LOW COMPLEXITY METHODS FOR DISCRETIZING MANIFOLDS VIA RIESZ ENERGY MINIMIZATION

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ABSTRACT. Let A be a compact d-rectifiable set embedded in Euclidean space $\mathbb{R}^p$, $d \le p$. For a given continuous distribution $\sigma(x)$ with respect to d-dimensional Hausdorff measure on A, our earlier results provided a method for generating N-point configurations on A that have asymptotic distribution $\sigma(x)$ as $N \to \infty$; moreover such configurations are "quasi-uniform" in the sense that the ratio of the covering radius to the separation distance is bounded independent of N. The method is based upon minimizing the energy of N particles constrained to A interacting via a weighted power law potential $w(x,y)|x-y|^{-s}$, where $s > d$ is a fixed parameter and $w(x,y) = (\sigma(x)\sigma(y))^{-(s/2d)}$.

Here we show that one can generate points on A with the above mentioned properties keeping in the energy sums only those pairs of points that are located at a distance of at most $r_N = C_N N^{-1/d}$ from each other, with C_N being a positive sequence tending to infinity arbitrarily slowly. To do this we minimize the energy with respect to a varying truncated weight $v_N(x,y) = \Phi(|x-y|/r_N)\, w(x,y)$, where $\Phi : (0,\infty) \to [0,\infty)$ is a bounded function with $\Phi(t) = 0$, $t \ge 1$, and $\lim_{t\to 0^+} \Phi(t) = 1$. This reduces, under appropriate assumptions, the complexity of generating N point 'low energy' discretizations to order NC_N^d computations.

1. Introduction

Points on a compact set A that minimize certain energy functions often have desirable properties that reflect special features of A. For $A = S^2$, the unit sphere in $\mathbb{R}^3$, the determination of minimal Coulomb energy points is the classic problem of Thomson [15, 5]. Other energy functions on higher dimensional spheres give rise to equilibrium points that are useful for a variety of applications including coding theory [8], cubature formulas [16], and the generation of finite normalized tight frames [1]. In this paper, we shall consider a generalized Thomson problem, namely minimal energy points for weighted Riesz potentials on rectifiable sets (where the weight varies as the cardinality of the configuration grows). Energy problems with varying weights arise, in particular, in physical problems involving potentials that are not scale invariant.

Our focus is on the hypersingular case when short range interaction between points is the dominant effect. Such energy functions are not treatable with classical potential theoretic methods, and so require different techniques of analysis.

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Let A be a compact set in $\mathbb{R}^p$ whose d-dimensional Hausdorff measure[1], $\mathcal{H}_d(A)$, is finite and positive. For a collection of $N \geq 2$ distinct points $\omega_N := \{x_1, \ldots, x_N\} \subset A$, 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

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

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

$$\mathcal{E}_s^w(A, N) := \inf\{E_s^w(\omega_N) : \omega_N \subset A, \#\omega_N = N\}, \tag{1}$$

where $\#X$ denotes the cardinality of a set X. If $v(x, y) = (w(x, y) + w(y, x))/2$, then $E_s^v(\omega_N) = E_s^w(\omega_N)$ for any N-point configuration $\omega_N \subset A$, and so, without loss of generality, we assume 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 every closed subset $B \subset A \times A \setminus D(A)$.

Here CPD stands for (almost everywhere) 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 $A \times A$). We mention that if a CPD-weight w is also lower semi-continuous on $A \times A$, then the infimum in (1) will be attained.

If $w \equiv 1$ on $A \times A$ (which we refer to as the *unweighted* case), we write $E_s(\omega_N)$ and $\mathcal{E}_s(A, N)$ for $E_s^w(\omega_N)$ and $\mathcal{E}_s^w(A, N)$, respectively. For the trivial cases $N = 0$ or 1 we put $E_s(\omega_N) = \mathcal{E}_s(A, N) = E_s^w(\omega_N) = \mathcal{E}_s^w(A, N) = 0$.

In previous works, the authors of this paper have investigated asymptotics as $N \to \infty$ for a fixed weight w for the energy $\mathcal{E}_s^w(A, N)$ as well as for the optimal configurations that achieve the minimum energy. Our focus in this article is a generalization that allows the weight w to vary with N. A primary motivation for this generalization is to lower the complexity of energy computations that typically are of order N^2 by incorporating a "cut-off" function into the weight that depends on N.

Before stating our main results we provide some needed notation and review some relevant prior work.

A set $A \subset \mathbb{R}^p$ is called *d-rectifiable* if $A = \phi(K)$, where $K \subset \mathbb{R}^d$ is a bounded set and $\phi : K \to \mathbb{R}^p$ is a Lipschitz mapping. A set $A \subset \mathbb{R}^p$ 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.

A sequence of Borel probability measures $\{\mu_N\}$ supported on a compact set A in $\mathbb{R}^p$ is said to *converge in the weak* sense* to a Borel probability measure μ (supported on

[1]For integer d, we normalize Hausdorff measure on $\mathbb{R}^p$ so that $\mathcal{H}_d(U) = 1$ if U is a d-dimensional unit cube embedded in $\mathbb{R}^p$.

A), if for every Borel subset B of A whose relative boundary $\partial_A B$ with respect to A has μ-measure zero, we have

$$\lim_{N\to\infty} \mu_N(B) = \mu(B).$$

In this case we write $\mu_N \xrightarrow{*} \mu$ as $N \to \infty$.

Let $\mathcal{L}_m$ denote the Lebesgue measure in $\mathbb{R}^m$ and let

$$K(\epsilon) := \{x \in \mathbb{R}^p : \operatorname{dist}(x, K) < \epsilon\}$$

denote the ϵ-neighborhood of the set K in $\mathbb{R}^p$. The *upper* and the *lower d-dimensional Minkowski content* of the set K are defined by

$$\overline{\mathcal{M}}_d(K) := \limsup_{\epsilon\to 0^+} \frac{\mathcal{L}_p(K(\epsilon))}{\beta_{p-d}\epsilon^{p-d}}$$

and

$$\underline{\mathcal{M}}_d(K) := \liminf_{\epsilon\to 0^+} \frac{\mathcal{L}_p(K(\epsilon))}{\beta_{p-d}\epsilon^{p-d}}$$

respectively, where β_m is the Lebesgue measure of the unit ball in $\mathbb{R}^m$, $m \in \mathbb{N}$, and $\beta_0 := 1$. If the limit

$$\mathcal{M}_d(K) := \lim_{\epsilon\to 0^+} \frac{\mathcal{L}_p(K(\epsilon))}{\beta_{p-d}\epsilon^{p-d}}$$

exists, it is called the *d-dimensional Minkowski content* of the set K. We also let δ_x denote the unit point mass at $x \in \mathbb{R}^p$.

