sets $g_{s,\alpha}(A)=0$ and $g_{\infty,\alpha}(A)=\infty$ and the minimal s-energy (as well as the best-packing radius) is the same for A and its closure.

Choose an arbitrary $\epsilon\in(0,1)$ and let $s>\alpha$. Let N be sufficiently large and $\omega_N^*:=\{x_{1,N},\ldots,x_{N,N}\}$ be an s-energy minimizing N-point collection on A. Set $N_\epsilon:=\lfloor(1-\epsilon)N\rfloor$, where $\lfloor t\rfloor$ is the floor function of t, and

$$r_{i,N}:=\min_{j:j\neq i}|x_{i,N}-x_{j,N}|.$$

Pick a point $x_{i_1,N} \in \omega_N^*$ with $r_{i_1,N} \leq \delta_N(A)$. In $\omega_N^* \setminus \{x_{i_1,N}\}$ pick a point $x_{i_2,N}$ so that $r_{i_2,N} \leq \delta_{N-1}(A)$. Continue this process until we pick a point $x_{i_{\lfloor \epsilon N \rfloor+1},N} \in \omega_N^* \setminus \{x_{i_1,N}, \ldots, x_{i_{\lfloor \epsilon N \rfloor},N}\}$ such that $r_{i_{\lfloor \epsilon N \rfloor+1},N} \leq \delta_{N-\lfloor \epsilon N \rfloor}(A)$. Then

$$\mathcal{E}_s(A,N) = E_s(\omega_N^*) \geq \sum_{k=1}^{\lfloor \epsilon N \rfloor+1} \frac{1}{(r_{i_k,N})^s} \geq \sum_{k=1}^{\lfloor \epsilon N \rfloor+1} \frac{1}{(\delta_{N-k+1}(A))^s} \geq \frac{\epsilon N}{(\delta_{N_\epsilon}(A))^s}.$$

Hence,

$$\overline{g}_{s,\alpha}(A) \geq \limsup_{N\to\infty} \frac{\epsilon}{(\delta_{N_\epsilon}(A))^s N^{s/\alpha}} = \frac{\epsilon(1-\epsilon)^{s/\alpha}}{\left(\liminf\limits_{N\to\infty} \delta_{N_\epsilon}(A) \cdot N_\epsilon^{1/\alpha}\right)^s} = \frac{\epsilon(1-\epsilon)^{s/\alpha}}{\left(\underline{g}_{\infty,\alpha}(A)\right)^s}, \tag{50}$$

since N_ϵ passes through all natural numbers. Similarly,

$$\underline{g}_{s,\alpha}(A) \geq \frac{\epsilon(1-\epsilon)^{s/\alpha}}{\left(\overline{g}_{\infty,\alpha}(A)\right)^s}. \tag{51}$$

Then, letting first $s \to \infty$ and then $\epsilon \to 0$, we get

$$\liminf_{s\to\infty} \left(\overline{g}_{s,\alpha}(A)\right)^{1/s} \geq \frac{1}{\underline{g}_{\infty,\alpha}(A)} \quad \text{and} \quad \liminf_{s\to\infty} \left(\underline{g}_{s,\alpha}(A)\right)^{1/s} \geq \frac{1}{\overline{g}_{\infty,\alpha}(A)}. \tag{52}$$

Upper estimates. Let, for every $N(\geq 2)$ fixed, $X_N = \{x, x_1, \ldots, x_{N-1}\} \subset \mathbb{R}^{d'}$ be such that $a := \delta(X_N) > 0$ and for every $k \in \mathbf{N}$ let M_k be the set of points from X_N contained in $B(x, a(k+1))$ but not in $B(x, ak)$, where $B(x,r)$ is the open ball in $\mathbf{R}^{d'}$ centered at x with radius r. Then, from a volume argument,

$$\#M_k \cdot \mathcal{L}_{d'}\left[B\left(0, a/2\right)\right] \leq \mathcal{L}_{d'}\left[B\left(x, a(k+3/2)\right) \setminus B\left(x, a(k-1/2)\right)\right],$$

and so $\#M_k \leq (2k+3)^{d'} - (2k-1)^{d'} \leq 4d'(2k+3)^{d'-1}$. Hence,

$$P_s(x, X_N) := \sum_{i=1}^{N-1} \frac{1}{|x-x_i|^s} = \sum_{k=1}^{\infty} \sum_{x_i \in M_k} \frac{1}{|x-x_i|^s}$$

$$\leq \sum_{k=1}^{\infty} \frac{\#M_k}{a^s k^s} \leq \frac{4d'}{a^s} \sum_{k=1}^{\infty} \frac{(2k+3)^{d'-1}}{k^s} \leq \frac{\eta_s}{a^s}, \quad s > d',$$

where $\eta_s := 4d' 5^{d'-1} \zeta(s - d' + 1)$.

Now let $\overline{\omega}_N := \{\overline{x}_{1,N}, \ldots, \overline{x}_{N,N}\}$ be a best-packing N-point configuration on A; that is, $\delta(\overline{\omega}_N) = \delta_N(A)$. Then, using the above estimate, for $s > d'$ we get

$$\mathcal{E}_s(A,N) \leq E_s(\overline{\omega}_N) = \sum_{i=1}^{N} P_s(\overline{x}_{i,N}, \overline{\omega}_N) \leq \frac{\eta_s N}{(\delta_N(A))^s}.$$

Hence, for $s > d'$ we have

$$\overline{g}_{s,\alpha}(A) \leq \limsup_{N\to\infty} \frac{\eta_s}{\left(\delta_N(A)\cdot N^{1/\alpha}\right)^s} = \frac{\eta_s}{\left(\underline{g}_{\infty,\alpha}(A)\right)^s}, \quad \underline{g}_{s,\alpha}(A) \leq \frac{\eta_s}{\left(\overline{g}_{\infty,\alpha}(A)\right)^s}. \tag{53}$$

Then, since $\eta_s^{1/s} \to 1$ as $s \to \infty$, we have

$$\limsup_{s\to\infty} \left(\overline{g}_{s,\alpha}(A)\right)^{1/s} \leq \frac{1}{\underline{g}_{\infty,\alpha}(A)}, \qquad \limsup_{s\to\infty} \left(\underline{g}_{s,\alpha}(A)\right)^{1/s} \leq \frac{1}{\overline{g}_{\infty,\alpha}(A)}. \tag{54}$$

Inequalities (52) and (54) yield relations (49). Propositions III.4.1—III.4.3 are proved.

III.5 Proofs for rectifiable sets

In this section we prove Theorems III.1.1 and III.1.2. Using (42) and Proposition III.4.2 we get Theorem III.1.2:

$$\lim_{s\to\infty} C_{s,d}^{1/s} = \lim_{s\to\infty} g_{s,d}([0,1]^d)^{1/s} = \frac{1}{g_{\infty,d}([0,1]^d)} = \frac{1}{C_{\infty,d}}.$$

Taking into account Theorem II.1.1, Proposition III.4.2 and Theorem III.1.2, we get equation (39):

$$g_{\infty,d}(A) = \frac{1}{\lim\limits_{s\to\infty} (g_{s,d}(A))^{1/s}} = \lim_{s\to\infty} \frac{\mathcal{H}_d(A)^{1/d}}{C_{s,d}^{1/s}} = C_{\infty,d}\mathcal{H}_d(A)^{1/d}.$$

Now suppose that A is d-rectifiable with $\mathcal{H}_d(A) > 0$, and $\{\overline{\omega}_N\}_{N=2}^{\infty}$ is a sequence of best-packing configurations on A such that $\#\overline{\omega}_N = N$, $N \geq 2$. To show that $\{\overline{\omega}_N\}_{N=2}^{\infty}$ is asymptotically uniformly distributed on A, choose any subset $B \subset A$ whose boundary relative to A has $\mathcal{H}_d$-measure zero. As before, $\overline{B}$ stands for the closure of the set B. Set $p_N := \#(\overline{\omega}_N \cap B)$ and let $\mathcal{N} \subset \mathbf{N}$ be any infinite subset such that the limit

$$p(\mathcal{N}) := \lim_{\mathcal{N}\ni N\to\infty} \frac{p_N}{N}$$

exists. If $p(\mathcal{N}) > 0$, then for sufficiently large $N \in \mathcal{N}$ we get

$$\delta_N(A) = \delta(\overline{\omega}_N) \le \delta(\overline{\omega}_N \cap B) \le \delta_{p_N}(B) \le \delta_{p_N}(\overline{B}).$$

Since $\overline{B}$, as a subset of A, is a closed d-rectifiable set and $\mathcal{H}_d(\overline{B}) = \mathcal{H}_d(B)$, using (39), we have

$$p(\mathcal{N}) \le \lim_{\mathcal{N} \ni N \to \infty} \frac{\delta_{p_N}(\overline{B})^d \cdot p_N}{\delta_N(A)^d \cdot N} = \left(\frac{g_{\infty,d}(\overline{B})}{g_{\infty,d}(A)}\right)^d = \frac{\mathcal{H}_d(B)}{\mathcal{H}_d(A)}. \tag{55}$$

If $p(\mathcal{N}) = 0$, then the inequality $p(\mathcal{N}) \le \mathcal{H}_d(B)/\mathcal{H}_d(A)$ is trivial. Thus,

$$\limsup_{N \to \infty} \frac{p_N}{N} \le \frac{\mathcal{H}_d(B)}{\mathcal{H}_d(A)}.$$

Next, let $q_N := \#\left(\overline{\omega}_N \cap (A \setminus B)\right)$. Since the boundary of $A \setminus B$ relative to A also has $\mathcal{H}_d$-measure zero, using the same argument we can write

$$\limsup_{N \to \infty} \frac{q_N}{N} \le \frac{\mathcal{H}_d(A \setminus B)}{\mathcal{H}_d(A)},$$

which implies that

$$\liminf_{N \to \infty} \frac{p_N}{N} \ge \frac{\mathcal{H}_d(B)}{\mathcal{H}_d(A)}.$$

This shows that

$$\lim_{N \to \infty} \frac{\#(\overline{\omega}_N \cap B)}{N} = \frac{\mathcal{H}_d(B)}{\mathcal{H}_d(A)}.$$

Hence, (41) holds.

To prove (40) we will need the following lemma. Denote $\mu_{d'} := \mathcal{L}_{d'}(B(0,2))$ and recall that $G(r)$ is the r-neighborhood of a set G in $\mathbb{R}^{d'}$.

Lemma III.5.1. *Let $0 < \alpha \le d'$, G and F be two sets in $\mathbf{R}^{d'}$ and assume that for some positive numbers c, γ and $\rho < (\gamma/\mu_{d'})^{1/\alpha}$ there holds*

$$\mathcal{L}_{d'}\left[G(\rho) \setminus F((c+1)\rho)\right] > \gamma \rho^{d'-\alpha}.$$

Then for $N = \lfloor \gamma/(\mu_{d'}\rho^\alpha) \rfloor + 1$ we have $\delta_N\left(G \setminus F(c\rho)\right) \ge \rho$.

Proof. Let $k \in \mathbf{N} \cup \{0\}$ be the largest number of pairwise disjoint balls of radius $\rho/2$ centered at points of $G \setminus F(c\rho)$. We just need to show that $k > \gamma/(\mu_{d'}\rho^\alpha)$. Assume the contrary. Choose points $x_1, \ldots, x_k \in G \setminus F(c\rho)$ such that $|x_i - x_j| \geq \rho$, $1 \leq i \neq j \leq k$. Then

$$\mathcal{L}_{d'}\left(\bigcup_{i=1}^{k} B(x_i, 2\rho)\right) \leq k\mu_{d'}\rho^{d'} \leq \gamma\rho^{d'-\alpha} < \mathcal{L}_{d'}\left[G(\rho) \setminus F((c+1)\rho)\right].$$

This means that there is a point $y \in G(\rho) \setminus F((c+1)\rho)$ such that $|y - x_i| \geq 2\rho$, $i = 1, \ldots, k$. Also, there exists a point $x_{k+1} \in G$ such that $|y - x_{k+1}| < \rho$. Hence, $\operatorname{dist}(x_{k+1}, F) \geq c\rho$. Thus, $x_{k+1} \in G \setminus F(c\rho)$ and $|x_{k+1} - x_i| > \rho$, $i = 1, \ldots, k$, and so we have $k+1$ pairwise disjoint balls of radius $\rho/2$ centered at points of $G \setminus F(c\rho)$ which contradicts to the maximality of k. Lemma III.5.1 is proved.

Another fact needed to show (40) is the left inequality in (47). We can assume that $\overline{\mathcal{M}}_\alpha(A) > 0$. Choose any $0 < M < \overline{\mathcal{M}}_\alpha(A)$. Then there is a sequence $\{r_m\}_{m=1}^\infty$, $r_m \searrow 0$, $m \to \infty$, such that

$$\mathcal{L}_{d'}\left(A(r_m)\right) > M\beta_{d'-\alpha} r_m^{d'-\alpha}, \quad m \in \mathbf{N}.$$

By Lemma III.5.1 (with $F = \emptyset$) for the sequence $N_m := \lfloor M\beta_{d'-\alpha}/(\mu_{d'} r_m^\alpha)\rfloor + 1$, $m \in \mathbf{N}$, we have

$$\delta_{N_m}(A) \geq r_m \geq \left(\frac{M\beta_{d'-\alpha}}{\mu_{d'} N_m}\right)^{1/\alpha}$$

for sufficiently large m. Hence, $\overline{g}_{\infty,\alpha}(A) \geq (M\beta_{d'-\alpha}/\mu_{d'})^{1/\alpha}$. Letting $M \to \overline{\mathcal{M}}_\alpha(A)$, gives the lower estimate in (47).

Proof of inequality (40). In the case $\mathcal{H}_d(A) = 0$ we have $\overline{\mathcal{M}}_d(A) > 0$ and by the left inequality in (47) there holds $\overline{g}_{\infty,d}(A) > 0 = C_{\infty,d}\mathcal{H}_d(A)^{1/d}$. Assume that $\mathcal{H}_d(A) > 0$ and set $d'' = d' - d$. Let $c_0 \in (0,1)$ be such that

$$(c_0 + 1)^{d''}\, \mathcal{H}_d(A) < \overline{\mathcal{M}}_d(A)$$

and $M_1, M_2 > 0$ be such numbers that

$$(c_0 + 1)^{d''}\, \mathcal{H}_d(A) < (c_0 + 1)^{d''}\, M_1 < M_2 < \overline{\mathcal{M}}_d(A).$$

Choose any $\epsilon \in (0,1)$. By definition of $(\mathcal{H}_d, d)$-rectifiability (or by Lemmas II.1.1 and II.1.2), there is a d-rectifiable compact subset $K_\epsilon \subset A$ such that $\mathcal{H}_d(K_\epsilon) > \mathcal{H}_d(A)(1-\epsilon)$. By definition (38) there is a sequence of positive numbers $\{r_m\}_{m=1}^{\infty}$, $r_m \searrow 0$, $m \to \infty$, such that

$$\mathcal{L}_{d'}\left(A(r_m)\right) > M_2 \beta_{d''} \cdot r_m^{d''}, \quad m \in \mathbf{N}.$$

By (14) we have $\mathcal{M}_d(K_\epsilon) = \mathcal{H}_d(K_\epsilon) < M_1$. Then, for sufficiently large m

$$\mathcal{L}_{d'}\left[K_\epsilon((c_0+1)r_m)\right] < M_1 \beta_{d''} \cdot (c_0+1)^{d''} r_m^{d''}$$

and hence,

$$\mathcal{L}_{d'}\left[A(r_m) \setminus K_\epsilon((c_0+1)r_m)\right] > \left(M_2 - (c_0+1)^{d''} M_1\right) \beta_{d''} \cdot r_m^{d''}.$$

By Lemma III.5.1 with $\alpha = d$, there is a constant $\nu_1 > 0$ independent of m and ϵ, such that for $k_m = \lfloor \nu_1 / r_m^d \rfloor + 1$ and m sufficiently large we have

$$\delta_{k_m}(A \setminus K_\epsilon(c_0 r_m)) \geq r_m.$$

Let $X_m \subset A \setminus K_\epsilon(c_0 r_m)$ be a best-packing collection of k_m points.