For $s > 0$ and a CPD-weight w on A, we say that a sequence $\{\omega_N\}_{N=2}^{\infty}$ of N-point configurations on A is *asymptotically (w, s)-energy minimizing* if

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

In the unweighted case ($w \equiv 1$) the asymptotic behavior of the minimal energy and the weak* limit distribution of energy minimizing configurations are known for wide classes of sets as stated in the following theorem.

Theorem 1.1. *Let $s > d$ and $p \geq d$, where d and p are integers. For every infinite compact $(\mathcal{H}_d, d)$-rectifiable set A in $\mathbb{R}^p$ with $\mathcal{M}_d(A) = \mathcal{H}_d(A)$, we have*

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

where $C_{s,d}$ is a positive and finite constant independent of A.

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

$$\frac{1}{N} \sum_{x\in\omega_N} \delta_x \xrightarrow{*} \frac{\mathcal{H}_d(\cdot \cap A)}{\mathcal{H}_d(A)}, \quad N \to \infty. \tag{2}$$

This result was proved for the case that A is a finite union of rectifiable Jordan arcs in [13, Theorems 3.2 and 3.4], a d-dimensional rectifiable manifold in [10, Theorem 2.4], a d-rectifiable closed set in [4, Theorems 1 and 2], and, in the form presented above, in [4, Theorems 1 and 2 and related remarks].

We remark that the constant $C_{s,1} = 2\zeta(s)$ for $s > 1$, where $\zeta(s)$ denotes the classical Riemann zeta function. For other values d, this constant is not yet known. However, for certain values of d, specifically $d = 2, 4, 8$ and 24, it is conjectured (cf. [6]) that $C_{s,d} = |\Lambda_d|^{s/d}\zeta_{\Lambda_d}(s)$ for $s > d$, where ζ_{Λ_d} denotes the *Epstein zeta function* for the hexagonal, D_4, E_8, and Leech lattices, respectively and $|\Lambda_d|$ denotes the co-volume of Λ_d.

Given a CPD-weight w on $A \times A$, define for any Borel set $B \subset A$,

$$\mathcal{H}_d^{s,w}(B) := \int_B w(x,x)^{-d/s} \mathrm{d}\mathcal{H}_d(x), \quad s > d.$$

If $0 < \mathcal{H}_d(A) < \infty$, the corresponding probability measure on A is

$$h_d^{s,w}(B) := \frac{\mathcal{H}_d^{s,w}(B)}{\mathcal{H}_d^{s,w}(A)}. \tag{3}$$

In the case of weighted energy the following asymptotic result is known, see [4, Theorem 2].

Theorem 1.2. *Let $A \subset \mathbb{R}^p$ be an infinite closed d-rectifiable set. Suppose $s > d$ and that w is a CPD-weight function on $A \times A$. Then*

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

where the constant $C_{s,d}$ is as in Theorem 1.1. Furthermore, if $\mathcal{H}_d(A) > 0$, any asymptotically (w,s)-energy minimizing sequence of N-point configurations on A is uniformly distributed with respect to the probability measure $h_d^{s,w}$ defined in (3), as $N \to \infty$.

One application of the above theorem is to generate points on a rectifiable set that have a specified limiting distribution with respect to Hausdorff measure on the set. More precisely, if A is as in Theorem 1.2 and σ is a probability density on A that is continuous almost everywhere with respect to $\mathcal{H}_d$ and is bounded above and below by positive constants, then for fixed $s > d$ and $w : A \times A \to [0, \infty)$ given by

$$w(x,y) := (\sigma(x)\sigma(y))^{-s/2d}, \tag{4}$$

a sequence of normalized counting measures associated with N-point (w,s)-energy minimizing configurations on A converges weak* (as $N \to \infty$) to $\sigma(\cdot)\,\mathrm{d}\mathcal{H}_d(\cdot)$ (see also, [4, Corollary 2]).

The outline of the paper is as follows. In the next section we state our main results. In Section 3, we provide complexity estimates for generating minimum weighted energy points that involve a cut-off function, and we illustrate the generation method with two examples—one for the sphere and another for a 3-dimensional spherical shell. Section 4 is devoted to the proof of Theorem 2.1, while Sections 5 and 6 are devoted to the proofs of Theorems 2.2 and 2.3. The proofs of Theorems 2.4 and 2.5 are given in Section 7 and the complexity assertions from Section 3 are justified in Section 8.

2. Main results

The main purpose of this paper is to present an efficient method for generating a large number of points on a manifold that are well-separated and approximate a given distribution. The low complexity of our method is accomplished by performing significantly fewer operations when computing energy sums and gradients.

We begin by stating the following result extending Theorem 1.2 to the wider class of $(\mathcal{H}_d, d)$-rectifiable sets whose Minkowski content of dimension d coincides with the d-dimensional Hausdorff measure. We note that this result also extends relation (2) of Theorem 1.1 to this class of sets. The proof of this result will appear in Section 4.

Theorem 2.1. *Let $A \subset \mathbb{R}^p$ be an infinite compact $(\mathcal{H}_d, d)$-rectifiable set with $\mathcal{H}_d(A) = \mathcal{M}_d(A)$ and suppose that w is a CPD-weight function on $A \times A$. If $s > d$, then*

$$\lim_{N\to\infty} \frac{\mathcal{E}_s^w(A,N)}{N^{1+s/d}} = \frac{C_{s,d}}{[\mathcal{H}_d^{s,w}(A)]^{s/d}}, \tag{5}$$

where the constant $C_{s,d}$ is as in Theorem 1.1.

Furthermore, if $\mathcal{H}_d(A) > 0$, any sequence $\widetilde{\omega}_N = \{x_1^N, \ldots, x_N^N\}$ of asymptotically (w, s)-energy minimizing configurations on A is uniformly distributed with respect to the probability measure $h_d^{s,w}$ as $N \to \infty$.

The following theorem, one of the main results of this paper, concerns asymptotic results in the case when the weight function includes a "cut-off" function depending on N. Given a sequence of non-negative weights $\mathbf{v} = \{v_N\}$ on $(A \times A) \setminus D(A)$, we say that a sequence of N-point configurations $\{\omega_N\}$ on A is *asymptotically* $(\mathbf{v}, s)$*-energy minimizing* if

$$\lim_{N\to\infty} \frac{E_s^{v_N}(\omega_N)}{\mathcal{E}_s^{v_N}(A,N)} = 1.$$

Theorem 2.2. *Let $A \subset \mathbb{R}^p$ be a compact $(\mathcal{H}_d, d)$-rectifiable set with $\mathcal{H}_d(A) = \mathcal{M}_d(A) > 0$ and let w be a CPD-weight function on $A \times A$. Suppose Φ is a non-negative, bounded function on $(0, \infty)$ such that $\lim_{t\to 0^+} \Phi(t) = 1$ and $\{r_N\}_{N\in\mathbb{N}}$ is a sequence of positive numbers such that*

$$\lim_{N\to\infty} r_N N^{1/d} = \infty. \tag{6}$$

For $N \in \mathbb{N}$, let $\mathbf{v} = \{v_N\}_{N\in\mathbb{N}}$ denote the sequence of weights

$$v_N(x,y) := \Phi\left(\frac{|x-y|}{r_N}\right) w(x,y), \quad x, y \in A, \quad x \neq y. \tag{7}$$

If $s > d$, then

$$\lim_{N\to\infty} \frac{\mathcal{E}_s^{v_N}(A,N)}{N^{1+s/d}} = \frac{C_{s,d}}{[\mathcal{H}_d^{s,w}(A)]^{s/d}}, \tag{8}$$

where the constant $C_{s,d}$ is as in Theorem 1.1. Furthermore, any sequence of asymptotically $(\mathbf{v}, s)$-energy minimizing N-point configurations on A is uniformly distributed with respect to the probability measure $h_d^{s,w}$, as $N \to \infty$.

The proof of Theorem 2.2 is given in Sections 5 and 6.

Remark: Note that *any* compact set $A \subset \mathbb{R}^d$ (i.e., $p = d$) is automatically a $(\mathcal{H}_d, d)$-rectifiable set with $\mathcal{H}_d(A) = \mathcal{M}_d(A)$ and so the conclusions of Theorem 2.2 hold for any compact $A \subset \mathbb{R}^d$ such that $\mathcal{H}_d(A) > 0$. The same is true for any $A \subset \mathbb{R}^p$ that is compact and d-rectifiable.

Theorem 2.2 implies, in particular, that the minimal (v_N, s)-energy has the same asymptotic dominant term on a wide class of compact rectifiable sets as the minimal (w, s)-energy (for $s > d$).

We note that if $\Phi(t) = 0$ for $t > 1$, then the energy sum $E_s^{v_N}(\omega_N)$ for this cutoff function simplifies since it only involves pairs of points from ω_N that are no further than r_N apart. In the next section, we discuss the complexity of computing such sums in more detail.

Theorem 2.2 is a consequence of a more general result, which we present next. It provides general conditions under which one can find the asymptotic behavior of the minimal weighted energy sum where the weight varies with N. In view of condition (b) of the definition of a CPD-weight, there is a number $\kappa > 0$ such that $w(x, y) > 0$, whenever $x, y \in A$ and $|x - y| < \kappa$. Given a non-negative function $v(x, y)$ on $A \times A \setminus D(A)$, for every $\delta \in (0, \kappa)$, define

$$I^w(v, \delta) = \inf\{\frac{v(x, y)}{w(x, y)} : (x, y) \in A \times A,\ 0 < |x - y| \leq \delta\} \tag{9}$$

and let

$$S^w(v, \delta) = \sup\{\frac{v(x, y)}{w(x, y)} : (x, y) \in A \times A,\ 0 < |x - y| \leq \delta\}. \tag{10}$$

Theorem 2.3. *Let $s > d$, $A \subset \mathbb{R}^p$ be a compact $(\mathcal{H}_d, d)$-rectifiable set with $\mathcal{H}_d(A) = \mathcal{M}_d(A) > 0$, w be a CPD-weight function on $A \times A$, and $\mathbf{v} = \{v_N\}_{N \in \mathbb{N}}$ be a sequence of non-negative functions on $A \times A \setminus D(A)$ such that for some constant $M > 0$,*

$$v_N(x, y) \leq M w(x, y), \quad (x, y) \in A \times A \setminus D(A),\ N \in \mathbb{N}, \tag{11}$$

and

$$\lim_{N\to\infty} I^w(v_N, aN^{-1/d}) = \lim_{N\to\infty} S^w(v_N, aN^{-1/d}) = 1 \tag{12}$$

for every positive constant a. Then

$$\lim_{N\to\infty} \frac{\mathcal{E}_s^{v_N}(A, N)}{N^{1+s/d}} = \frac{C_{s,d}}{[\mathcal{H}_d^{s,w}(A)]^{s/d}}, \tag{13}$$

where the constant $C_{s,d}$ is as in Theorem 1.1.

Furthermore, any sequence of asymptotically $(\mathbf{v}, s)$*-energy minimizing* N*-point configurations on* A *is uniformly distributed with respect to the probability measure* $h_d^{s,w}$ *as* $N \to \infty$*.*

The proof Theorem 2.3 is given in Section 6.

We next find conditions that guarantee that a sequence of (v_N, s)-energy minimizing N-point configurations is *quasi-uniform*, that is, the ratios of the covering radius[2] to the separation distance of the configurations stay bounded as $N \to \infty$. For a point configuration X in $\mathbb{R}^p$, we define its *separation distance* by

$$\delta(X) := \inf_{\substack{x,y \in X \\ x \neq y}} |x - y|, \tag{14}$$

and its *covering radius relative to a set* A *in* $\mathbb{R}^p$ by

$$\rho(X, A) := \sup_{y \in A} \inf_{x \in X} |x - y|. \tag{15}$$

We shall establish quasi-uniformity of (v_N, s)-energy minimizing N-point configurations ω_N^s in A by showing that both $\delta(\omega_N^s)$ and $\rho(\omega_N^s, A)$ are of order $N^{-1/d}$.

Theorem 2.4. *Let* $s > d$*,* $A \subset \mathbb{R}^p$ *be a compact set with* $\mathcal{H}_d(A) > 0$*, and* $\{v_N\}$ *be a uniformly bounded sequence of non-negative lower semi-continuous functions on* $A \times A$ *such that for* N *sufficiently large, there holds*

$$v_N(x, y) > \alpha_0, \qquad (x, y) \in A \times A,\ 0 < |x - y| \le a_0 N^{-1/d}, \tag{16}$$

for some positive constants a_0 *and* α_0*. Then for every sequence* $\{\omega_N^s\}$ *of* N*-point* (v_N, s)*-energy minimizing configurations on* A*, there holds*

$$\liminf_{N \to \infty} \delta(\omega_N^s) N^{1/d} > 0. \tag{17}$$

We note that Theorem 2.4 holds under the assumptions on s, A, and $\{v_N\}$ in Theorem 2.3 provided that the v_N's are uniformly bounded and lower semi-continuous on $A \times A$.