Set $\nu := C_{\infty,d} \mathcal{H}_d(A)^{1/d}$. By (39) and the choice of K_ϵ, for sufficiently large N, we have

$$\delta_N(K_\epsilon) > \nu(1-\epsilon)^{1/d} N^{-1/d}.$$

For every m sufficiently large, choose N_m to be the largest integer such that

$$\delta_{N_m}(K_\epsilon) \geq \nu(1-\epsilon)^{1/d} N_m^{-1/d} \geq c_0 r_m$$

and denote by Y_m the best-packing collection of N_m points on K_ϵ. Since $\mathrm{dist}(X_m, K_\epsilon) \geq c_0 r_m$, we have that $\delta(X_m \cup Y_m) \geq c_0 r_m$ for m sufficiently large. Hence,

$$\overline{g}_{\infty,d}(A) \geq \limsup_{m\to\infty} \delta_{k_m+N_m}(A)(k_m+N_m)^{1/d} \geq$$

$$\geq \limsup_{m\to\infty} c_0 r_m \left(\frac{\nu_1}{r_m^d} + \frac{\nu^d(1-\epsilon)}{c_0^d r_m^d} - 1\right)^{1/d} = \left(c_0^d \nu_1 + \nu^d (1-\epsilon)\right)^{1/d}.$$

Letting $\epsilon \to 0$, we get

$$\overline{g}_{\infty,d}(A) \geq \left(c_0^d \nu_1 + \nu^d\right)^{1/d} > \nu = C_{\infty,d}\mathcal{H}_d(A)^{1/d}.$$

This completes the proof of Theorem III.1.1.

III.6 Proof of Proposition III.1.3 and remarks for general sets.

Using Proposition III.4.1, Theorem III.1.2, and inequality (40), for every $(\mathcal{H}_d, d)$-rectifiable compact set A with $\overline{\mathcal{M}}_d(A) > \mathcal{H}_d(A)$, we have

$$\lim_{s\to\infty}\left(\frac{\underline{g}_{s,d}(A)}{C_{s,d}\mathcal{H}_d(A)^{-s/d}}\right)^{1/s} = \frac{C_{\infty,d}\mathcal{H}_d(A)^{1/d}}{\overline{g}_{\infty,d}(A)} < 1,$$

and inequality (43) follows for sufficiently large s. Proposition III.1.3 is proved.

We only need to prove (46) and (47) in proposition III.2.1 since the upper estimates in (44) and (45) will follow from (53) and the lower estimates in (46) and (47). Analogously, the lower estimates in (44) and (45) are obtained from the upper estimates in (46) and (47), using (50) or (51) with ϵ equal, say 1/2. We remark that (50), (51) and (53) hold for any infinite set A.

Since we do not look for sharp constants, redefine

$$\underline{\mathcal{M}}_\alpha(A) := \liminf_{r\to 0^+}\frac{\mathcal{L}_{d'}(A(r))}{r^{d'-\alpha}} \quad \text{and} \quad \overline{\mathcal{M}}_\alpha(A) := \limsup_{r\to 0^+}\frac{\mathcal{L}_{d'}(A(r))}{r^{d'-\alpha}}$$

for all $0 < \alpha \leq d'$. To show the lower estimate in (46), assume that $\underline{\mathcal{M}}_\alpha(A) > 0$ (otherwise it is trivial). Pick any $0 < M < \underline{\mathcal{M}}_\alpha(A)$ and set

$$r_N := \left(\frac{M}{\mu_{d'}N}\right)^{1/\alpha}.$$

Then, for N sufficiently large $\mathcal{L}_{d'}(A(r_N)) > M r_N^{d'-\alpha}$. By Lemma III.5.1 (with $F = \emptyset$), for $k_N = \lfloor M/(\mu_{d'} r_N^\alpha)\rfloor + 1$ (k_N will be greater that N) we have

$$\delta_N(A) \geq \delta_{k_N}(A) \geq r_N = (M/(\mu_{d'}N))^{1/\alpha}$$

for sufficiently large N. Hence, $\underline{g}_{\infty,\alpha}(A) \geq \mu_{d'}^{-1/\alpha} M^{1/\alpha}$. Letting $M \to \underline{\mathcal{M}}_\alpha(A)$, we get the lower estimate in (46). We need the following lemma for the upper estimate.

Lemma III.6.1. *Let $0 < \alpha \le d'$, $A \neq \emptyset$ be a set in $\mathbf{R}^{d'}$, and for some positive numbers γ and $\rho < (\gamma/\beta_{d'})^{1/\alpha}$, assume that there holds*

$$\mathcal{L}_{d'}(A(\rho)) < \gamma\rho^{d'-\alpha}.$$

Then for any $N > \gamma/(\beta_{d'}\rho^\alpha)$ we have $\delta_N(A) \le 2\rho$.

Proof. Suppose $k \ge 2$ is an integer such that $\delta_k(A) > 2\rho$, and let $x_1, \dots, x_k \in A$ be a collection of distinct points with separation at least 2ρ. Then

$$\mathcal{L}_{d'}\left(\bigcup_{i=1}^{k} B(x_i, \rho)\right) = k\beta_{d'}\rho^{d'} \le \mathcal{L}_{d'}(A(\rho)) < \gamma\rho^{d'-\alpha}.$$

Hence, $k \le \gamma/(\beta_{d'}\rho^\alpha)$, and so for any $N > \gamma/(\beta_{d'}\rho^\alpha)$ we have $\delta_N(A) \le 2\rho$, which proves the lemma.

To get the upper estimate in (46), we can assume that $\underline{\mathcal{M}}_\alpha(A) < \infty$. Choose any $M > \underline{\mathcal{M}}_\alpha(A)$. There is a sequence of positive numbers $\{r_m\}_{m=1}^\infty$, $r_m \searrow 0$, $m \to \infty$, such that

$$\mathcal{L}_{d'}(A(r_m)) < M r_m^{d'-\alpha}, \quad m \in \mathbf{N}.$$

Set $N_m := \lfloor M/(\beta_{d'} r_m^\alpha)\rfloor + 1$. By Lemma III.6.1 we have $\delta_{N_m}(A) \le 2r_m$ for sufficiently large m. Consequently,

$$\underline{g}_{\infty,\alpha}(A) \le \liminf_{m\to\infty} \delta_{N_m}(A) N_m^{1/\alpha} \le \liminf_{m\to\infty} 2r_m N_m^{1/\alpha} = 2\beta_{d'}^{-1/\alpha} M^{1/\alpha}.$$

Letting $M \to \underline{\mathcal{M}}_\alpha(A)$ completes the proof of (46).

The left inequality in (47) was shown before the proof of inequality (40). Thus, it remains to prove the right inequality in (47) for the case $\overline{\mathcal{M}}_\alpha(A) < \infty$. Pick any $M > \overline{\mathcal{M}}_\alpha(A)$ and let

$$r_N := \left(\frac{M}{\beta_{d'}(N-1)}\right)^{1/\alpha}, \quad N \ge 2.$$

Then $\mathcal{L}_{d'}\left(A\left(r_N\right)\right) < M r_N^{d'-\alpha}$ for N sufficiently large. Since, $N > M/(\beta_{d'} r_N^\alpha)$, by Lemma III.6.1 we get

$$\delta_N(A) \le 2r_N = 2(M/(\beta_{d'}(N-1)))^{1/\alpha}.$$

Hence, $\overline{g}_{\infty,\alpha}(A) \leq 2\beta_{d'}^{-1/\alpha} M^{1/\alpha}$. Letting $M \to \overline{\mathcal{M}}_\alpha(A)$ completes the proof of (47) and Proposition III.2.1.

III.7 Proof of the divergence results.

In this section we show Proposition III.3.1. It was shown in [30] (see also [38, Theorem 4.14]) that for any set $K \in \mathcal{K}$ there are constants $c_1, c_2 > 0$ such that

$$c_1 r^\lambda \leq \mathcal{H}_\lambda\left(K \cap B(x,r)\right) \leq c_2 r^\lambda, \quad x \in K, \quad 0 < r < 1, \tag{56}$$

(we will call λ-regular every set satisfying (56)). Using an argument analogous to the proof of Lemma III.6.1, one can show that $\overline{g}_{\infty,\lambda}(K) < \infty$. Since for any set $K \in \mathcal{K}$ we have

$$\underline{\mathcal{M}}_\lambda(K) \geq C\mathcal{H}_\lambda(K) > 0$$

with $C > 0$ being independent of K (cf. e.g. [38, p. 79]), by (46) we have $\underline{g}_{\infty,\lambda}(K) > 0$.

Assume that $g_{\infty,\lambda}(K)$ exists (it must be positive and finite). Let $S_1, \ldots, S_p : \mathbb{R}^{d'} \to \mathbb{R}^{d'}$ be the similitudes with the same contraction coefficient $\sigma \in (0,1)$ such that relations (48) hold. Set $h := \min_{i \neq j} \operatorname{dist}\left(S_i(K), S_j(K)\right)$ and choose $k \in \mathbf{N}$ so that $\delta_k(K) < h$.

Let $m \in \mathbf{N}$ and for $\mathbf{i} = (i_1, \ldots, i_m) \in \{1, \ldots, p\}^m =: Z_p^m$ put $F_{\mathbf{i}} := S_{i_1} \circ \ldots \circ S_{i_m}$. Then

$$\operatorname{dist}\left(F_{\mathbf{i}}(K), F_{\mathbf{j}}(K)\right) \geq h\sigma^{m-1} > \sigma^{m-1}\delta_k(K), \quad \mathbf{i} \neq \mathbf{j}, \tag{57}$$

and $\bigcup_{\mathbf{i} \in Z_p^m} F_{\mathbf{i}}(K) = K$. Let $\overline{\omega}_k \subset K$ be a collection of k points such that $\delta(\overline{\omega}_k) = \delta_k(K)$, and $\omega_m := \cup_{\mathbf{i} \in Z_p^m} F_{\mathbf{i}}\left(\overline{\omega}_k\right)$. In view of (57), it is not difficult to see that

$$\delta_{kp^m}(K) \geq \delta(\omega_m) = \sigma^m \delta_k(K).$$

On the other hand, from any collection of $c_m := (k-1)p^m + 1$ points on K at least k must belong to the same $F_{\mathbf{i}}(K)$, and hence, $\delta_{c_m}(K) \leq \sigma^m \delta_k(K)$. Since $c_m \leq kp^m$, we have $\delta_{kp^m}(K) = \delta_{c_m}(K)$ and

$$g_{\infty,\lambda}(K) = \lim_{m\to\infty} \delta_{kp^m}(K)\left(kp^m\right)^{1/\lambda} = \lim_{m\to\infty} \delta_{c_m}(K)\left(kp^m\right)^{1/\lambda} =$$

$$= g_{\infty,\lambda}(K) \lim_{m\to\infty} \left(\frac{kp^m}{c_m}\right)^{1/\lambda} = g_{\infty,\lambda}(K) \left(\frac{k}{k-1}\right)^{1/\lambda} > g_{\infty,\lambda}(K),$$

since $0 < g_{\infty,\lambda}(K) < \infty$. Contradiction. Hence, $0 < \underline{g}_{\infty,\lambda}(K) < \overline{g}_{\infty,\lambda}(K) < \infty$. Taking into account Propositions III.4.1 and III.4.3, we get Proposition III.3.1.

CHAPTER IV

WEIGHTED ENERGY PROBLEM

As we proved in Chapter II, Theorem B holds, in particular, for closed d-rectifiable sets (see Definition II.1.1) and $s > d$. In this chapter we extend this result and relation (5) which holds for $s = d$ to the case of weighted energy, and obtain separation estimates for minimal weighted energy configurations when the Hausdorff dimension of the compact set is an arbitrary positive number.

We consider separately the case of a strictly positive weight and a weight with isolated zeros.

IV.1 Asymptotic behavior of the minimlal weighted s-energy. The case of a positive weight.

Let $d \le d'$ be two positive integers and A be a compact set in $\mathbb{R}^{d'}$ whose d-dimensional Hausdorff measure, $\mathcal{H}_d(A)$ is finite (recall that we choose such normalization of $\mathcal{H}_d$ that $\mathcal{H}_d|_{\mathbb{R}^d} = \mathcal{L}_d$). For a collection of $N(\ge 2)$ distinct points $\omega_N := \{x_1, \dots, x_N\} \subset A$, a non-negative weight function w on $A \times A$ (we shall specify additional conditions on w shortly), and $s > 0$, the *weighted Riesz s-energy of ω_N* is defined by

$$E_s^w(\omega_N) := \sum_{1 \le i \ne j \le N} \frac{w(x_i, x_j)}{|x_i - x_j|^s} = \sum_{i=1}^{N} \sum_{\substack{j=1 \\ j \ne i}}^{N} \frac{w(x_i, x_j)}{|x_i - x_j|^s},$$

while the *N-point weighted Riesz s-energy of A* is defined by

$$\mathcal{E}_s^w(A, N) := \inf\{E_s^w(\omega_N) : \omega_N \subset A, \#\omega_N = N\}, \tag{58}$$

where as before, $\#X$ denotes the cardinality of a set X. Since, for the weight $\widetilde{w}(x,y) := (w(x,y) + w(y,x))/2$, we have

$$E_s^w(\omega_N) = E_s^{\widetilde{w}}(\omega_N) = 2 \sum_{1 \le i < j \le N} \frac{\widetilde{w}(x_i, x_j)}{|x_i - x_j|^s},$$

we shall assume, without loss of generality, throughout this chapter that w is symmetric, i.e., $w(x,y) = w(y,x)$ for $x, y \in A$. We call $w : A \times A \to [0, \infty]$ a *CPD-weight function on $A \times A$* if

(a) w is continuous (as a function on $A \times A$) at $\mathcal{H}_d$-almost every point of the diagonal $D(A) := \{(x,x) : x \in A\}$,

(b) there is some neighborhood G of $D(A)$ (relative to $A \times A$) such that $\inf_G w > 0$, and

(c) w is bounded on any closed subset $B \subset A \times A$ such that $B \cap D(A) = \emptyset$.

Here CPD stands for (almost) continuous and positive on the diagonal. In particular, conditions (a), (b), and (c) hold if w is bounded on $A \times A$ and continuous and positive at every point of the diagonal $D(A)$ (where continuity at a diagonal point (x_0, x_0) is meant in the sense of limits taken on $A \times A$).

If $w \equiv 1$ on $A \times A$, we get the non-weighted minimal energy problem considered in Chapter II. For the trivial cases $N = 0$ or 1 we put $E_s^w(\omega_N) = \mathcal{E}_s^w(A, N) = 0$.

If A is a compact set in $\mathbb{R}^{d'}$ and w is a CPD-weight function on $A \times A$, then for $s \geq d$ we define the *weighted Hausdorff measure* $\mathcal{H}_d^{s,w}$ on Borel sets $B \subset A$ by

$$\mathcal{H}_d^{s,w}(B) := \int_B (w(x,x))^{-d/s} d\mathcal{H}_d(x), \tag{59}$$

and its normalized form

$$h_d^{s,w}(B) := \frac{\mathcal{H}_d^{s,w}(B)}{\mathcal{H}_d^{s,w}(A)}, \tag{60}$$

if $\mathcal{H}_d(A) > 0$.

We say, that a sequence $\{\widetilde{\omega}_N\}_{N=2}^{\infty}$ of N-point configurations in A is *asymptotically (w,s)-energy minimizing for A* if

$$\lim_{N \to \infty} \frac{E_s^w(\widetilde{\omega}_N)}{\mathcal{E}_s^w(A, N)} = 1.$$

The main results of this section are stated below.