For the next result concerning the covering radius, we recall the notion of a *d-regular* set. A compact set $\tilde{A} \subset \mathbb{R}^p$ is said to be *d-regular* if there exists a finite positive Borel measure μ supported on $\tilde{A}$ that is both upper and lower d-regular, that is, there are positive constants c_0, C_0 such that

$$c_0^{-1} r^d \le \mu(B(x, r)) \le C_0 r^d, \qquad (x \in \tilde{A},\ 0 < r < \operatorname{diam} \tilde{A}), \tag{18}$$

where $B(x, r)$ denotes the open ball in $\mathbb{R}^p$ centered at x of radius $r > 0$.

Theorem 2.5. *Assume that* s*,* A*, and* $\{v_N\}$ *are as in Theorem 2.3. In addition, assume that the* v_N*'s are uniformly bounded and lower semi-continuous on* $A \times A$*, and that* A *is a subset of a* d*-regular set* $\tilde{A} \subset \mathbb{R}^p$*. Then for every sequence* $\{\omega_N^s\}$ *of* N*-point configurations on* A *such that* ω_N^s *minimizes the* (v_N, s)*-energy,* $N \in \mathbb{N}$*, there holds*

$$\limsup_{N \to \infty} \rho(\omega_N^s, A) N^{1/d} < \infty. \tag{19}$$

[2]The covering radius of a configuration (relative to a set A) is also referred to as the *fill radius* or the *mesh-norm* of the configuration.

The proofs of Theorems 2.4 and 2.5 are given in Section 7.

In applications with a non-uniform limiting density, it can be useful to allow the 'cutoff' radius $r_N = r_N(x, y)$ in (6) to depend on $(x, y) \in A\times A$. The following immediate corollary of Theorems 2.3, 2.4 and 2.5 addresses this case.

Corollary 2.6. *Let $s > d$, $A \subset \mathbb{R}^p$ be a compact $(\mathcal{H}_d, d)$-rectifiable set with $\mathcal{H}_d(A) = \mathcal{M}_d(A) > 0$ and let w be a CPD-weight function on $A\times A$. Suppose $r_N : A\times A \to (0,\infty)$ is a symmetric function such that*

$$r_N(x, y)N^{1/d} \to \infty \tag{20}$$

uniformly on $A \times A$ as $N \to \infty$, and $\Phi : (0,\infty) \to [0,\infty)$ is bounded and satisfies $\lim_{t\to 0^+} \Phi(t) = 1$. For $N \geq 1$, let

$$v_N(x, y) := \Phi\left(\frac{|x-y|}{r_N(x, y)}\right) w(x, y), \quad x, y \in A, \quad x \neq y. \tag{21}$$

Then the conclusions of Theorem 2.3 hold.

If, in addition, each v_N is lower semi-continuous, w is bounded, and A is contained in a d-regular set $\tilde{A} \subset \mathbb{R}^p$, then every sequence of N-point (v_N, s)-energy minimizing configurations on A is quasi-uniform on A.

Indeed with v_N, r_N and Φ as in the above corollary, it is easy to verify that v_N satisfies (11) and (12).

Finally, we further elucidate the behavior of a sequence of weights $\{v_N\}$ satisfying conditions of form (12) in Theorem 2.3. Given a non-negative function v on $A\times A\setminus D(A)$ and a point $x_0 \in A$, let

$$L(v, x_0) := \limsup_{\substack{(x,y)\to(x_0,x_0)\\ x\neq y}} v(x, y) \quad \text{and} \quad l(v, x_0) := \liminf_{\substack{(x,y)\to(x_0,x_0)\\ x\neq y}} v(x, y).$$

Proposition 2.7. *Let w be a CPD-weight defined on $A \times A$ and $\{v_N\}$ be a sequence of non-negative functions on $A \times A \setminus D(A)$. If for some positive sequence $\{\alpha_N\}$ that tends to zero, one has*

$$\lim_{N\to\infty} I^w(v_N, \alpha_N) = \lim_{N\to\infty} S^w(v_N, \alpha_N) = 1 \tag{22}$$

(in particular, if condition (12) holds), then

$$\lim_{N\to\infty} \frac{L(v_N, x_0)}{L(w, x_0)} = 1 \quad \text{and} \quad \lim_{N\to\infty} \frac{l(v_N, x_0)}{l(w, x_0)} = 1 \tag{23}$$

uniformly over $x_0 \in A$.

If, in addition, w is continuous on $D(A)$, then condition (22) holds for some positive sequence $\{\alpha_N\}$ with zero limit if and only if

$$\lim_{N\to\infty} L(v_N, x_0) = \lim_{N\to\infty} l(v_N, x_0) = w(x_0, x_0) \tag{24}$$

with both sequences converging uniformly for $x_0 \in A$.

The proof of Proposition 2.7 is given in Appendix A.

If $L(w,x_0)=\infty$ in (23), we agree that $L(v_N,x_0)/L(w,x_0)=0$ when $L(v_N,x_0)<\infty$ and $L(v_N,x_0)/L(w,x_0)=1$ when $L(v_N,x_0)=\infty$. A similar agreement is also in place for the lower limits $l(\cdot,x_0)$.

We also remark that if the limit of w at some point $(x_0,x_0)\in D(A)$ does not exist, one can construct a sequence of weights $\{v_N\}$ such that (22) fails for any positive sequence $\{\alpha_N\}$ converging to zero. This can be done even if w is assumed to be bounded on $A\times A$.

3. Complexity estimates and numerical experiments

Throughout this section we assume that Φ is a 'cutoff' function as in Theorem 2.2 such that

$$\Phi(t)=0 \text{ for } t>1.$$

For such Φ, we consider the complexity of evaluating

$$f(x_1,\ldots,x_N):=E_s^{v_N}(\omega_N)=\sum_{(i,j):i\neq j}\Phi\left(\frac{|x_i-x_j|}{r_N(x_i,x_j)}\right)\frac{w(x_i,x_j)}{|x_i-x_j|^s}, \tag{25}$$

where $\omega_N=\{x_1,\ldots,x_N\}$. Assuming Φ, r_N, and w are sufficiently smooth, and A is a compact set in $\mathbb{R}^d$ of positive Lebesgue measure with boundary of measure zero, we also shall consider the complexity of evaluating the gradient of f; i.e., the vector in $\mathbb{R}^{Nd}$ with $(d(i-1)+\ell)^{\text{th}}$ component given by

$$\partial_{x_{i,\ell}}f(x_1,\ldots,x_N)=2\sum_{j:j\neq i}\partial_{x_{i,\ell}}\left(\Phi\left(\frac{|x_i-x_j|}{r_N(x_i,x_j)}\right)\frac{w(x_i,x_j)}{|x_i-x_j|^s}\right), \tag{26}$$

where $x_{i,\ell}$ denotes the ℓ^{th} component of x_i for $i=1,\ldots,N$ and $\ell=1,\ldots,d$, as well as the complexity of evaluating the Hessian of f; i.e., the $Nd\times Nd$ matrix with $(d(i-1)+\ell,d(j-1)+k)$ component given by

$$\partial_{x_{i,\ell}}\partial_{x_{j,k}}f(x_1,\ldots,x_N)=2\partial_{x_{i,\ell}}\partial_{x_{j,k}}\left(\Phi\left(\frac{|x_i-x_j|}{r_N(x_i,x_j)}\right)\frac{w(x_i,x_j)}{|x_i-x_j|^s}\right) \tag{27}$$

for $1\le i\neq j\le N$ and $\ell,k=1,\ldots,d$, and

$$\partial_{x_{i,\ell}}\partial_{x_{i,k}}f(x_1,\ldots,x_N)=2\sum_{j:j\neq i}\partial_{x_{i,\ell}}\partial_{x_{i,k}}\left(\Phi\left(\frac{|x_i-x_j|}{r_N(x_i,x_j)}\right)\frac{w(x_i,x_j)}{|x_i-x_j|^s}\right) \tag{28}$$

for $i=1,\ldots,N$ and $\ell,k=1,\ldots,d$.

The number of non-zero terms in (25) of the form

$$\Phi\left(\frac{|x_i-x_j|}{r_N(x_i,x_j)}\right)\frac{w(x_i,x_j)}{|x_i-x_j|^s} \tag{29}$$

does not exceed the cardinality of $\{(x,y)\in\omega_N\times\omega_N : 0<|x-y|\le r_N(x,y)\}$, and so, if $r_N(x,y)\le\delta_N$ for all $x,y\in A$, then the quantity

$$Z(\omega_N,\delta_N):=\#\{(x,y)\in\omega_N\times\omega_N : 0<|x-y|\le\delta_N\}, \tag{30}$$

times the maximal complexity of evaluating a single term provides an upper bound for the complexity of computing $E_s^{v_N}(\omega_N)$. Similarly, the number of nonzero terms of the form

$$\partial_{x_{i,\ell}}\left(\Phi\left(\frac{|x_i-x_j|}{r_N(x_i,x_j)}\right)\frac{w(x_i,x_j)}{|x_i-x_j|^s}\right)$$

required to compute the gradient of f is bounded above by $dZ(\omega_N,\delta_N)$, while the number of nonzero elements of the Hessian (each of the form in (27) or (28)) is bounded above by $2d^2Z(\omega_N,\delta_N)$. Hence, the computational complexity of one step in a gradient descent optimization scheme (or to evaluate f and its gradient and Hessian, as required in one step of a second-order optimization scheme) is bounded by a constant (determined by the maximal complexity of the individual terms and the dimension d) times $Z(\omega_N,\delta_N)$. Finally, we mention that determining the set $\{(x,y)\in\omega_N\times\omega_N : 0<|x-y|\le\delta_N\}$ is known as the *fixed-radius near neighbor problem* which can be solved using so-called *bucketing algorithms* with (expected) complexity of order $O(N+Z(\omega_N,\delta_N))$ (cf. [2]).

We further provide bounds on $Z(\omega_N,\delta_N)$ based on geometrical and/or energy properties of ω_N. In order to use Theorem 2.2 and Corollary 2.6, we must have that δ_N is of the form $\delta_N=C_NN^{-1/d}$, for some positive sequence C_N with infinite limit and we shall assume this form in the following. We first observe that

$$Z(\omega_N,\delta_N)\le N\max_{x\in\omega_N}\#\left(\omega_N\cap B[x,\delta_N]\right), \tag{31}$$

where $B[x,r]$ denotes the closed ball in $\mathbb{R}^p$ with radius r and center x. Hence, if $\{\omega_N\}$ is a sequence of N-point configurations on A such that

$$\max_{x\in\omega_N}\#\left(\omega_N\cap B[x,\delta_N]\right)=O(N\delta_N^d)=O(C_N^d),\quad N\to\infty, \tag{32}$$

then $Z(\omega_N,\delta_N)=O(NC_N^d)$, $N\to\infty$.

If A is a compact subset of $\mathbb{R}^d$ with boundary of positive Lebesgue measure or A is a d-regular subset of $\mathbb{R}^p$, we can still estimate the number of non-zero terms in (25) of form (29). We can show that a well-separated sequence of configurations ω_N on a compact d-regular set A satisfies (32) and so we obtain:

Proposition 3.1. *Let A be a compact d-regular set in $\mathbb{R}^p$, $d\le p$, and $\{\omega_N\}$ be a sequence of N-point configurations on A such that*

$$\liminf_{N\to\infty}\delta(\omega_N)N^{1/d}>0. \tag{33}$$

If $\delta_N=C_NN^{-1/d}$, where $\{C_N\}$ is a positive sequence bounded below by some $c>0$, then

$$Z(\omega_N,\delta_N)=O(NC_N^d),\quad N\to\infty.$$

The following estimate is the most important for our applications to calculating low energy configurations.

Proposition 3.2. *Let $s>0$, A be a compact set in $\mathbb{R}^p$ and ω be arbitrary finite configuration on A. Then*

$$Z(\omega,\delta)\le\delta^sE_s(\omega).$$

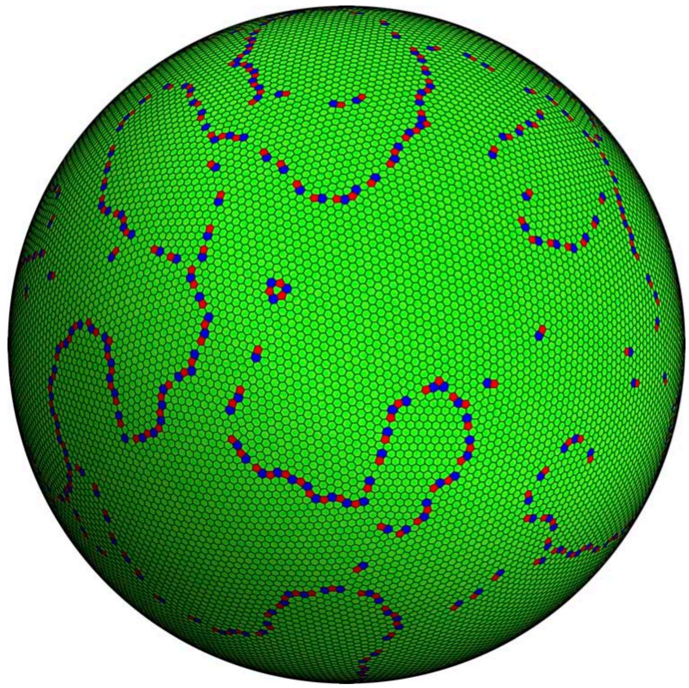

FIGURE 1. **A configuration of 30,000 near optimal $s = 3.5$ energy points on the sphere.**