Theorem IV.1.1. *Let $A \subset \mathbb{R}^{d'}$ be a compact d-rectifiable set. Suppose that $s > d$ and w is a CPD-weight function on $A \times A$. Then*

$$\lim_{N \to \infty} \frac{\mathcal{E}_s^w(A, N)}{N^{1+s/d}} = \frac{C_{s,d}}{\left[\mathcal{H}_d^{s,w}(A)\right]^{s/d}}, \tag{61}$$

where $C_{s,d}$ is as in (42).

Furthermore, if $\mathcal{H}_d(A) > 0$, any asymptotically (w, s)-energy minimizing sequence of configurations $\widetilde{\omega}_N = \{x_1^N, \ldots, x_N^N\}$, $N = 2, 3, \ldots$, for A has limit distribution according to the measure $h_d^{s,w}$; that is,

$$\frac{1}{N}\sum_{k=1}^{N}\delta_{x_k^N} \xrightarrow{\ *\ } h_d^{s,w}, \quad N \to \infty. \tag{62}$$

Recall that constant β_d was defined in (12).

Theorem IV.1.2. *Let A be a compact subset of a d-dimensional C^1-manifold in $\mathbb{R}^{d'}$ with $\mathcal{H}_d(A) < \infty$, and suppose w is a CPD-weight function on $A \times A$. Then*

$$\lim_{N\to\infty} \frac{\mathcal{E}_d^w(A, N)}{N^2 \log N} = \frac{\beta_d}{\mathcal{H}_d^{d,w}(A)}. \tag{63}$$

Furthermore, if $\mathcal{H}_d(A) > 0$, any asymptotically (w, d)-energy minimizing sequence of configurations $\widetilde{\omega}_N = \{x_1^N, \ldots, x_N^N\}$, $N = 2, 3, \ldots$, on A has limit distribution with measure $h_d^{d,w}$; that is, (62) holds with $s = d$.

Remarks. In the case $\mathcal{H}_d(A) = 0$, the right-hand sides of (61) and (63) are understood to be infinity.

In order to obtain a finite collection of points distributed with a given density $\rho(x)$ on a closed d-rectifiable set A, we can take any $s > d$ and the weight

$$w(x, y) := (\rho(x)\rho(y) + |x - y|)^{-s/2d}, \tag{64}$$

where the term $|x-y|$ is included to ensure that w is locally bounded off of $D(A)$. By Theorem IV.1.1 any asymptotically (w, s)-energy minimizing sequence of N-point configurations will converge to the required distribution as $N \to \infty$. We thus obtain

Corollary IV.1.1. *Let $A \subset \mathbb{R}^{d'}$ be a compact d-rectifiable set with $\mathcal{H}_d(A) > 0$. Suppose ρ is a bounded probability density on A (with respect to $\mathcal{H}_d$) that is continuous $\mathcal{H}_d$-almost everywhere on A. Then, for $s > d$ and w given by (64), the normalized counting measures for any asymptotically (w, s)-energy minimizing sequence of configurations ω_N converge weak* (as $N \to \infty$) to $\rho\, d\mathcal{H}_d$.*

Furthermore, if $\inf_A \rho > 0$ and ρ is upper semi-continuous, then any (w, s)-energy minimizing sequence of configurations ω_N is well-separated in the sense of Theorem IV.5.1 with $\alpha = d$.

Remark: The first part of Corollary IV.1.1 holds for $s = d$ when A is contained in a C^1 d-dimensional manifold.

IV.2 Proofs for the case of a positive weight.

In this section we present proofs of Theorems IV.1.1 and IV.1.2. First, we prove several lemmas which are central to the proofs of our main theorems.

Divide and conquer. In this subsection we provide two lemmas relating the minimal energy problem on $A = B \cup D$ to the minimal energy problems on B and D, respectively.

In order to unify our computations for the cases $s > d$ and $s = d$, we define, for integers $N > 1$,

$$\tau_{s,d}(N) := \begin{cases} N^{1+s/d}, & s > d, \\ N^2 \log N, & s = d \end{cases}$$

and set $\tau_{s,d}(N) = 1$ for $N = 0$ or 1. For a set $A \subset \mathbb{R}^{d'}$ and $s \geq d$, let

$$\underline{g}^w_{s,d}(A) := \liminf_{N\to\infty} \frac{\mathcal{E}^w_s(A,N)}{\tau_{s,d}(N)}, \qquad \overline{g}^w_{s,d}(A) := \limsup_{N\to\infty} \frac{\mathcal{E}^w_s(A,N)}{\tau_{s,d}(N)},$$

and

$$g^w_{s,d}(A) := \lim_{N\to\infty} \frac{\mathcal{E}^w_s(A,N)}{\tau_{s,d}(N)}$$

if this limit exists (these quantities are allowed to be infinite). In the case $w(x,y) \equiv 1$, we use the notations $\underline{g}_{s,d}(A)$, $\overline{g}_{s,d}(A)$ and $g_{s,d}(A)$, respectively.

The following two lemmas extend to the weighted case Lemmas II.4.1 and II.4.2 whose proof is given in [28]. (We remark that the following results hold when quantities are 0 or infinite using $0^{-d/s} = 0^{-s/d} = \infty$ and $\infty^{-d/s} = \infty^{-s/d} = 0$.)

Lemma IV.2.1. *Let $s \geq d$ and suppose that B and D are sets in $\mathbb{R}^{d'}$ such that* $\operatorname{dist}(B, D) > 0$. *Suppose $w : (B \cup D) \times (B \cup D) \to [0, \infty]$ is bounded on the subset $B \times D$. Then*

$$\overline{g}^w_{s,d}(B \cup D)^{-d/s} \geq \overline{g}^w_{s,d}(B)^{-d/s} + \overline{g}^w_{s,d}(D)^{-d/s}.$$

Proof. Assume that $0 < \overline{g}^w_{s,d}(B),\ \overline{g}^w_{s,d}(D) < \infty$. Denote

$$\alpha^* := \frac{\overline{g}^w_{s,d}(D)^{d/s}}{\overline{g}^w_{s,d}(B)^{d/s} + \overline{g}^w_{s,d}(D)^{d/s}}.$$

For $N \in \mathbb{N}$, let $N_B := \lfloor \alpha^* N \rfloor$ (recall that $\lfloor x \rfloor$ denotes the greatest integer less than or equal to x), $N_D := N - N_B$ and $\omega_N^B \subset B$ and $\omega_N^D \subset D$ be configurations of N_B and N_D points respectively such that $E^w_s(\omega_N^B) < \mathcal{E}^w_s(B, N_B) + 1$ and $E^w_s(\omega_N^D) < \mathcal{E}^w_s(D, N_D) + 1$. Let $\gamma_0 := \operatorname{dist}(B, D) > 0$. Then

$$\begin{aligned}\mathcal{E}^w_s(B \cup D, N) &\leq E^w_s(\omega_N^B \cup \omega_N^D)\\ &= E^w_s(\omega_N^B) + E^w_s(\omega_N^D) + 2 \sum_{x \in \omega_N^B,\ y \in \omega_N^D} \frac{w(x,y)}{|x-y|^s}\\ &\leq \mathcal{E}^w_s(B, N_B) + \mathcal{E}^w_s(D, N_D) + 2 + 2\gamma_0^{-s} N^2 \|w\|_{B\times D},\end{aligned}$$

where $\|w\|_{B\times D}$ denotes the supremum of w over $B \times D$. Dividing by $\tau_{s,d}(N)$ and taking into account that $\tau_{s,d}(N_B)/\tau_{s,d}(N) \to (\alpha^*)^{1+s/d}$ as $N \to \infty$, we obtain

$$\begin{aligned}\overline{g}^w_{s,d}(B \cup D) &\leq \limsup_{N\to\infty} \frac{\mathcal{E}^w_s(B, N_B)}{\tau_{s,d}(N)} + \limsup_{N\to\infty} \frac{\mathcal{E}^w_s(D, N_D)}{\tau_{s,d}(N)}\\ &= \limsup_{N\to\infty} \frac{\mathcal{E}^w_s(B, N_B)}{\tau_{s,d}(N_B)} \cdot \frac{\tau_{s,d}(N_B)}{\tau_{s,d}(N)} + \limsup_{N\to\infty} \frac{\mathcal{E}^w_s(D, N_D)}{\tau_{s,d}(N_D)} \cdot \frac{\tau_{s,d}(N_D)}{\tau_{s,d}(N)}\\ &\leq \overline{g}^w_{s,d}(B) \cdot (\alpha^*)^{1+s/d} + \overline{g}^w_{s,d}(D) \cdot (1-\alpha^*)^{1+s/d}\\ &= \left(\overline{g}^w_{s,d}(B)^{-d/s} + \overline{g}^w_{s,d}(D)^{-d/s}\right)^{-s/d}.\end{aligned}$$

The remaining cases when $\overline{g}^w_{s,d}(B)$ or $\overline{g}^w_{s,d}(D)$ are 0 or ∞ easily follow from the monotonicity of $\overline{g}^w_{s,d}$.

The following statement in particular shows sub-additivity of $\underline{g}^w_{s,d}(\cdot)^{-d/s}$.

Lemma IV.2.2. *Let $s \geq d$ and $B, D \subset \mathbb{R}^{d'}$. Suppose $w : (B \cup D) \times (B \cup D) \to [0, \infty]$. Then*

$$\underline{g}^w_{s,d}(B \cup D)^{-d/s} \leq \underline{g}^w_{s,d}(B)^{-d/s} + \underline{g}^w_{s,d}(D)^{-d/s}. \tag{65}$$

Furthermore, if $\underline{g}^w_{s,d}(B), \underline{g}^w_{s,d}(D) > 0$ and at least one of these quantities is finite, then

$$\lim_{\mathcal{N} \ni N \to \infty} \frac{\#\left(\widetilde{\omega}_N \cap B\right)}{N} = \frac{\underline{g}^w_{s,d}(D)^{d/s}}{\underline{g}^w_{s,d}(B)^{d/s} + \underline{g}^w_{s,d}(D)^{d/s}} \tag{66}$$

holds for any sequence $\{\widetilde{\omega}_N\}_{N\in\mathcal{N}}$ *of* N*-point configurations in* $B\cup D$ *such that*

$$\lim_{\mathcal{N}\ni N\to\infty}\frac{E_s^w(\widetilde{\omega}_N)}{\tau_{s,d}(N)}=\left(\underline{g}_{s,d}^w(B)^{-d/s}+\underline{g}_{s,d}^w(D)^{-d/s}\right)^{-s/d}, \tag{67}$$

where $\mathcal{N}$ *is some infinite subset of* $\mathbb{N}$.

In the case $\underline{g}_{s,d}^w(D)=\infty$ the right-hand side of relation (66) is understood to be 1.

Proof. Assume that $\underline{g}_{s,d}^w(B),\underline{g}_{s,d}^w(D)>0$ and $\underline{g}_{s,d}^w(B)<\infty$. We agree that $\infty\cdot a=\infty$ for any $a>0$ and $\infty\cdot 0=0$. Let an infinite subset $\mathcal{N}_1\subset\mathbb{N}$ and a sequence of point configurations $\{\omega_N\}_{N\in\mathcal{N}_1}$, $\omega_N\subset B\cup D$, be such that $\lim_{\mathcal{N}_1\ni N\to\infty}\#(\omega_N\cap B)/N=\alpha$, where $0\le\alpha\le 1$. Set $N_B:=\#(\omega_N\cap B)$ and $N_D:=\#(\omega_N\setminus B)$. Then

$$E_s^w(\omega_N)\ge E_s^w(\omega_N\cap B)+E_s^w(\omega_N\setminus B)\ge\mathcal{E}_s^w(B,N_B)+\mathcal{E}_s^w(D,N_D),$$

and we have

$$\begin{aligned}\liminf_{\mathcal{N}_1\ni N\to\infty}\frac{E_s^w(\omega_N)}{\tau_{s,d}(N)}&\ge\liminf_{\mathcal{N}_1\ni N\to\infty}\frac{\mathcal{E}_s^w(B,N_B)}{\tau_{s,d}(N_B)}\cdot\frac{\tau_{s,d}(N_B)}{\tau_{s,d}(N)}\\&\quad+\liminf_{\mathcal{N}_1\ni N\to\infty}\frac{\mathcal{E}_s^w(D,N_D)}{\tau_{s,d}(N_D)}\cdot\frac{\tau_{s,d}(N_D)}{\tau_{s,d}(N)}\\&\ge F(\alpha):=\underline{g}_{s,d}^w(B)\alpha^{1+s/d}+\underline{g}_{s,d}^w(D)(1-\alpha)^{1+s/d}.\end{aligned}\tag{68}$$

Let

$$\widetilde{\alpha}:=\frac{\underline{g}_{s,d}^w(D)^{d/s}}{\underline{g}_{s,d}^w(B)^{d/s}+\underline{g}_{s,d}^w(D)^{d/s}},$$

and $\{\widetilde{\omega}_N\}_{N\in\mathcal{N}}$ be any sequence of point sets satisfying (67). If $\mathcal{N}_2\subset\mathcal{N}$ is any infinite subsequence such that the quantity $\#(\widetilde{\omega}_N\cap B)/N$ has a limit as $\mathcal{N}_2\ni N\to\infty$ (denote it by α_1), then by (67) and (68) we have

$$F(\widetilde{\alpha})=\lim_{\mathcal{N}_2\ni N\to\infty}\frac{E_s^w(\widetilde{\omega}_N)}{\tau_{s,d}(N)}\ge F(\alpha_1).$$

It is not difficult to see that $\widetilde{\alpha}$ is the only minimum point of $F(t)$ on $[0,1]$. Hence $\alpha_1=\widetilde{\alpha}$, which proves (66).

Now let $\{\overline{\omega}_N\}_{N\in\mathcal{N}_3}$ be a sequence of N-point configurations in $B\cup D$ such that

$$\underline{g}_{s,d}^w(B\cup D)=\lim_{\mathcal{N}_3\ni N\to\infty}\frac{E_s^w(\overline{\omega}_N)}{\tau_{s,d}(N)}$$

($\overline{\omega}_N$'s can be chosen for example so that $E_s^w(\overline{\omega}_N) < \mathcal{E}_s^w(B \cup D, N) + 1$). If $\mathcal{N}_4 \subset \mathcal{N}_3$ is such an infinite set that $\lim_{\mathcal{N}_4 \ni N \to \infty} \#\left(\overline{\omega}_N \cap B\right)/N$ exists (denote it by α_2), then by (68) we obtain

$$\begin{aligned} \underline{g}_{s,d}^w(B \cup D) &= \lim_{\mathcal{N}_4 \ni N \to \infty} \frac{E_s^w(\overline{\omega}_N)}{\tau_{s,d}(N)} \geq F(\alpha_2) \\ &\geq F(\widetilde{\alpha}) = \left(\underline{g}_{s,d}^w(B)^{-d/s} + \underline{g}_{s,d}^w(D)^{-d/s}\right)^{-s/d}, \end{aligned}$$

which implies (65).