In particular, if $s > d > 0$ and a sequence $\{\omega_N\}$ of N-point configurations on A is such that

$$E_s(\omega_N) = O(N^{1+s/d}), \quad N \to \infty, \quad \text{and} \quad \delta_N = C_N N^{-1/d},$$

where $\{C_N\}$ is a positive sequence bounded below by some $c > 0$, then

$$Z(\omega_N, \delta_N) = O(NC_N^s), \quad N \to \infty.$$

Remark. Note that if w is a bounded CPD weight on $A \times A$ and $s > d$, then $E_s(\omega_N) = O(N^{1+s/d})$ if and only if $E_s^w(\omega_N) = O(N^{1+s/d})$ and so either of these energies can be used in the assumptions of Proposition 3.2.

To illustrate the utility of our results, we present two examples of low-energy discretizations. The first, shown in Figure 1, shows the Voronoi decomposition of the unit sphere $\mathbb{S}^2$ for a configuration of 30,000 points on the sphere obtained from a random starting configuration followed by 500 iterations of gradient descent. We used $s = 3.5$, $w(x, y) = 1$, $\Phi(t) = (1 - t^2)^3 \chi_{[0,1]}(t)$, where $\chi_{[0,1]}(t)$ is the characteristic function of the interval $[0, 1]$, and $r_N(x, y) = (\ln N)N^{-1/2}$ ($\ln N \approx 10$ for $N = 30,000$). We observe (and this is almost always the case for large low energy configurations on the sphere) that all of Voronoi cells are either pentagons, hexagons, or heptagons, with the large majority being nearly regular hexagons. This hexagonal dominant local structure lends support to the conjectured value of $C_{s,2}$ given in the discussion following Theorem 1.1.

The second example consists of a configuration of $500,000$ low energy points computed in a 3-dimensional spherical shell with inner radius $R_0 = .55$ and outer radius $R_1 = 1$.

We used the same s, w, and Φ as in the previous example. In this case we chose $r_N(x,y) = (1/4)(\ln N)N^{-1/3}$. The configuration was obtained by applying 1000 gradient descent iterations to a random starting configuration. In Figure 2 we show the energy for the configuration at each iteration step and in Figure 3 we show a portion of the configuration near a slice of the shell for the final 1000-th iteration.

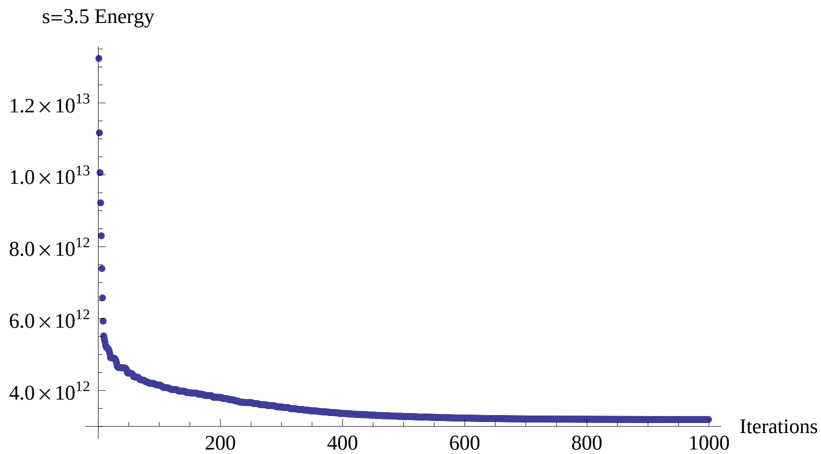

Figure 2. **The energy ($s = 3.5$) of a sequence of 500,000 point configurations in a spherical shell resulting from 1000 gradient descent iterations starting from a random configuration.**

4. Proof of Theorem 2.1

Given a sequence of CPD-weight functions $\mathbf{v} = \{v_N\}$ on $A \times A$, let

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

and, if the limit (possibly infinite) exists,

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

For a constant sequence $v_N = w$, we write $\underline{g}^{w}_{s,d}(A)$, $\overline{g}^{w}_{s,d}(A)$, $g^{w}_{s,d}(A)$ for these respective quantities. In particular, when $v_N \equiv 1$, we omit the superscript.

We shall need the following known results from geometric measure theory.

Theorem 4.1. ([9, Theorem 3.2.39]) *If $W \subset \mathbb{R}^p$ is a closed d-rectifiable set, then $\mathcal{M}_d(W) = \mathcal{H}_d(W)$.*

A mapping $\varphi : K \to \mathbb{R}^p$, $K \subset \mathbb{R}^d$, is called *bi-Lipschitz* with constant $L > 1$ if

$$L^{-1}|x-y| \le |\varphi(x) - \varphi(y)| \le L\,|x-y|, \quad x, y \in K.$$

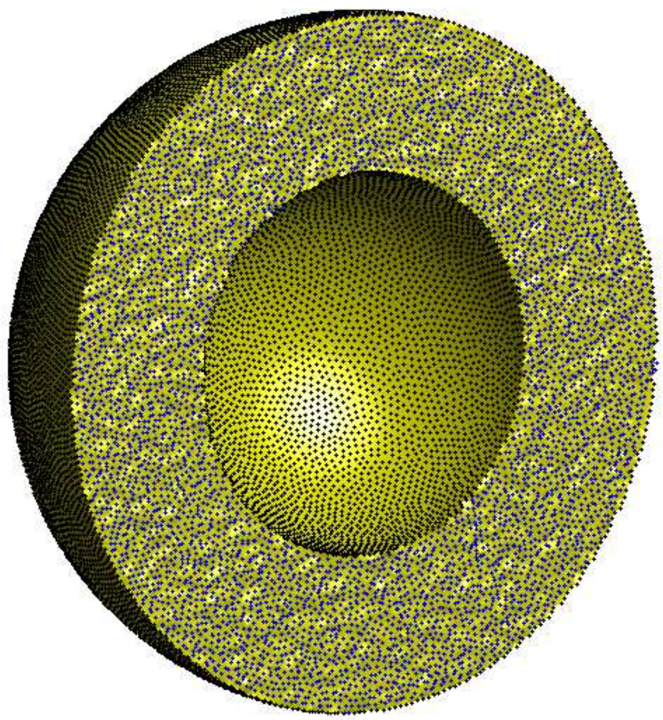

FIGURE 3. **A configuration of 500,000 near optimal $s = 3.5$ energy points on a spherical shell for geoscience (earth's mantle) applications.**

Lemma 4.2. *(see [9, 3.2.18]) Let $W \subset \mathbb{R}^p$ be an $(\mathcal{H}_d, d)$-rectifiable set. Then for every $\epsilon > 0$, there exist (at most countably many) compact sets $K_1, K_2, K_3, \ldots \subset \mathbb{R}^d$ and bi-Lipschitz mappings $\psi_i : K_i \to \mathbb{R}^p$ 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*

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

We start by proving the following auxiliary statement.

Lemma 4.3. *Let $A \subset \mathbb{R}^p$ be a compact $(\mathcal{H}_d, d)$-rectifiable set with $\mathcal{M}_d(A) = \mathcal{H}_d(A)$. Then every compact subset $K \subset A$ is also $(\mathcal{H}_d, d)$-rectifiable and $\mathcal{M}_d(K) = \mathcal{H}_d(K)$.*

Proof. Let $K \subset A$ be compact. It is not difficult to verify that K is also $(\mathcal{H}_d, d)$-rectifiable. Then, if $\epsilon > 0$, it follows from the definition of $(\mathcal{H}_d, d)$-rectifiability that there is some d-rectifiable compact set $J \subset K$ such that $\mathcal{H}_d(J) \geq \mathcal{H}_d(K) - \epsilon$. Using

Theorem 4.1, we obtain

$$\underline{\mathcal{M}}_d(K) \geq \mathcal{M}_d(J) = \mathcal{H}_d(J) \geq \mathcal{H}_d(K) - \epsilon,$$

and so $\underline{\mathcal{M}}_d(K) \geq \mathcal{H}_d(K)$.

It remains to show that $\overline{\mathcal{M}}_d(K) \leq \mathcal{H}_d(K)$. Let $\epsilon > 0$. Since, by assumption $\overline{\mathcal{M}}_d(A) < \infty$, we must have $\overline{\mathcal{M}}_d(K) < \infty$. Hence, we can find a compact set $L \subset A \setminus K$ such that $\mathcal{H}_d(L) + \mathcal{H}_d(K) > \mathcal{H}_d(A) - \epsilon$. Since $\operatorname{dist}(K, L) > 0$, it is easily seen that $\overline{\mathcal{M}}_d(K \cup L) \geq \overline{\mathcal{M}}_d(K) + \underline{\mathcal{M}}_d(L)$ and so, using the first part of this proof, we obtain

$$\mathcal{H}_d(A) = \mathcal{M}_d(A) \geq \overline{\mathcal{M}}_d(K \cup L) \geq \overline{\mathcal{M}}_d(K) + \underline{\mathcal{M}}_d(L) \geq \overline{\mathcal{M}}_d(K) + \mathcal{H}_d(L).$$

Hence,

$$\overline{\mathcal{M}}_d(K) \leq \mathcal{H}_d(A) - \mathcal{H}_d(L) \leq \mathcal{H}_d(K) + \epsilon,$$

and it follows that $\overline{\mathcal{M}}_d(K) \leq \mathcal{H}_d(K)$. □

In view of Lemma 4.3, applying Theorem 1.1, we have $g_{s,d}(K) = C_{s,d}\mathcal{H}_d(K)^{-s/d}$ for every compact subset $K \subset A$. Hence, Theorem 2.1 is a consequence of the following known lemma.

Lemma 4.4. *(see [4, Lemma 6]) Suppose that $s > d$, A is a compact set in $\mathbb{R}^p$ 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*

$$g_{s,d}(K) = \frac{C_{s,d}}{\mathcal{H}_d(K)^{s/d}}. \tag{34}$$

Then $g^w_{s,d}(A)$ exists and is given by

$$g^w_{s,d}(A) = C_{s,d} \left(\mathcal{H}^{s,w}_d(A)\right)^{-s/d}. \tag{35}$$

Moreover, 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

$$\frac{1}{N}\sum_{k=1}^{N} \delta_{x_k^N} \xrightarrow{\ *\ } h^{s,w}_d, \quad N \to \infty. \tag{36}$$

5. A special case of Theorem 2.2

We first establish the following special case of Theorem 2.2.

Proposition 5.1. *With the assumptions of Theorem 2.2 and the additional hypotheses that* (a) $\Phi(t) \leq 1$ *for* $t \in (0, \infty)$ *and* (b) $\Phi(t) = 0$ *for* $t > 1$*, the conclusions of Theorem 2.2 hold; i.e., for $s > d$, we have*

$$g^{\mathbf{v}}_{s,d}(A) = \lim_{N\to\infty} \frac{\mathcal{E}^{v_N}_s(A, N)}{N^{1+s/d}} = \frac{C_{s,d}}{\left[\mathcal{H}^{s,w}_d(A)\right]^{s/d}}, \tag{37}$$

where the constant $C_{s,d}$ is as in Theorem 1.1. Furthermore, any sequence of asymptotically $(\mathbf{v}, s)$-energy minimizing N-point configurations on A is uniformly distributed with respect to the probability measure $h^{s,w}_d$ as $N \to \infty$.

We start by proving the following basic estimate.

Lemma 5.2. *Let $s > d$ and $\omega \subset \mathbb{R}^d$ be a point configuration such that $\delta(\omega) \geq a > 0$. Then for every $R > a$ and $x \in \omega$,*

$$U_s(\omega; x, R) := \sum_{\substack{y\in\omega \\ |y-x|>R}} \frac{1}{|y-x|^s} \leq \frac{d5^d}{a^s} \sum_{i=[R/a]}^{\infty} \frac{1}{i^{s-d+1}}.$$

Proof. For every point $x \in \omega$, let

$$T_i(x) = \{y \in \omega : ai \leq |y-x| < a(i+1)\}, \quad i \in \mathbb{N}.$$

Then since the collection of open balls of radius $a/2$ centered at points of ω is pairwise disjoint, we have

$$\begin{aligned} \#T_i(x) &\leq \frac{\mathcal{L}_d\left(B(x,(i+3/2)a) \setminus B(x,(i-1/2)a)\right)}{\mathcal{L}_d(B(\mathbf{0},a/2))} \\ &= \frac{(i+3/2)^d a^d - (i-1/2)^d a^d}{(a/2)^d} = (2i+3)^d - (2i-1)^d \\ &\leq 4d(2i+3)^{d-1} \leq d5^d i^{d-1}, \quad i \in \mathbb{N}. \end{aligned} \tag{38}$$