Proofs of Theorems IV.1.1 and IV.1.2. The following lemma relates the weighted minimal energy problem ($s \geq d$) on a set $A \subset \mathbb{R}^{d'}$ to the unweighted minimal energy problem on compact subsets of A. Theorems IV.1.1 and IV.1.2 then follow easily from this lemma. For convenience, we denote

$$C_{d,d} := \beta_d, \quad d \in \mathbb{N}.$$

and recall that when $w(x,y) \equiv 1$, we set

$$\underline{g}_{s,d}(A) = \underline{g}_{s,d}^w(A), \quad \overline{g}_{s,d}(A) = \overline{g}_{s,d}^w(A), \quad \text{and} \quad g_{s,d}(A) = g_{s,d}^w(A).$$

Lemma IV.2.3. *Suppose $s \geq d$, $A \subset \mathbb{R}^{d'}$ is compact with $\mathcal{H}_d(A) < \infty$, and that w is a CPD-weight function on $A \times A$. Furthermore, suppose that for any compact subset $K \subset A$, the limit $g_{s,d}(K)$ exists and is given by*

$$g_{s,d}(K) = \frac{C_{s,d}}{\mathcal{H}_d(K)^{s/d}}. \tag{69}$$

Then

(a) $g_{s,d}^w(A)$ exists and is given by

$$g_{s,d}^w(A) = C_{s,d}\left(\mathcal{H}_d^{s,w}(A)\right)^{-s/d}, \tag{70}$$

and,

(b) if a sequence $\{\widetilde{\omega}_N\}_{N=2}^{\infty}$, where $\widetilde{\omega}_N = \{x_1^N, \ldots, x_N^N\}$, is asymptotically (w,s)-energy minimizing on the set A and $\mathcal{H}_d(A) > 0$, then

$$\frac{1}{N}\sum_{k=1}^{N} \delta_{x_k^N} \xrightarrow{\ *\ } h_d^{s,w}, \quad N \to \infty. \tag{71}$$

Remark. If $\mathcal{H}_d(K) = 0$, condition (69) is understood as $g_{s,d}(K) = \infty$.

Proof. To prove the first part of this statement, we break A into disjoint "pieces" of small diameter and estimate the (w, s)-energy of A by replacing w with its supremum or infinum on each of the "pieces" and applying Lemmas IV.2.1 and IV.2.2.

For $\delta > 0$, suppose that $\mathcal{P}_\delta$ is a partition of A such that $\operatorname{diam} P \leq \delta$ and $\mathcal{H}_d(\overline{P}) = \mathcal{H}_d(P)$ for $P \in \mathcal{P}_\delta$, where $\overline{B}$ denotes the closure of a set B. For each $P \in \mathcal{P}_\delta$, choose a closed subset $Q_P \subset P$ so that $\mathcal{Q}_\delta := \{Q_P : P \in \mathcal{P}_\delta\}$ satisfies

$$\sum_{P \in \mathcal{P}_\delta} \mathcal{H}_d(Q_P) \geq \mathcal{H}_d(A) - \delta, \tag{72}$$

and

$$\operatorname{dist}(Q_{P_1}, Q_{P_2}) > 0, \quad P_1 \neq P_2 \in \mathcal{P}_\delta.$$

An example of such systems $\mathcal{P}_\delta$ and $\mathcal{Q}_\delta$ can be constructed as follows. Let $G_j[t]$ be the hyperplane in $\mathbb{R}^{d'}$ consisting of all points whose j-th coordinate equals t. If $(-a, a)^{d'}$ is a cube containing A, then for $\mathbf{i} = (i_1, \ldots, i_{d'}) \in \{1, \ldots, m\}^{d'}$, let

$$R_{\mathbf{i}} := [t^1_{i_1 - 1}, t^1_{i_1}) \times \cdots \times [t^{d'}_{i_{d'} - 1}, t^{d'}_{i_{d'}}),$$

where m and partitions $-a = t^j_0 < t^j_1 < \ldots < t^j_m = a$, $j = 1, \ldots, d'$, are chosen so that the diameter of every $R_{\mathbf{i}}$, $\mathbf{i} \in \{1, \ldots, m\}^{d'}$, is less than δ and $\mathcal{H}_d(G_j[t^j_i] \cap A) = 0$ for all i and j. (Since $\mathcal{H}_d(A) < \infty$, there are at most countably many values of t such that $\mathcal{H}_d(G_j[t] \cap A) > 0$.) Then, we may choose

$$\mathcal{P}_\delta = \{R_{\mathbf{i}} \cap A : \mathbf{i} \in \{1, \ldots, m\}^{d'}\}$$

and $\gamma \in (0, 1)$ sufficiently close to 1 such that (72) holds for $\mathcal{Q}_\delta = \{Q_{\mathbf{i}} : \mathbf{i} \in \{1, \ldots, m\}^{d'}\}$, where $Q_{\mathbf{i}} = \big(\gamma(\overline{R}_{\mathbf{i}} - c_{\mathbf{i}}) + c_{\mathbf{i}}\big) \cap A$ and $c_{\mathbf{i}}$ denotes the center of $R_{\mathbf{i}}$.

To continue the proff for $B \subset A$, let

$$\overline{w}_B = \sup_{x,y \in B} w(x, y) \text{ and } \underline{w}_B = \inf_{x,y \in B} w(x, y)$$

and define the simple functions

$$\overline{w}_\delta(x) := \sum_{P\in\mathcal{P}_\delta} \overline{w}_P \cdot \chi_P(x) \quad \text{and} \quad \underline{w}_\delta(x) := \sum_{P\in\mathcal{P}_\delta} \underline{w}_P \cdot \chi_P(x),$$

where χ_K denotes the characteristic function of a set K. Since the distance between any two sets from $\mathcal{Q}_\delta$ is strictly positive, Lemma IV.2.1 and equation (69) imply

$$\begin{aligned} \overline{g}^w_{s,d}(A)^{-d/s} &\geq \overline{g}^{\overline{w}_\delta}_{s,d}\left(\bigcup_{Q\in\mathcal{Q}_\delta} Q\right)^{-d/s} \geq \sum_{\substack{Q\in\mathcal{Q}_\delta\\ Q\neq\emptyset}} \left(\overline{w}_Q \cdot \overline{g}_{s,d}(Q)\right)^{-d/s} \\ &= C_{s,d}^{-d/s} \sum_{\substack{Q\in\mathcal{Q}_\delta\\ Q\neq\emptyset}} \overline{w}_Q^{-d/s} \cdot \mathcal{H}_d(Q) \geq C_{s,d}^{-d/s} \int\limits_{\bigcup\limits_{Q\in\mathcal{Q}_\delta} Q} (\overline{w}_\delta(x))^{-d/s} d\mathcal{H}_d(x). \end{aligned} \tag{73}$$

Applying Lemma IV.2.2 and relation (69), we similarly have

$$\begin{aligned} \underline{g}^w_{s,d}(A)^{-d/s} &\leq \sum_{P\in\mathcal{P}_\delta} \left(\underline{w}_P \cdot \underline{g}_{s,d}(P)\right)^{-d/s} = \sum_{P\in\mathcal{P}_\delta} \left(\underline{w}_P \cdot \underline{g}_{s,d}(\overline{P})\right)^{-d/s} \\ &= C_{s,d}^{-d/s} \sum_{P\in\mathcal{P}_\delta} \underline{w}_P^{-d/s} \cdot \mathcal{H}_d(\overline{P}) = C_{s,d}^{-d/s} \int\limits_A (\underline{w}_\delta(x))^{-d/s} d\mathcal{H}_d(x). \end{aligned} \tag{74}$$

Since w is a CPD-weight function on $A \times A$, there is some neighborhood G of $D(A)$ such that $\eta := \inf_G w > 0$. For $\delta > 0$ sufficiently small, we have $P \times P \subset G$ for all $P \in \mathcal{P}_\delta$, and hence

$$\overline{w}_\delta(x) \geq w(x,x) \geq \underline{w}_\delta(x) \geq \eta$$

for $x \in A$. Furthermore, w is continuous at $(x,x) \in D(A)$ for $\mathcal{H}_d$-almost all $x \in A$ and thus, for any such x, it follows that $\overline{w}_\delta(x)$ and $\underline{w}_\delta(x)$ converge to $w(x,x)$ as $\delta \to 0$. Therefore, by the Lebesgue Dominated Convergence Theorem, the integrals

$$\int\limits_{\bigcup\limits_{Q\in\mathcal{Q}_\delta} Q} \left(\overline{w}_\delta(x)\right)^{-d/s} d\mathcal{H}_d(x) \text{ and } \int_A \left(\underline{w}_\delta(x)\right)^{-d/s} d\mathcal{H}_d(x)$$

both converge to $\mathcal{H}_d^{s,w}(A)$ as $\delta \to 0$. Hence, using (73) and (74), we obtain (70).

Now suppose that $\mathcal{H}_d(A) > 0$ and $\widetilde{\omega}_N = \{x_1^N, \ldots, x_N^N\}$, $N \in \mathbb{N}$, is an asymptotically (w,s)-energy minimizing sequence of N-point configurations on A. As we have noted in Section II.1, the weak* convergence result given in (71) is equivalent to the assertion that

$$\lim_{N\to\infty} \frac{\#\left(\widetilde{\omega}_N \bigcap B\right)}{N} = h_d^{s,w}(B) \tag{75}$$

holds for any subset $B \subset A$, whose boundary with respect to A has $\mathcal{H}_d$-measure zero. For any such set $B \subset A$, since each of sets $\overline{B}$ and $\overline{A \setminus B}$ as compact subsets of A, satisfies the hypotheses of Lemma IV.2.3, relation (70) implies

$$\begin{aligned}\lim_{N\to\infty} \frac{E_s^w(\widetilde{\omega}_N)}{\tau_{s,d}(N)} &= C_{s,d}\left(\mathcal{H}_d^{s,w}(A)\right)^{-s/d} \\ &= C_{s,d}\left(\mathcal{H}_d^{s,w}(\overline{B}) + \mathcal{H}_d^{s,w}(\overline{A\setminus B})\right)^{-s/d} \\ &= \left(g_{s,d}^w(\overline{B})^{-d/s} + g_{s,d}^w(\overline{A\setminus B})^{-d/s}\right)^{-s/d}.\end{aligned}$$

Using relation (66) in Lemma IV.2.2 and (70) for $\overline{B}$ and $\overline{A\setminus B}$, we get

$$\lim_{N\to\infty} \frac{\#\left(\widetilde{\omega}_N \bigcap B\right)}{N} = \frac{g_{s,d}^w(\overline{A\setminus B})^{d/s}}{g_{s,d}^w(\overline{B})^{d/s} + g_{s,d}^w(\overline{A\setminus B})^{d/s}} = h_d^{s,w}(B)$$

showing that (71) holds.

Theorems IV.1.1 and IV.1.2 then follow from Lemma IV.2.3 and Theorems II.1.1 for closed d-rectifiable sets and Theorem B for $s = d$ as we now explain. If $s > d$ and $A \subset \mathbb{R}^{d'}$ is a closed d-rectifiable set, then every compact subset $B \subset A$ is also closed and d-rectifiable and Theorem II.1.1 implies that B satisfies condition (69) and so Theorem IV.1.1 then follows from Lemma IV.2.3. If $s = d$ and A is a compact subset of a d-dimensional C^1-manifold in $\mathbb{R}^{d'}$, then applying Theorem B for $s = d$ to every compact subset of A, we get (69). Consequently Theorem IV.1.2 follows from Lemma IV.2.3 with $s = d$.

IV.3 The case of a weight with zeros.

Finally, we consider weight functions with isolated zeros. For $t > 0$, we say that a function $w : A \times A \to \mathbb{R}$ has a *zero at* $(a, a) \in D(A)$ *of order at most* t if there are positive constants C and δ such that

$$w(x, y) \geq C|x - a|^t \qquad (x, y \in A \cap B(a, \delta)), \tag{76}$$

where as above, $B(a,r)$ denotes the open ball in $\mathbb{R}^{d'}$ centered at a point a with radius $r > 0$. If w has a zero $a \in A$ whose order is too large, then a may act as an attractive "sink" with $\mathcal{E}_s^w(A,N) = 0$. For example, let A be the closed unit ball in $\mathbb{R}^d$, $w(x,y) = |x|^t + |y|^t$ for $x, y \in A$ with $t > s > d$. If $\omega_N = \{x_1, \ldots, x_N\}$ is a configuration of N distinct points in A, then

$$E_s^w(\gamma\omega_N) = \gamma^{t-s} E_s^w(\omega_N)$$

for any $0 < \gamma < 1$. Taking $\gamma \to 0$, shows that $\mathcal{E}_s^w(A,N) = 0$.

We say that a closed set $A \subset \mathbb{R}^{d'}$ is *α-regular at $a \in A$* if there are positive constants C_0 and δ such that

$$(C_0)^{-1} r^\alpha \leq \mathcal{H}_\alpha(A \cap B(x,r)) \leq C_0 r^\alpha \tag{77}$$

for all $x \in A \cap B(a,\delta)$ and $0 < r < \delta$.

Theorem IV.3.1. *Let $A \subset \mathbb{R}^{d'}$ be a compact d-rectifiable set and $s > d$. Suppose A is α_i-regular with $\alpha_i \leq d$ at a_i, $i = 1, \ldots, n$, for a finite collection of points $a_1, \ldots, a_n$ in A and that $w : A \times A \to [0,\infty]$ is a CPD-weight function on $K \times K$ for any compact $K \subset A \setminus \{a_1, \ldots, a_n\}$. If w has a zero of order at most $t < s$ at each (a_i, a_i), then the conclusions of Theorem IV.1.1 hold.*

Remark: The hypotheses of Theorem IV.3.1 imply that

$$\int_A (w(x,x))^{-d/s} d\mathcal{H}_d(x) < \infty$$

(see Section IV.4).

IV.4 Proof for the case of a weight with zeros.

In this section we prove Theorem IV.3.1. The essential ingredient in the proof of Theorem IV.3.1 is the following lemma which assumes lower regularity. We say that a set $K \subset \mathbb{R}^{d'}$ is *lower α-regular* if there are positive constants C_0 and r_0 so that

$$(C_0)^{-1} r^\alpha \leq \mathcal{H}_\alpha(K \cap B(x,r)) \tag{78}$$

for all $x \in K$ and $r < r_0$.

Lemma IV.4.1. *Suppose $K \subset \mathbb{R}^{d'}$ is compact and lower α-regular and $a \in K$. Further suppose $s > \alpha$ and $w : K \times K \to [0,\infty]$ is a CPD-weight function on $K' \times K'$ for any compact set $K' \subset K \setminus \{a\}$. If w has a zero of order at most t at (a,a), where $0 < t < s$, then there is a constant $C_1 > 0$ such that*

$$\underline{g}^w_{s,\alpha}(K) \geq C_1 C_0^{-s/\alpha} 2^{-(s+t)} \left(\int_K \frac{1}{|x-a|^{(t\alpha)/s}} \, d\mathcal{H}_\alpha(x) \right)^{-s/\alpha}. \tag{79}$$

Proof. Let $\omega_N = \{x_1, \ldots, x_N\}$ be a configuration of N distinct points in K. For $i = 1, \ldots, N$, let $\rho_i = |x_i - a|$, $r_i = \min_{j:j\neq i} |x_i - x_j|$, and choose $y_i \in \omega_N$ such that $|x_i - y_i| = r_i$. Since K is bounded, there is some finite L (independent of N) such that there are at most $L-1$ of the points $x_i \in \omega_N$ with the property that $r_i \geq r_0$ (where r_0 is from the definition of lower α-regularity and $r_0 \leq \delta$, where δ comes from the definition of a zero of order at most t at (a,a)). We order the points in ω_N so that $\rho_N \leq \rho_i$ for $i = 1, \ldots, N$ and so that $r_i < r_0$ for $i = 1, \ldots, N-L$. It follows from Cauchy's and Jensen's inequality (or see (29) of [28]) that if $\gamma_1, \ldots, \gamma_M$ are positive numbers, then

$$\sum_{i=1}^{M} \gamma_i^{-s} \geq M^{1+s/\alpha} \left(\sum_{i=1}^{M} \gamma_i^{\alpha} \right)^{-s/\alpha} \tag{80}$$

from which we obtain

$$\begin{aligned} E_s^w(\omega_N) &\geq \sum_{i=1}^{N-L} \frac{w(x_i,y_i)}{r_i^s} \geq C_1 \sum_{i=1}^{N-L} \frac{\rho_i^t}{r_i^s} = C_1 \sum_{i=1}^{N-L} \left(\rho_i^{-t/s} r_i \right)^{-s} \\ &\geq C_1 (N-L)^{1+s/\alpha} \left(\sum_{i=1}^{N-L} \frac{r_i^\alpha}{\rho_i^{t\alpha/s}} \right)^{-s/\alpha}. \end{aligned} \tag{81}$$

For $i = 1, \ldots, N-1$, observe that

$$r_i = \min_{j:j\neq i} |x_i - x_j| \leq |x_i - a| + \min_{j:j\neq i} |a - x_j| \leq \rho_i + \rho_N \leq 2\rho_i$$

and so

$$|x-a| \leq |x - x_i| + |x_i - a| \leq r_i/2 + \rho_i \leq 2\rho_i, \qquad x \in B(x_i, r_i/2). \tag{82}$$

Using (78) and (82) we have

$$\frac{r_i^\alpha}{\rho_i^{t\alpha/s}} \leq C_0 2^{(t+s)\alpha/s} (2\rho_i)^{-\alpha t/s} \mathcal{H}_\alpha \left(K \cap B\left(x_i, r_i/2\right) \right)$$

$$\leq C_0 2^{(\alpha/s)(s+t)} \int_{K\cap B(x_i,r_i/2)} \frac{1}{|x-a|^{t\alpha/s}}\, d\mathcal{H}_\alpha(x)$$

for $i = 1, \ldots, N-L$. Since $B(x_i, r_i/2)$ and $B(x_j, r_j/2)$ are disjoint for $i \neq j$, it follows that

$$\sum_{i=1}^{N-L} \frac{r_i^\alpha}{\rho_i^{t\alpha/s}} \leq C_0 2^{(\alpha/s)(s+t)} \int_K \frac{1}{|x-a|^{t\alpha/s}}\, d\mathcal{H}_\alpha(x).$$

From (81) we get

$$E_s(\omega_N) \geq C_1 C_0^{-s/\alpha} 2^{-(s+t)} (N-L)^{1+s/\alpha} \left(\int\limits_K \frac{1}{|x-a|^{(t\alpha)/s}}\, d\mathcal{H}_\alpha(x) \right)^{-s/\alpha}.$$

In view of arbitrariness of ω_N, we get the requiured inequality. Lemma IV.4.1 is proved.

Remark: If K is α-regular at a in the above lemma, then the integral

$$\int\limits_K \frac{1}{|x-a|^{(t\alpha)/s}}\, d\mathcal{H}_\alpha(x)$$

appearing in (79) is finite (cf. [38, p. 109]) and thus the Lebesgue Dominated Convergence Theorem (or absolute continuity of the lebesgue integral) gives

$$\lim_{\delta\to 0} \int\limits_{K\cap B(a,\delta)} \frac{1}{|x-a|^{(t\alpha)/s}}\, d\mathcal{H}_\alpha(x) = 0$$

and so $\lim_{\delta\to 0} \underline{g}^w_{s,\alpha}(K\cap B(a,\delta)) = \infty$.

Now we are prepared to complete the proof of Theorem IV.3.1. First note that the hypotheses of Theorem IV.3.1 (namely that A is α_i-regular at a_i and w has a zero of order of at most $t < s$ at a_i for $i = 1, \ldots, n$) imply that

$$\int\limits_A w(x,x)^{-d/s}\, d\mathcal{H}_d(x) < \infty.$$

Suppose $\epsilon > 0$. By Lemma IV.4.1 and Lemma IV.2.2 we can find $\delta > 0$ such that $B_\epsilon := \bigcup_{i=1}^n (A \cap B(a_i, \delta))$ satisfies $\underline{g}^w_{s,d}(B_\epsilon) \geq \epsilon^{-1}$ (note that if $\alpha < d$ and $\underline{g}^w_{s,\alpha}(K) > 0$, then $\underline{g}^w_{s,d}(K) = \infty$) and

$$\mathcal{H}_d^{s,w}(A_\epsilon) = \int_{A_\epsilon} w(x,x)^{-s/d}\, d\mathcal{H}_d(x) \geq (1-\epsilon)\mathcal{H}_d^{s,w}(A),$$

where $A_\epsilon := A \setminus B_\epsilon$.

Since w is a CPD-weight function on $A_\epsilon \times A_\epsilon$, it follows from Theorem IV.1.1 that $g^w_{s,d}(A_\epsilon)$ exists and equals $C_{s,d}\mathcal{H}^{s,w}_d(A_\epsilon)^{-s/d}$. Lemma IV.2.2 then gives

$$\begin{aligned}\underline{g}^w_{s,d}(A) &\geq (g^w_{s,d}(A_\epsilon)^{-d/s} + \underline{g}^w_{s,d}(B_\epsilon)^{-d/s})^{-s/d} \\ &\geq (C^{-d/s}_{s,d}\mathcal{H}^{s,w}_d(A_\epsilon) + \epsilon^{d/s})^{-s/d} \\ &\geq (C^{-d/s}_{s,d}\mathcal{H}^{s,w}_d(A) + \epsilon^{d/s})^{-s/d}.\end{aligned} \tag{83}$$

Also, we clearly have

$$\overline{g}^w_{s,d}(A) \leq g^w_{s,d}(A_\epsilon) = C_{s,d}\mathcal{H}^{s,w}_d(A_\epsilon)^{-s/d} \leq C_{s,d}(1-\epsilon)^{-s/d}\mathcal{H}^{s,w}_d(A)^{-s/d}. \tag{84}$$

Taking $\epsilon \to 0$ in (83) and (84) shows that $g^w_{s,d}(A)$ exists and equals $C_{s,d}\mathcal{H}^{s,w}_d(A)^{-s/d}$.

If $\mathcal{H}^{s,w}_d(A) > 0$, then, as in the proof of Theorem IV.1.1, Lemma IV.2.2 implies that (62) holds for any asymptotically (w,s)-energy minimizing sequence of configurations $\widetilde{\omega}_N = \{x^N_1, \ldots, x^N_N\}$, $N = 2, 3, \ldots$, for A which will complete the proof of Theorem IV.3.1. Indeed, choose any subset $B \subset A$ with $\mathcal{H}_d(\partial_A B) = 0$ (∂_A denotes the boundary of a subset of A relative to A). Since each a_i is α_i-regular with $\alpha_i \leq d$ and $\mathcal{H}_d(A) < \infty$, for almost all $\delta \in (0, \delta_0)$, where δ_0 is a sufficiently small number, we can write:

$$\mathcal{H}_d(A \cap S(a_i, \delta)) = 0, \quad i = 1, \ldots, n, \tag{85}$$

where $S(a_i, \delta)$ is the sphere in $\mathbb{R}^{d'}$ centered at point a_i of radius δ, and

$$\mathcal{H}_d\left(A \cap (\cup^n_{i=1} B(a_i, \delta))\right) \leq C\delta^d, \tag{86}$$

for some $C > 0$. For $\delta \in (0, \delta_0)$ such that (85) and (86) hold, denote

$$B_\delta := B \cup (\cup^n_{i=1} B[a_i, \delta] \cap A),$$

where $B[a, r]$ is a closed ball in $\mathbb{R}^{d'}$ centered at a point a of radius $r > 0$. Then, $\mathcal{H}_d(\partial_A B_\delta) = \mathcal{H}_d(\partial_A(A \setminus B_\delta)) = 0$. Set $\overline{B}_\delta$ satisfies the assumptions of the Theorem IV.3.1 and set $\overline{A \setminus B_\delta}$ satisfies even assumptions of Theorem IV.1.1. We already proved that they both will satisfy (61).

Using argument, analogous to the proof of (62) (or (71)), we get that

$$\limsup_{N\to\infty} \frac{\#(B\cap\widetilde{\omega}_N)}{N} \leq \lim_{N\to\infty} \frac{\#(B_\delta\cap\widetilde{\omega}_N)}{N} = h_d^{s,w}(B_\delta).$$

On the other hand, let $D_\delta := B \setminus (\cup_{i=1}^n B(a_i,\delta))$. It is not difficult to see that $\mathcal{H}_d(\partial_A D_\delta) = \mathcal{H}_d(\partial_A(A\setminus D_\delta)) = 0$. Both $\overline{D}_\delta$ and $\overline{A\setminus D_\delta}$ satisfy (61). Using again the argument from the proof of (62), we get that

$$\liminf_{N\to\infty} \frac{\#(B\cap\widetilde{\omega}_N)}{N} \geq \lim_{N\to\infty} \frac{\#(D_\delta\cap\widetilde{\omega}_N)}{N} = h_d^{s,w}(D_\delta).$$

Letting $\delta\to 0$ so that (85) and (86) hold, we get that $\mathcal{H}_d(B_\delta)\to\mathcal{H}_d(B)$, $\mathcal{H}_d(D_\delta)\to\mathcal{H}_d(B)$, and

$$\lim_{N\to\infty} \frac{\#(B\cap\widetilde{\omega}_N)}{N} = h_d^{s,w}(B).$$

Theorem IV.3.1 is proved.

IV.5 Separation results

For an N-point configuration $\omega_N = \{x_1,\ldots,x_N\}\subset A$ let

$$\delta(\omega_N) := \min_{1\leq i\neq j\leq N} |x_i - x_j| \tag{87}$$

be its separation distance (or separation radius). We obtain estimates for the separation radius of minimal weighted energy configurations on a class of sets including sets of arbitrary Hausdorff dimension α. We remark that the normalization for the Hausdorff measure $\mathcal{H}_\alpha$ plays no essential role here.

Theorem IV.5.1. *Let $0<\alpha\leq d'$. Suppose $A\subset\mathbb{R}^{d'}$ is a compact set with $\mathcal{H}_\alpha(A)>0$ and let w be a CPD-weight function that is bounded and lower semi-continuous on $A\times A$. Then, for every $s\geq\alpha$ there is a constant $c_s = c_s(A,w,\alpha)>0$ such that any (w,s)-energy minimizing configuration ω_N^* on A, with N points, satisfies the inequality*

$$\delta(\omega_N^*) \geq \begin{cases} c_s N^{-1/\alpha}, & s>\alpha, \\ c_\alpha (N\log N)^{-1/\alpha}, & s=\alpha, \quad N\geq 2. \end{cases}$$

As a consequence of the proof of Theorem IV.5.1 we establish the following estimates. Recall that

$$\mathcal{H}_\alpha^\infty(A) := \inf\{\sum_i (\text{diam } G_i)^\alpha : A \subset \bigcup_i G_i\}$$

and $\|w\|_{A\times A} = \sup\{w(x,y) : x, y \in A\}$.

Corollary IV.5.1. *Under the assumptions of Theorem IV.5.1, for $N \geq 2$,*

$$\mathcal{E}_s^w(A,N) \leq \begin{cases} M_{s,\alpha}\|w\|_{A\times A}\mathcal{H}_\alpha^\infty(A)^{-s/\alpha}N^{1+s/\alpha}, & s > \alpha, \\ M_\alpha N^2 \log N, \quad s = \alpha, \end{cases}$$

where the constant $M_{s,\alpha} > 0$ is independent of A, w and N, and the constant M_α is independent of N.

Known separation results on curves for $s > 1$ [39] and on d-rectifiable manifolds for $s > d$ [34], [28], [13] use the following upper regularity assumption. There are constants $M, \delta > 0$ such that for every $x \in A$ and $0 < r < \delta$ we have

$$\mathcal{H}_d(A \cap B(x,r)) \leq Mr^d. \tag{88}$$

We base the proof of our results on Frostman's lemma establishing the existence of a non-trivial measure on a set A with $\mathcal{H}_d(A) > 0$ satisfying a regularity assumption similar to (88).

Lemma IV.5.1. *(see e.g. [38, Theorem 8.8]). Let $\alpha > 0$ and A be a Borel set in $\mathbb{R}^{d'}$. Then $\mathcal{H}_\alpha(A) > 0$ if and only if there is a Radon measure μ on $\mathbb{R}^{d'}$ with compact support contained in A such that $0 < \mu(A) < \infty$ and*

$$\mu[B(x,r)] \leq r^\alpha, \quad x \in \mathbb{R}^{d'}, \quad r > 0. \tag{89}$$

Moreover, one can find μ so that $\mu(A) \geq c_{d',\alpha}\mathcal{H}_\alpha^\infty(A)$, where $c_{d',\alpha} > 0$ is independent of A.

We proceed using the technique developed in [34]. Let $\omega_N^* := \{x_1, \dots, x_N\}$, $N \in \mathbb{N}$, $N \geq 2$, be a (w,s)-energy minimizing configuration on A (for convenience, we dropped the subscript N in writing energy minimizing points $x_{k,N}$). For $i = 1, \dots, N$ let

$$U_i(x) := \sum_{j:j\neq i} \frac{w(x, x_j)}{|x - x_j|^s}, \quad x \in A.$$

From the minimization property we have that $U_i(x_i) \leq U_i(x)$, $x \in A$, $i = 1, \dots, N$. If μ is a measure from Lemma IV.5.1, set

$$r_0 := \left(\frac{\mu(A)}{2N}\right)^{1/\alpha}$$

and let

$$D_i := A \setminus \bigcup_{j:j\neq i} B(x_j, r_0), \quad i = 1, \dots, N.$$

Then, by the properties of μ, we have

$$\mu(D_i) \geq \mu(A) - \sum_{j:j\neq i} \mu\left[B(x_j, r_0)\right] \geq \mu(A) - (N-1)r_0^\alpha > \frac{\mu(A)}{2} > 0,$$

$i = 1, \dots, N$. Consequently,

$$\begin{aligned} U_i(x_i) &\leq \frac{1}{\mu(D_i)} \int\limits_{D_i} U_i(x) d\mu(x) \leq \frac{2}{\mu(A)} \sum_{j:j\neq i} \int\limits_{D_i} \frac{w(x, x_j)}{|x - x_j|^s} d\mu(x) \\ &\leq \frac{2\|w\|}{\mu(A)} \sum_{j:j\neq i} \int\limits_{A\setminus B(x_j, r_0)} \frac{1}{|x - x_j|^s} d\mu(x), \quad i = 1, \dots, N, \end{aligned}$$

where $\|w\| := \sup\{|w(x, y)| : x, y \in A\}$. Let $R := \operatorname{diam} A$. Then by (89) we have $\mu(A) \leq R^\alpha$. For every $y \in A$ and $r \in (0, R]$, using (89) we also get

$$\begin{aligned} T_s(y, r) &:= \int\limits_{A\setminus B(y,r)} \frac{1}{|x - y|^s} d\mu(x) = \int\limits_0^{r^{-s}} \mu\{x \in A : \frac{1}{|x - y|^s} > t\} dt \\ &= \frac{\mu(A)}{R^s} + \int\limits_{R^{-s}}^{r^{-s}} \mu\left[B\left(y, t^{-1/s}\right)\right] dt \leq R^{\alpha - s} + \int\limits_{R^{-s}}^{r^{-s}} t^{-\alpha/s} dt \\ &\leq \begin{cases} \frac{s}{(s-\alpha)} r^{\alpha - s}, & s > \alpha, \\ 1 + \alpha \ln \frac{R}{r}, & s = \alpha. \end{cases} \end{aligned}$$

Then for $i = 1, \ldots, N$ and $s > \alpha$ we have

$$U_i(x_i) \leq \frac{2\|w\|}{\mu(A)} \sum_{j \neq i} T_s(x_j, r_0) \leq \frac{2s(N-1)\|w\|}{(s-\alpha)\mu(A) r_0^{s-\alpha}} \leq C_1 \|w\| \left(\frac{N}{\mu(A)} \right)^{s/\alpha}, \tag{90}$$

where $C_1 > 0$ is a constant independent of A, w and N. Hence,

$$\mathcal{E}_s^w(A, N) = E_s^w(\omega_N^*) = \sum_{i=1}^{N} U_i(x_i) \leq \frac{M_{s,\alpha}\|w\|}{\mathcal{H}_\alpha^\infty(A)^{s/\alpha}} N^{1+s/\alpha},$$

where $M_{s,\alpha} > 0$ is a constant independent of A, w, and N. In particular, when $w \equiv 1$, we get

$$\mathcal{E}_s(A, N) \leq \frac{s 2^{s/\alpha} N^{1+s/\alpha}}{(s-\alpha)(c_{d',\alpha})^{s/\alpha} \mathcal{H}_\alpha^\infty(A)^{s/\alpha}}.$$

Since w is a CPD-weight function, there are $\eta, \rho > 0$ such that $w(x, y) > \eta$ whenever $|x - y| < \rho$. If $\delta(\omega_N^*) < \rho$, let i_s and j_s be such that $\delta(\omega_N^*) = |x_{i_s} - x_{j_s}|$. Then with some constant $C_2 > 0$ independent of N and the choice of ω_N^* we obtain from (90)

$$C_2 N^{s/\alpha} \geq U_{i_s}(x_{i_s}) \geq \frac{w(x_{i_s}, x_{j_s})}{|x_{i_s} - x_{j_s}|^s} \geq \frac{\eta}{|x_{i_s} - x_{j_s}|^s} = \frac{\eta}{\delta(\omega_N^*)^s}.$$

Hence,

$$\delta(\omega_N^*) \geq C_0 N^{-1/\alpha},$$

where $C_0 = C_0(A, w, \alpha, s) > 0$. Thus, in any case,

$$\delta(\omega_N^*) \geq \min\{\rho, C_0 N^{-1/\alpha}\} \geq C_s N^{-1/\alpha}, \quad N \geq 2,$$

for a sufficiently small constant $C_s > 0$ independent of N and ω_N^*. In particular, when $w \equiv 1$, we have

$$\delta(\omega_N^*) \geq \frac{c_{s,\alpha}}{(\mathcal{H}_\alpha^\infty(A) \cdot N)^{1/\alpha}},$$

where $c_{s,\alpha} > 0$ does not depend on A and N. This proves Theorem II.3.1. The case $s = \alpha$ is handled analogously, which completes the proofs of Theorem IV.5.1 and Corollary IV.5.1.

CHAPTER V

NEXT ORDER TERMS OF MINIMAL ENERGY ON SMOOTH CURVES.

Theorem A in the Introduction in particular, gives the main (dominant) term in the asymptotics of minimal s-energy on curves for $s \geq 1$.

Restricting our consideration to sufficiently smooth simple closed curves we shall determine the lower-order term in the asymptotic decomposition of the quantity $\mathcal{E}_s(\Gamma, N)$ as $N \to \infty$, for all $s \geq 1$, $s \neq s_0$, where this exceptional value s_0 satisfies $1 \leq s_0 < 3$. We also get a better estimate of the separation distance. We also find the order of the next term on non-closed smooth curves for $s \geq 2$.

V.1 Next order term and separation results for closed curves.

Notation and definitions. We say that a curve $\Gamma \subset \mathbb{R}^d$ is *simple*, if it has no self-intersections (except possibly coincidence of endpoints). We call Γ a C^n *curve*, if it has a non-zero tangent vector at every point and admits an n-times continuously differentiable parametrization.

For a rectifiable curve Γ, let $L := |\Gamma|$ be its length and λ_Γ be the normalized arclength measure supported on Γ.

Assume that $\Gamma \subset \mathbb{R}^d$ is a simple and closed C^3 curve. Let $\kappa(x)$ be the curvature of Γ at a given point x and $L(x, y)$ be the length of the smaller arc of Γ, connecting points x and y on it.

Define

$$g_s(x, y) := |x - y|^{-s} - L(x, y)^{-s}. \tag{91}$$

and

$$\Phi_s(\Gamma) := \int_\Gamma \int_\Gamma g_s(x, y) d\lambda_\Gamma(x) d\lambda_\Gamma(y). \tag{92}$$

It is not difficult to see that under the above assumptions on Γ, this integral is convergent iff $s < 3$. Denote also

$$\kappa(\Gamma) := \int_\Gamma \kappa^2(x) d\lambda_\Gamma$$

and let

$$\gamma := \lim_{N\to\infty}\left(\sum_{k=1}^{N} k^{-1} - \ln N\right).$$

be the Euler constant, and

$$\zeta(s) := \sum_{k=1}^{\infty} k^{-s}, \quad s > 1,$$

be the Riemann zeta-function.

Results for closed curves. According to Theorem A, on a Jordan curve Γ in $\mathbb{R}^d$ we have for $s > 1$

$$\mathcal{E}_s(\Gamma, N) \sim 2\zeta(s)\,|\Gamma|^{-s}\,N^{s+1}, \quad N \to \infty,$$

and

$$\mathcal{E}_1(\Gamma, N) \sim 2\,|\Gamma|^{-1}\,N^2 \ln N, \quad N \to \infty.$$

We obtain the following result.

Theorem V.1.1. *Let $\Gamma \subset \mathbb{R}^d$, $d \in \mathbb{N}$, be a simple and closed C^3 curve. Then, if $s > 3$, we have*

$$\lim_{N\to\infty} \frac{\mathcal{E}_s(\Gamma, N) - 2\zeta(s)L^{-s}N^{s+1}}{N^{s-1}} = \frac{s\zeta(s-2)}{12L^{s-2}}\kappa(\Gamma), \tag{93}$$

and for $s = 3$ there holds

$$\lim_{N\to\infty} \frac{\mathcal{E}_3(\Gamma, N) - 2\zeta(3)L^{-3}N^4}{N^2 \ln N} = \frac{\kappa(\Gamma)}{4L}. \tag{94}$$

If $1 < s < 3$, then

$$\lim_{N\to\infty} \frac{\mathcal{E}_s(\Gamma, N) - 2\zeta(s)L^{-s}N^{s+1}}{N^2} = \Phi_s(\Gamma) - \frac{2^s}{(s-1)L^s} \tag{95}$$

and when $s = 1$, there holds

$$\lim_{N\to\infty} \frac{\mathcal{E}_s(\Gamma, N) - 2L^{-1}N^2 \ln N}{N^2} = \Phi_1(\Gamma) + 2L^{-1}(\gamma - \ln 2). \tag{96}$$

Remark. There is a unique $s_0 \in (1, 3)$ for which the right-hand side of (95) is zero. The value (95) is negative for $1 < s < s_0$ and tends to $-\infty$ as $s \to 1$, and is positive for $s_0 < s < 3$, and goes to ∞ as $s \to 3$. For the value $s = s_0$ Theorem V.1.1 tells only that the next order term of the minimal s-energy is $o(N^2)$.

Choose an orientation on Γ and denote by $l(x, y)$ the length of the arc from point x to point y

on Γ in the direction of the orientation of Γ. For an N-point collection $\omega_N = \{x_1, \ldots, x_N\} \subset \Gamma$ we as usually denote

$$\delta(\omega_N) := \min_{1 \le i \ne j \le N} |x_i - x_j|$$

and let

$$\Delta(\omega_N) := \max_{i=1,\ldots,N} l(x_i, x_{i+1}),$$

where $x_{N+1} = x_1$. We will always assume that the index i for $x_i \in \omega_N$ grows in the direction of the orientation of the curve.

Known results provide only the order of the separation radius on different classes of sets. In the theorem below, we get its asymptotic behavior on smooth closed curves.

Theorem V.1.2. *Let $s > 2$ and $\Gamma \subset \mathbb{R}^d$, $d \in \mathbb{N}$, be a simple and closed C^3 curve. If $\{\omega_N^*\}_{N=2}^{\infty}$ is a sequence of s-energy minimizing collections on Γ, $\#\omega_N^* = N$, $N \ge 2$, then*

$$\lim_{N\to\infty} \delta(\omega_N^*) \cdot N = \lim_{N\to\infty} \Delta(\omega_N^*) \cdot N = L. \tag{97}$$

This theorem implies that for $s > 2$ the maximal and the minimal arclength between neighboring points of optimal configurations asymptotically equals L/N, $N \to \infty$.

V.2 Remarks for non-closed arcs.

For smooth non-closed curves the second term is negative and has order N^s for $s > 2$.

Proposition V.2.1. *Let $\Gamma \subset \mathbb{R}^d$, $d \in \mathbb{N}$, be a simple non-closed rectifiable C^2 curve. If $s > 2$, there exist two negative constants C_1, C_2 such that, for sufficiently large N,*

$$C_1 N^s < \mathcal{E}_s(\Gamma, N) - 2\zeta(s)L^{-s}N^{s+1} < C_2 N^s. \tag{98}$$

If $s = 2$, one can find negative constants C_1, C_2 so that

$$C_1 N^2 \ln N < \mathcal{E}_2(\Gamma, N) - 2\zeta(2)L^{-2}N^3 < C_2 N^2 \ln N. \tag{99}$$

Conclusions. The next order term of the minimal s-energy on smooth curves reflects whether the curve is closed or not. On closed curves for $s > 3$ the next term is positive with the order N^{s-1}, and has order $N^2 \ln N$ for $s = 3$ and N^2 for $1 \le s < 3$. At the same time, on non-closed curves for $s > 2$, it is negative and has order N^s, or $N^2 \ln N$ for $s = 2$, $N \to \infty$. Hence, making a smooth simple curve into a closed one increases its s-energy for $s \ge 2$.

Similar to the break of the order of the main term of s-energy on curves which happens at $s = 1$ (see Theorem A), the next order term for closed curves changes its order from N^2 to N^{s-1} when $s = 3$. On non-closed curves such a transition happens at $s = 2$.

V.3 Auxiliary definitions and results.

Let Γ be a simple closed curve in $\mathbb{R}^d$. For an N-point collection $\omega_N = \{x_1, \dots, x_N\} \subset \Gamma$ we denote

$$F_s(\omega_N) := \sum_{1 \le i \ne j \le N} \frac{1}{L(x_i, x_j)^s}$$

and

$$G_s(\omega_N) := E_s(\omega_N) - F_s(\omega_N) = \sum_{1 \le i \ne j \le N} g_s(x_i, x_j),$$

where $g_s(x, y)$ is defined in (91). Denote by $\overline{\omega}_N = \{\overline{x}_1, \dots, \overline{x}_N\}$ a collection of equally spaced points on Γ, i.e. a collection such that $L(\overline{x}_i, \overline{x}_{i+1}) = L/N$, $i = 1, \dots, N-1$. This collection will be optimal in the following sense.

Lemma V.3.1. *Let $\Gamma \subset \mathbb{R}^d$ be a simple closed curve and $s > 0$. Then,*

$$F_s(\omega_N) \ge F_s(\overline{\omega}_N) \tag{100}$$

for every N-point configuration $\omega_N = \{x_1, \dots, x_N\} \subset \Gamma$.

Proof. Denote $x_{i+N} := x_i$ and $x_{i-N} := x_i$, $i = 1, \dots, N$. Then,

$$F_s(\omega_N) = \sum_{1 \le i \ne j \le N} L(x_i, x_j)^{-s} = \sum_{\substack{j=-\lfloor (N-1)/2 \rfloor \\ j \ne 0}}^{\lfloor N/2 \rfloor} \sum_{k=1}^{N} L(x_k, x_{k+j})^{-s} \ge$$

$$\ge N \sum_{\substack{j=-\lfloor (N-1)/2 \rfloor \\ j \ne 0}}^{\lfloor N/2 \rfloor} \left(\frac{1}{N} \sum_{k=1}^{N} L(x_k, x_{k+j}) \right)^{-s} \ge N \sum_{j=1}^{\lfloor N/2 \rfloor} \left(\frac{1}{N} \sum_{k=1}^{N} \sum_{i=1}^{j} l(x_{k+i-1}, x_{k+i}) \right)^{-s} +$$

$$+N\sum_{j=1}^{\lfloor (N-1)/2\rfloor}\left(\frac{1}{N}\sum_{k=1}^{N}\sum_{i=1}^{j}l(x_{k-i},x_{k-i+1})\right)^{-s} = N^{s+1}\sum_{j=1}^{\lfloor N/2\rfloor}\left(\sum_{i=1}^{j}\sum_{k=1}^{N}l(x_{k+i-1},x_{k+i})\right)^{-s} +$$

$$+N^{s+1}\sum_{j=1}^{\lfloor (N-1)/2\rfloor}\left(\sum_{i=1}^{j}\sum_{k=1}^{N}l(x_{k-i},x_{k-i+1})\right)^{-s} = N\sum_{\substack{j=-\lfloor (N-1)/2\rfloor\\ j\neq 0}}^{\lfloor N/2\rfloor}\left(\frac{|j|\,L}{N}\right)^{-s} = F_s(\overline{\omega}_N).$$

Lemma V.3.1 is proved.

The following statement shows by how much the distance between two points on Γ and the length of the shorter arc between them differ as the points get close to each other. For a function $F:\Gamma\times\Gamma\to\mathbb{R}$ we write $F(x,y)\underset{\longrightarrow}{\longrightarrow}0$ as $L(x,y)\to 0$, if for every $\epsilon>0$ there is a number $\delta>0$ such that $|F(x,y)|<\epsilon$, whenever $x,y\in\Gamma$ and $0<L(x,y)<\delta$.

Lemma V.3.2. *Let $s>0$ and $\Gamma\subset\mathbb{R}^d$ be a simple closed C^3 curve. Then, for any points $x,y\in\Gamma$,*

$$g_s(x,y) = \frac{s\cdot\kappa(y)^2}{24}L(x,y)^{2-s} + \alpha(x,y)L(x,y)^{2-s}, \tag{101}$$

where $\alpha(x,y)\underset{\longrightarrow}{\longrightarrow}0$ as $L(x,y)\to 0$.

In particular, for every $s>0$ there are constants $M_s>0$ and $\delta_s\in(0,L/2)$ such that

$$g_s(x,y)\le M_s\cdot L(x,y)^{2-s},\qquad x,y\in\Gamma,\ 0<L(x,y)<\delta_s. \tag{102}$$

Our argument does not work if Γ is only two times differentiable, since under such an assumption the Taylor formula only guarantees that $g_s(x,y)=o(L(x,y)^{1-s})$.

Proof of Lemma V.3.2. Given an interval I and a function $f:I\times I\to\mathbb{R}^d$, we write $f(t_1,t_2)\underset{\longrightarrow}{\longrightarrow}0$, as $|t_1-t_2|\to 0$, if for every $\epsilon>0$ there is $\delta>0$ such that $|f(t_1,t_2)|<\epsilon$ whenever $|t_1-t_2|<\delta$.

Let $\varphi:\mathbb{R}\to\mathbb{R}^d$ be a three times continuously differentiable L-periodic arclength parametrization for Γ. Then,

$$\varphi(t_1)-\varphi(t_2) = (t_1-t_2)\varphi'(t_2) + \frac{(t_1-t_2)^2}{2}\varphi''(t_2)$$

$$+\frac{(t_1-t_2)^3}{6}\varphi'''(t_2) + (t_1-t_2)^3\alpha_3^{\varphi}(t_1,t_2),$$

where in view of uniform continuity of φ''' we have $\alpha_3^{\varphi}(t_1,t_2)\underset{\longrightarrow}{\longrightarrow}0$ as $|t_1-t_2|\to 0$. Since $|\varphi'|=1$, we get $\frac{\mathrm{d}}{\mathrm{d}t}|\varphi'|^2 = 2\langle\varphi',\varphi''\rangle = 0$ and $\frac{\mathrm{d}}{\mathrm{d}t}\langle\varphi',\varphi''\rangle = |\varphi''|^2+\langle\varphi',\varphi'''\rangle = 0$, that is, $|\varphi''|^2 = -\langle\varphi',\varphi'''\rangle$.

Hence,

$$|\varphi(t_1)-\varphi(t_2)|^2=(t_1-t_2)^2-\frac{(t_1-t_2)^4}{12}\left|\varphi''(t_2)\right|^2+(t_1-t_2)^4\beta(t_1,t_2),$$

where $\beta(t_1,t_2)\underset{\longrightarrow}{\longrightarrow}0$ as $|t_1-t_2|\to 0$. Then,

$$|\varphi(t_1)-\varphi(t_2)|^{-s}=|t_1-t_2|^{-s}\left(1-\frac{(t_1-t_2)^2}{12}\left|\varphi''(t_2)\right|^2+(t_1-t_2)^2\beta(t_1,t_2)\right)^{-s/2}=$$

$$=|t_1-t_2|^{-s}\left[1+\frac{s(t_1-t_2)^2}{24}\left|\varphi''(t_2)\right|^2+(t_1-t_2)^2\gamma(t_1,t_2)\right], \tag{103}$$

where $\gamma(t_1,t_2)\underset{\longrightarrow}{\longrightarrow}0$ as $|t_1-t_2|\to 0$, and (101) follows.

As in previous chapters, let δ_x be the atomic probability measure in $\mathbb{R}^d$ centered at point x and $\omega_N:=\{x_{1,N},\ldots,x_{N,N}\}\subset\Gamma$, $N\in\mathbb{N}$, be a sequence of N-point sets. Denote by

$$\nu(\omega_N):=\frac{1}{N}\sum_{k=1}^{N}\delta_{x_{k,N}}$$

the normalized counting measure supported at points of ω_N. We write

$$\nu(\omega_N)\xrightarrow{\ *\ }\lambda_\Gamma,\quad N\to\infty, \tag{104}$$

if for every continuous function $f:\Gamma\to\mathbb{R}$

$$\frac{1}{N}\sum_{k=1}^{N}f(x_{k,N})\to\int_\Gamma f(x)d\lambda_\Gamma,\quad N\to\infty.$$

According to Theorem A the following statement is true.

Lemma V.3.3. *Let $s\geq 1$ and $\Gamma=\cup_{j=1}^{m}\Gamma_j$, where each Γ_j is a rectifiable Jordan arc, and $|\Gamma|=\sum_{j=1}^{m}|\Gamma_j|$. If $\{\omega_N^*\}_{N=2}^{\infty}$ is a sequence of s-energy minimizing configurations on Γ ($\#\omega_N^*=N$, $N\geq 2$), then*

$$\nu(\omega_N^*)\xrightarrow{\ *\ }\lambda_\Gamma,\quad N\to\infty.$$

V.4 Proofs for closed curves.

In this section we prove Theorems V.1.1 and V.1.2. Recall, that $\overline{\omega}_N$ denotes a collection of N equally spaced points on Γ and $\omega_N^*=\{x_1^*,\ldots,x_N^*\}$ is an s-energy minimizing N-point collection on Γ. To prove Theorem V.1.1 we look for the main term of the difference $\mathcal{E}_s(\Gamma, N) - F_s(\overline{\omega}_N)$. For $s \geq 1$ we have

$$\mathcal{E}_s(\Gamma, N) - F_s(\overline{\omega}_N) \leq E_s(\overline{\omega}_N) - F_s(\overline{\omega}_N) = G_s(\overline{\omega}_N),$$

and by Lemma V.3.1

$$\mathcal{E}_s(\Gamma, N) - F_s(\overline{\omega}_N) = E_s(\omega_N^*) - F_s(\overline{\omega}_N) \geq E_s(\omega_N^*) - F_s(\omega_N^*) = G_s(\omega_N^*).$$

Thus,

$$G_s(\omega_N^*) \leq \mathcal{E}_s(\Gamma, N) - F_s(\overline{\omega}_N) \leq G_s(\overline{\omega}_N). \tag{105}$$

Case $1 \leq s < 3$**.** We shall show that

$$\lim_{N\to\infty} \frac{G_s(\omega_N^*)}{N^2} = \lim_{N\to\infty} \frac{G_s(\overline{\omega}_N)}{N^2} = \Phi_s(\Gamma). \tag{106}$$

Indeed, choose arbitrary $\epsilon \in (0, \delta_s)$, where δ_s is from (102). Let

$$U_\epsilon = \{(x, y) \in \Gamma \times \Gamma : L(x, y) \geq \epsilon\}$$

and

$$V_\epsilon = \{(x, y) \in \Gamma \times \Gamma : L(x, y) \leq \epsilon\}.$$

By Urysohn's lemma there is a continuous function $f_\epsilon : \mathbb{R}^{2d} \to [0, 1]$ such that $f_\epsilon(x, y) = 1$, $(x, y) \in U_\epsilon$, and $f_\epsilon(x, y) = 0$, $(x, y) \in V_{\epsilon/2}$. Then, since $\nu(\omega_N^*) \xrightarrow{\ *\ } \lambda_\Gamma$, $N \to \infty$, we obtain

$$\liminf_{N\to\infty} \frac{G_s(\omega_N^*)}{N^2} = \liminf_{N\to\infty} \frac{1}{N^2} \sum_{1\leq i\neq j\leq N} g_s(x_i^*, x_j^*)$$

$$\geq \lim_{N\to\infty} \frac{1}{N^2} \sum_{1\leq i,j\leq N} g_s(x_i^*, x_j^*) f_\epsilon(x_i^*, x_j^*)$$

$$= \int_\Gamma \int_\Gamma g_s(x, y) f_\epsilon(x, y) d\lambda_\Gamma d\lambda_\Gamma \geq \int_{U_\epsilon} g_s(x, y) \quad d\lambda_\Gamma \times \lambda_\Gamma.$$

Hence, in view of arbitrariness of ϵ, we get

$$\liminf_{N\to\infty} \frac{G_s(\omega_N^*)}{N^2} \geq \Phi_s(\Gamma). \tag{107}$$

On the other hand,

$$G_s(\overline{\omega}_N) = \sum_{0<L(\overline{x}_i,\overline{x}_j)<\epsilon} g_s(\overline{x}_i,\overline{x}_j) + \sum_{L(\overline{x}_i,\overline{x}_j)\geq\epsilon} g_s(\overline{x}_i,\overline{x}_j). \tag{108}$$

Since $\nu(\overline{\omega}_N) \xrightarrow{*} \lambda_\Gamma$, $N\to\infty$,

$$\limsup_{N\to\infty} \frac{1}{N^2} \sum_{L(\overline{x}_i,\overline{x}_j)\geq\epsilon} g_s(\overline{x}_i,\overline{x}_j) \leq \lim_{N\to\infty} \frac{1}{N^2} \sum_{1\leq i,j\leq N} g_s(\overline{x}_i,\overline{x}_j) f_\epsilon(\overline{x}_i,\overline{x}_j) =$$

$$= \int_\Gamma \int_\Gamma g_s(x,y) f_\epsilon(x,y) d\lambda_\Gamma d\lambda_\Gamma \leq \Phi_s(\Gamma).$$

Below, we will write $o(\cdot)$ and $O(\cdot)$ with respect to $N\to\infty$. Using (102) and the equality

$$\sum_{k=1}^N k^s = \frac{N^{s+1}(1+o(1))}{s+1}, \quad s>-1, \tag{109}$$

we obtain

$$\sum_{0<L(\overline{x}_i,\overline{x}_j)<\epsilon} g_s(\overline{x}_i,\overline{x}_j) \leq M_s \sum_{0<L(\overline{x}_i,\overline{x}_j)<\epsilon} L(\overline{x}_i,\overline{x}_j)^{2-s}$$

$$\leq 2M_s L^{2-s} N^{s-1} \sum_{k=1}^{\lfloor \epsilon N/L \rfloor} \frac{1}{k^{s-2}} = \frac{2M_s \epsilon^{3-s} N^2 (1+o(1))}{(3-s)L}. \tag{110}$$

Thus,

$$\limsup_{N\to\infty} \frac{G_s(\overline{\omega}_N)}{N^2} \leq \frac{2M_s\epsilon^{3-s}}{(3-s)L} + \Phi_s(\Gamma).$$

Letting $\epsilon\to 0$, we have

$$\limsup_{N\to\infty} \frac{G_s(\overline{\omega}_N)}{N^2} \leq \Phi_s(\Gamma), \tag{111}$$

which together with (107) and (105) yields (106). From (105) and (106) it follows that

$$\lim_{N\to\infty} \frac{\mathcal{E}_s(\Gamma,N) - F_s(\overline{\omega}_N)}{N^2} = \Phi_s(\Gamma). \tag{112}$$

Using the representation

$$\sum_{k=1}^N \frac{1}{k^s} = \zeta(s) - \frac{1}{s-1}\cdot\frac{1}{N^{s-1}} + o\left(\frac{1}{N^{s-1}}\right), \quad s>1, \tag{113}$$

one can show that

$$F_s(\overline{\omega}_N) = 2L^{-s}N^{s+1}\sum_{k=1}^{\lfloor N/2\rfloor} k^{-s} + O(N) =$$

$$= 2L^{-s}N^{s+1}\zeta(s) - \frac{2^s N^2}{(s-1)L^s} + o(N^2), \quad s>1. \tag{114}$$

Taking into account the equality

$$\sum_{k=1}^{N}\frac{1}{k} = \ln N + \gamma + o(1), \tag{115}$$

where γ is the Euler constant, one can also derive that

$$F_1(\overline{\omega}_N) = 2L^{-1}N^2\ln N + 2L^{-1}(\gamma - \ln 2)N^2 + o(N^2). \tag{116}$$

From (112) with $1 < s < 3$ and the representation (114) we get (95). Taking into account (112) with $s = 1$ and (116) we deduce (96).

Case $s \geq 3$. Upper estimate. Choose again any $\epsilon > 0$ and let $\delta \in (0, \epsilon)$ be chosen for this ϵ from the definition of $\alpha(x, y) \overset{\longrightarrow}{\longrightarrow} 0$, $L(x, y) \to 0$, in Lemma V.3.2. Then,

$$G_s(\overline{\omega}_N) = \sum_{0<L(\overline{x}_i,\overline{x}_j)<\delta} g_s(\overline{x}_i,\overline{x}_j) + \sum_{L(\overline{x}_i,\overline{x}_j)\geq\delta} g_s(\overline{x}_i,\overline{x}_j).$$

The function $g_s(x, y)$ is bounded as a continuous function on a compact set U_δ. Thus,

$$\sum_{L(\overline{x}_i,\overline{x}_j)\geq\delta} g_s(\overline{x}_i,\overline{x}_j) = O(N^2).$$

For convenience, set $\zeta(1) := 1$ and

$$\rho_s(N) := \begin{cases} N^{s-1}, & s>3, \\ N^2\ln N, & s=3. \end{cases}$$

From Lemmas V.3.2 and V.3.3 we have

$$\sum_{0<L(\overline{x}_i,\overline{x}_j)<\delta} g_s(\overline{x}_i,\overline{x}_j) \leq \sum_{0<L(\overline{x}_i,\overline{x}_j)<\delta} \left(\epsilon + \frac{s}{24}\kappa^2(\overline{x}_j)\right) L(\overline{x}_i,\overline{x}_j)^{2-s}$$

$$\leq 2\sum_{j=1}^{N}\left(\epsilon+\frac{s}{24}\kappa^2(\overline{x}_j)\right)\sum_{i=1}^{\lfloor \delta N/L\rfloor}\left(\frac{iL}{N}\right)^{2-s}$$

$$\leq \frac{2\zeta(s-2)}{L^{s-2}}\int_\Gamma\left(\epsilon+\frac{s\kappa^2(x)}{24}\right)d\lambda_\Gamma\cdot\rho_s(N)(1+o(1)).$$

Letting $N\to\infty$ and then letting $\epsilon\to 0$, we finally have

$$\limsup_{N\to\infty}\frac{G_s(\overline{\omega}_N)}{\rho_s(N)}\leq\frac{s\zeta(s-2)\kappa(\Gamma)}{12L^{s-2}}. \tag{117}$$

Next, we use these inequalities to obtain Theorem V.1.2, which in turn, is used to prove the lower estimate for $s\geq 3$.

Proof of Theorem V.1.2. Let $s>2$ and $\{\omega_N^*\}_{N=2}^\infty$ be a sequence of s-energy minimizing configurations on Γ, where we redenote $\omega_N^*=\{x_{1,N},\ldots,x_{N,N}\}$, $N\in\mathbb{N}$. Set $x_{i-N,N}:=x_{i,N}$, $x_{i+N,N}:=x_{i,N}$, $i=1,\ldots,N$, and let $\{(x_{j_N,N},x_{j_N+1,N})\}_{N=2}^\infty$ be any sequence of pairs of points from ω_N^* located next to each other on Γ. Denote

$$C_N:=l(x_{j_N,N},x_{j_N+1,N})\cdot N.$$

We shall show that $\lim_{N\to\infty}C_N=L$.

Let $\mathcal{N}\subset\mathbb{N}$ be any infinite set such that the limit $a:=\lim_{\mathcal{N}\ni N\to\infty}C_N$ is a finite number or infinity. For every $N\in\mathcal{N}$, using convexity of the function $y(t)=t^{-s}$, we have

$$\mathcal{E}_s(\Gamma,N)=E_s(\omega_N^*)\geq\sum_{k=2}^{\lfloor N/2\rfloor}\sum_{i=1}^{N}l(x_{i,N},x_{i+k,N})^{-s}$$

$$+\sum_{k=1}^{\lfloor (N-1)/2\rfloor}\sum_{i=1}^{N}l(x_{i-k,N},x_{i,N})^{-s}+l(x_{j_N,N},x_{j_N+1,N})^{-s}+\sum_{\substack{i=1\\ i\neq j_N}}^{N}l(x_{i,N},x_{i+1,N})^{-s}$$

$$\geq N^{s+1}\sum_{k=2}^{\lfloor N/2\rfloor}\left(\sum_{i=1}^{N}l(x_{i,N},x_{i+k,N})\right)^{-s}+N^{s+1}\sum_{k=1}^{\lfloor (N-1)/2\rfloor}\left(\sum_{i=1}^{N}l(x_{i-k,N},x_{i,N})\right)^{-s}+$$

$$+N^sC_N^{-s}+(N-1)^{s+1}\left(\sum_{\substack{i=1\\ i\neq j_N}}^{N}l(x_{i,N},x_{i+1,N})\right)^{-s}\geq N^{s+1}\sum_{\substack{k=-\lfloor (N-1)/2\rfloor\\ k\neq 0,1}}^{\lfloor N/2\rfloor}(|k|\,L)^{-s}$$

$$+N^sC_N^{-s}+(N-1)^{s+1}\left(L-\frac{C_N}{N}\right)^{-s}=F_s(\overline{\omega}_N)-L^{-s}N^{s+1}+N^sC_N^{-s}$$

$$+L^{-s}N^{s+1}\left(1-\frac{1}{N}\right)^{s+1}\left(1-\frac{C_N}{LN}\right)^{-s}. \qquad (118)$$

It is not difficult to see, that for $b \geq 1$ and $x \geq -1/b$ or for $b \leq 0$ and $-1 < x < 0$ we have $(1+x)^b \geq 1 + bx \geq 0$. We also have $l(x_{j_N,N}, x_{j_N+1,N}) \to 0$, $N \to \infty$. Hence, we can write for large $N \in \mathcal{N}$

$$\mathcal{E}_s(\Gamma, N) \geq F_s(\overline{\omega}_N) - L^{-s}N^{s+1} + N^s C_N^{-s} + L^{-s}N^{s+1}\left(1-\frac{s+1}{N}\right)\left(1+\frac{sC_N}{LN}\right) \geq$$

$$\geq F_s(\overline{\omega}_N) + N^s C_N^{-s} + \frac{sC_N N^s}{L^{s+1}} - \frac{(s+1)N^s}{L^s} + o(N^s), \quad N \to \infty, \quad N \in \mathcal{N}. \qquad (119)$$

By (105) and (117) for $s \geq 3$ or (112) for $2 < s < 3$, we have

$$\tau_s(\Gamma) := \limsup_{N\to\infty} \frac{\mathcal{E}_s(\Gamma, N) - F_s(\overline{\omega}_N)}{N^s} \leq \limsup_{N\to\infty} \frac{G_s(\overline{\omega}_N)}{N^s} = 0, \quad s > 2. \qquad (120)$$

On the other hand, from the (119), we have

$$\tau_s(\Gamma) \geq a^{-s} + \frac{sa}{L^{s+1}} - \frac{s+1}{L^s} := f(a).$$

Function $f(a)$ has a unique global minimum $f(L) = 0$ on $[0, \infty]$. Then, in view of (120) we can only have $a = L$. In view of the arbitrariness of the subsequence $\{C_N\}_{N\in\mathcal{N}}$ we have

$$\lim_{N\to\infty} l(x_{j_N,N}, x_{j_N+1,N}) \cdot N = L. \qquad (121)$$

Taking sequence $\{j_N\}$ so that $l(x_{j_N,N}, x_{j_N+1,N}) = \Delta(\omega_N^*)$, $N \in \mathbb{N}$, we get that the second equality in (97).

It is not difficult to see that uniformly over $x, y \in \Gamma$

$$\lim_{|x-y|\to 0} \frac{|x-y|}{L(x,y)} = 1. \qquad (122)$$

Let sequences of indexes $\{i_N\}_{N=2}^{\infty}$ and $\{p_N\}_{N=2}^{\infty}$ be such that $1 \leq i_N, p_N \leq N$ be such that $\delta(\omega_N^*) = |x_{i_N,N} - x_{p_N,N}|$, $N \in \mathbb{N}$. Choose $j_N = i_N$, if $l(x_{i_N,N}, x_{p_N,N}) = L(x_{i_N,N}, x_{p_N,N})$, and $j_N = p_N$, if $l(x_{p_N,N}, x_{i_N,N}) = L(x_{i_N,N}, x_{p_N,N})$, $N \in \mathbb{N}$. Since $\delta(\omega_N^*) \leq \Delta(\omega_N^*)$ we also have

$|x_{i_N,N} - x_{p_N,N}| \to 0$. Then, as $N \to \infty$

$$1 \leftarrow \frac{|x_{i_N,N} - x_{p_N,N}|}{L(x_{i_N,N}, x_{p_N,N})} \le \frac{\delta(\omega_N^*)}{l(x_{j_N,N}, x_{j_N+1,N})} \le \frac{|x_{j_N,N} - x_{j_N+1,N}|}{l(x_{j_N,N}, x_{j_N+1,N})} \le 1.$$

Hence,

$$\lim_{N\to\infty} \frac{\delta(\omega_N^*)}{l(x_{j_N,N}, x_{j_N+1,N})} = 1.$$

Taking into account (121), we get the first equality in (97). Theorem V.1.2 is proved.

Lower estimate for $s \ge 3$. Let $\{\omega_N^*\}_{N=2}^{\infty}$ be a sequence of s-energy minimizing configurations on Γ ($\omega_N^* = \{x_{1,N}, \dots, x_{N,N}\}$, $N \in \mathbb{N}$).

Choose any $\epsilon > 0$ and by this ϵ take $0 < h < \min\{\epsilon, L/4\}$ from the definition of the fact that $\alpha(x,y) \underset{\longrightarrow}{\longrightarrow} 0$, $L(x,y) \to 0$ in Lemma V.3.2. Denote $r(N) := \Delta(\omega_N^*) \cdot N - L$. By Theorem V.1.2, we have $r(N) \to 0$, $N \to \infty$. Then, for N sufficiently large and $k \le m_N := \lfloor hN/(2L) \rfloor$ we have

$$L(x_{i,N}, x_{i+k,N}) \le k\Delta(\omega_N^*) \le h(L + r(N))/2L < h.$$

Hence, by Lemma V.3.2,

$$G_s(\omega_N^*) \ge 2 \sum_{k=1}^{m_N} \sum_{i=1}^{N} g_s(x_{i,N}, x_{i+k,N})$$

$$\ge \sum_{k=1}^{m_N} \sum_{i=1}^{N} \left(\frac{s}{12}\kappa^2(x_{i,N}) - 2\epsilon\right) L(x_{i,N}, x_{i+k,N})^{2-s}$$

$$\ge \frac{N^{s-2}}{(L + r(N))^{s-2}} \sum_{i=1}^{N} \left(\frac{s}{12}\kappa^2(x_{i,N}) - 2\epsilon\right) \sum_{k=1}^{m_N} k^{2-s}.$$

Then, using Lemma V.3.3, we have for $s \ge 3$ (recall that $\zeta(1) = 1$)

$$\liminf_{N\to\infty} \frac{G_s(\omega_N^*)}{\rho_s(N)} \ge \frac{\zeta(s-2)}{L^{s-2}} \lim_{N\to\infty} \frac{1}{N} \sum_{i=1}^{N} \left(\frac{s}{12}\kappa^2(x_{i,N}) - 2\epsilon\right)$$

$$= \frac{s\zeta(s-2)(\kappa(\Gamma) - 24\epsilon/s)}{12L^{s-2}}. \tag{123}$$

Letting $\epsilon \to 0$ in (123) and combining it with (117) and (105), we have

$$\lim_{N\to\infty} \frac{\mathcal{E}_s(\Gamma, N) - F_s(\overline{\omega}_N)}{\rho_s(N)} = \frac{s\zeta(s-2)\kappa(\Gamma)}{12L^{s-2}}.$$

Using representation (114) we get (93) and (94).

V.5 Proofs for non-closed curves.

In this section we prove Proposition V.2.1. Under its assumptions, curve Γ allows a C^2 arclength parametrization $\varphi : [0, L] \to \mathbb{R}^d$ with $L := |\Gamma|$ being the length of Γ.

1. Auxiliary statements. Let $s \geq 2$. Note, that $|\varphi'| = 1$ and $\langle \varphi', \varphi'' \rangle = 0$. By the Taylor formula

$$\varphi(t_1) - \varphi(t_2) = (t_1 - t_2)\varphi'(t_2) + \frac{(t_1 - t_2)^2}{2}\varphi''(t_2)$$

$$+(t_1 - t_2)^2 \alpha_2^{\varphi}(t_1, t_2),$$

where in view of uniform continuity of φ'' we have $\alpha_2^{\varphi}(t_1, t_2) \rightrightarrows 0$ as $|t_1 - t_2| \to 0$. Then, taking into account that $|\varphi'|$ and $|\varphi''|$ are bounded, we have

$$|\varphi(t_1) - \varphi(t_2)|^2 = (t_1 - t_2)^2 \left|\varphi'(t_2)\right|^2 + (t_1 - t_2)^3 \langle \varphi'(t_2), \varphi''(t_2) \rangle +$$

$$+(t_1 - t_2)^3 \beta(t_1, t_2) = (t_1 - t_2)^2 \left(1 + (t_1 - t_2)\beta(t_1, t_2)\right),$$

where $\beta(t_1, t_2) \rightrightarrows 0$, $|t_1 - t_2| \to 0$. For $t_1 \neq t_2$ we have

$$|\varphi(t_1) - \varphi(t_2)|^{-s} = |t_1 - t_2|^{-s} \left(1 + (t_1 - t_2)\beta(t_1, t_2)\right)^{-s/2} =$$

$$= |t_1 - t_2|^{-s} \left(1 + |t_1 - t_2| \gamma(t_1, t_2)\right), \tag{124}$$

where $\gamma(t_1, t_2) \rightrightarrows 0$, $|t_1 - t_2| \to 0$.

For a non-closed curve $l(x, y)$ simply denotes the length of the part of Γ between points x and y on it. By (122), there exists a number $w_0 > 0$ such that $l(x, y) \leq 2|x - y|$ whenever $x, y \in \Gamma$, $0 < |x - y| < w_0$.

Take arbitrary $\epsilon \in (0, \frac{1}{2})$ and choose $0 < \delta_\epsilon < \min\{\frac{1}{2}, w_0\}$ from the definition of the fact, that $\gamma(t_1, t_2) \rightrightarrows 0$, $|t_1 - t_2| \to 0$ in (124). Let $Z_N^* = \{z_0^*, z_1^*, \ldots, z_N^*\}$ be such that $z_i^* = \varphi(\frac{iL}{N})$, $i = 0, \ldots, N$. Then

$$\mathcal{E}_s(\Gamma, N+1) \leq E_s(Z_N^*) = \sum_{0 \leq i \neq j \leq N} \left|z_i^* - z_j^*\right|^{-s} =$$

$$= \sum_{\substack{0\le i\neq j\le N \\ \left|z_i^*-z_j^*\right|<\delta_\epsilon/2}} \left|z_i^*-z_j^*\right|^{-s} + \sum_{\substack{0\le i\neq j\le N \\ \left|z_i^*-z_j^*\right|\ge\delta_\epsilon/2}} \left|z_i^*-z_j^*\right|^{-s} \le$$

$$\le \sum_{\substack{0\le i\neq j\le N \\ \left|z_i^*-z_j^*\right|<\delta_\epsilon/2}} \left|\varphi\left(iL/N\right)-\varphi\left(jL/N\right)\right|^{-s} + (2/\delta_\epsilon)^s N(N+1).$$

Since $\left|z_i^*-z_j^*\right| < \delta_\epsilon/2 < w_0$, we have $|i-j|\,L/N < 2\left|z_i^*-z_j^*\right| < \delta_\epsilon$. Then, using (124), we obtain

$$\mathcal{E}_s(\Gamma, N+1) \le \sum_{\substack{0\le i\neq j\le N \\ \left|z_i^*-z_j^*\right|<\delta_\epsilon/2}} \left[(|i-j|\,L/N)^{-s} + \epsilon\,(|i-j|\,L/N)^{-s+1}\right] + O(N^2).$$

Denote

$$D_a(N) := \sum_{0\le i\neq j\le N} |i-j|^{-a}, \quad N\in\mathbb{N}, \quad a\ge 1.$$

Then

$$\mathcal{E}_s(\Gamma, N+1) \le (N/L)^s\, D_s(N) + \epsilon\,(N/L)^{s-1}\, D_{s-1}(N) + O(N^2), \quad N\to\infty. \tag{125}$$

Using (113) and (115), it is not difficult to verify the following statement.

Lemma V.5.1. *As $N\to\infty$, the quantity $D_a(N)$ has the following representation*

$$D_a(N) = 2\zeta(a)N + 2(\zeta(a)-\zeta(a-1)) + O(N^{2-a}), \quad a>2,$$

$$D_2(N) = \frac{\pi^2}{3}N - 2\ln N + O(1),$$

$$D_a(N) = 2\zeta(a)N + O(N^{2-a}), \quad 1<a<2,$$

$$D_1(N) = 2N\ln N + O(N).$$

Using this lemma, for $s>2$ we have

$$\mathcal{E}_s(\Gamma, N+1) \le 2\zeta(s)L^{-s}N^{s+1} + 2(\zeta(s)-\zeta(s-1))L^{-s}N^s +$$

$$+2\epsilon\zeta(s-1)L^{s-1}N^s + o(N^s), \quad N\to\infty.$$

Since $\epsilon>0$ can be taken arbitrarily small, we get

$$\limsup_{N\to\infty} \frac{\mathcal{E}_s(\Gamma, N+1) - 2\zeta(s)L^{-s}N^{s+1}}{N^s} \le 2(\zeta(s)-\zeta(s-1))L^{-s}.$$

Hence,

$$\limsup_{N\to\infty} \frac{\mathcal{E}_s(\Gamma,N) - 2\zeta(s)L^{-s}N^{s+1}}{N^s} \le -2(s\zeta(s)+\zeta(s-1))L^{-s}. \tag{126}$$

Let $s=2$. Then from (125) and Lemma V.5.1 we have

$$\mathcal{E}_2(\Gamma,N) \le L^{-2}N^2 D_2(N) + \epsilon L^{-1} N D_1(N) + O(N^2) =$$

$$= \frac{\pi^2}{3}L^{-2}N^3 - 2L^{-2}N^2\ln N + 2\epsilon L^{-1}N^2\ln N + O(N^2), \quad N\to\infty.$$

Since $\epsilon>0$ can be taken arbitrarily small, we get

$$\limsup_{N\to\infty} \frac{\mathcal{E}_2(\Gamma,N) - 3^{-1}\pi^2L^{-2}N^3}{N^2\ln N} = \limsup_{N\to\infty} \frac{\mathcal{E}_2(\Gamma,N+1) - 3^{-1}\pi^2L^{-2}N^3}{N^2\ln N} \le -2L^{-2}. \tag{127}$$

A lower estimate can be obtained from the following inequality [39, relation (4.8)] which is true for $s>1$:

$$\mathcal{E}_s(\Gamma,N) \ge \frac{2(N-1)^{s+1}}{L^s}\sum_{k=1}^{N-1}\left(1-\frac{k-1}{N-1}\right)^{s+1}\cdot\frac{1}{k^s}.$$

Let $s>2$. For $0<t<1$, we have $(1-t)^{s+1} > 1-(s+1)t$. Hence, we have

$$\mathcal{E}_s(\Gamma,N) \ge 2L^{-s}N^{s+1}\left(1-\frac{s+1}{N}\right)\sum_{k=1}^{N-1}\left(1-\frac{k-1}{N-1}\right)^{s+1}\cdot\frac{1}{k^s}.$$

Using (113), for N sufficiently large, we get

$$\mathcal{E}_s(\Gamma,N) \ge 2L^{-s}N^{s+1}\left(1-\frac{s+1}{N}\right)\sum_{k=1}^{N-1}\left(1-\frac{(s+1)k}{N-1}\right)\cdot\frac{1}{k^s} =$$

$$= 2L^{-s}N^{s+1}\left(1-\frac{s+1}{N}\right)\left(\sum_{k=1}^{N-1}\frac{1}{k^s} - \frac{(s+1)}{N-1}\sum_{k=1}^{N-1}\frac{1}{k^{s-1}}\right) =$$

$$= 2L^{-s}N^{s+1}\left(1-\frac{s+1}{N}\right)\left(\zeta(s) - \frac{(s+1)\zeta(s-1)}{N} + o(\frac{1}{N})\right) =$$

$$= 2L^{-s}N^{s+1}\left(\zeta(s) - \frac{(s+1)(\zeta(s-1)+\zeta(s))}{N} + o(\frac{1}{N})\right), \quad N\to\infty.$$

Then

$$\liminf_{N\to\infty} \frac{\mathcal{E}_s(\Gamma,N) - 2\zeta(s)L^{-s}N^{s+1}}{N^s} \ge -2L^{-s}(s+1)\left(\zeta(s-1)+\zeta(s)\right). \tag{128}$$

Combining (126) and (128), we get (98).

Let $s = 2$. Then,

$$\mathcal{E}_2(\Gamma, N) \geq 2L^{-2} \sum_{k=1}^{N-1} (N-k)^3 \cdot \frac{1}{k^2} =$$

$$= 2L^{-2} \left(N^3 \sum_{k=1}^{N-1} \frac{1}{k^2} - 3N^2 \sum_{k=1}^{N-1} \frac{1}{k} + 3N(N-1) - \sum_{k=1}^{N-1} k \right) =$$

$$= 2L^{-2} \left(\zeta(2) N^3 - 3N^2 \ln N + O(N^2) \right), \quad N \to \infty.$$

Hence,

$$\liminf_{N \to \infty} \frac{\mathcal{E}_2(\Gamma, N) - 2\zeta(2) L^{-2} N^3}{N^2 \ln N} \geq -6L^{-2}.$$

Combining this relation with (127), we get (99). Proposition V.2.1 is proved.

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