Hence,

$$U_s(\omega; x, R) \leq \sum_{i=[R/a]}^{\infty} \sum_{y\in T_i(x)} \frac{1}{|y-x|^s} \leq \sum_{i=[R/a]}^{\infty} \frac{\#T_i(x)}{(ai)^s} \leq \frac{d5^d}{a^s} \sum_{i=[R/a]}^{\infty} \frac{1}{i^{s-d+1}},$$

which concludes the proof. □

Proof of Proposition 5.1. From (7) and the additional hypotheses on Φ we have $v_N(x,y) \leq w(x,y)$, $x, y \in A$, $x \neq y$. Hence, in view of Theorem 2.1, there holds for $s > d$,

$$\overline{g}^{\mathbf{v}}_{s,d}(A) = \limsup_{N\to\infty} \frac{\mathcal{E}_s^{v_N}(A,N)}{N^{1+s/d}} \leq \lim_{N\to\infty} \frac{\mathcal{E}_s^{w}(A,N)}{N^{1+s/d}} = \frac{C_{s,d}}{[\mathcal{H}_d^{s,w}(A)]^{s/d}}, \tag{39}$$

proving the upper estimate for (37).

Bounded weight. We first establish the required lower bound for (37) under the assumption that the CPD-weight w is bounded on $A \times A$. Let h and κ be positive numbers such that $w(x,y) > h$ whenever $x, y \in A$ and $|x-y| < \kappa$. Such numbers h and κ exist in view of condition (b) in the definition of the CPD-weight. Define

$$\overline{\Phi}(t) := \inf_{u\in(0,t]} \Phi(u), \quad t > 0. \tag{40}$$

Let $\{\omega_N\}$ be any sequence of point configurations on A such that $\#\omega_N = N$ and

$$|\mathcal{E}_s^{v_N}(A,N) - E_s^{v_N}(\omega_N)| = o(N^{1+s/d}), \quad N \to \infty. \tag{41}$$

Let

$$C_N := r_N N^{1/d} \qquad (N = 2, 3, \ldots). \tag{42}$$

Our goal is to show that the total energy of the pairs of points in ω_N that are at least $\sqrt{C_N}N^{-1/d}$ away from each other is $o(N^{1+s/d})$, from which the lower bound will follow. The argument consists of the following five steps:

Step 1. For a sufficiently small positive constant C, we remove from ω_N all those points whose $CN^{-1/d}$-neighborhood contains another point from ω_N and show that the configuration $\omega_{N,C}$ of the remaining points has sufficiently large cardinality.

Step 2. We choose a subset $D \subset A$ that consists of finitely many pairwise disjoint bi-Lipschitz embeddings of compact subsets of $\mathbb{R}^d$ and whose complement with respect to A has small $\mathcal{H}_d$-measure and show that the set $\eta_{N,C}$ of points from $\omega_{N,C}$ that are sufficiently close to D still has a sufficiently large cardinality.

Step 3. We move each point in $\eta_{N,C}$ to a close point in D and show that the resulting configuration $z_{N,C}$ has almost the same separation as $\eta_{N,C}$.

Step 4. We prove that the total energy of the pairs of points in $z_{N,C}$ that are sufficiently separated from each other is $o(N^{1+s/d})$. Since the bi-Lipschitz pieces of D are metrically separated, only the pairs of points from the same piece will make a significant contribution. This allows us to switch to estimating energies in $\mathbb{R}^d$ using Lemma 5.2.

Step 5. Since $\lim_{t\to 0^+}\Phi(t) = 1$, by varying the constant C the leading term of the (w, s)-energy of $\eta_{N,C}$ can be made as close as we like to the leading term of (v_N, s)-energy of ω_N thus giving us a sharp lower estimate for $\mathcal{E}_s^{v_N}(A, N)$.

For Step 1, choose a number $C \in (0, 1/2)$ such that

$$\alpha_C := 3^{d+1}\beta_{p-d}\beta_p^{-1}C^{2d} + C^s h^{-1} g_{s,d}^w(A) < 1 \tag{43}$$

and set

$$\omega_{N,C} := \{x \in \omega_N : \operatorname{dist}(x, \omega_N \setminus \{x\}) > CN^{-1/d}\}, \quad N \in \mathbb{N}.$$

Let y_x be a point in $\omega_N \setminus \{x\}$ closest to a given point $x \in \omega_N$. Then, for every N sufficiently large,

$$\begin{aligned}
E_s^{v_N}(\omega_N) &= \sum_{x\in\omega_N}\sum_{y\in\omega_N\setminus\{x\}} \frac{v_N(x,y)}{|x-y|^s} \geq \sum_{x\in\omega_N\setminus\omega_{N,C}} \frac{\Phi\left(|x-y_x|\, r_N^{-1}\right) w(x,y_x)}{|x-y_x|^s} \\
&\geq \sum_{x\in\omega_N\setminus\omega_{N,C}} \frac{\overline{\Phi}\left(CN^{-1/d} r_N^{-1}\right) w(x,y_x)}{|x-y_x|^s} \geq h\overline{\Phi}\left(\frac{C}{C_N}\right) \sum_{x\in\omega_N\setminus\omega_{N,C}} \frac{1}{|x-y_x|^s} \\
&\geq \#(\omega_N\setminus\omega_{N,C}) \cdot hC^{-s}\overline{\Phi}\left(\frac{C}{C_N}\right) N^{s/d}.
\end{aligned}$$

Consequently,

$$\begin{aligned}
g_{s,d}^w(A) &= \lim_{N\to\infty} \frac{\mathcal{E}_s^w(A,N)}{N^{1+s/d}} \geq \limsup_{N\to\infty} \frac{\mathcal{E}_s^{v_N}(A,N)}{N^{1+s/d}} \\
&= \limsup_{N\to\infty} \frac{E_s^{v_N}(\omega_N)}{N^{1+s/d}} \geq hC^{-s} \limsup_{N\to\infty} \frac{\#(\omega_N\setminus\omega_{N,C})}{N}.
\end{aligned} \tag{44}$$

By Theorem 2.1, since $\mathcal{H}_d(A) > 0$, the quantity $g^w_{s,d}(A)$ is finite. Hence, from (44), we have

$$\liminf_{N\to\infty} \frac{\#\omega_{N,C}}{N} \geq 1 - C^s h^{-1} g^w_{s,d}(A), \tag{45}$$

which completes Step 1.

To proceed with Step 2, let $\delta = C^{4d}$. In view of Lemma 4.2, there exist compact sets $K_1, K_2, \dots, K_m \subset \mathbb{R}^d$ and bi-Lipschitz mappings $\psi_i : K_i \to \mathbb{R}^p$ with bi-Lipschitz constant λ, $i = 1, \dots, m$, such that the set

$$D := \bigcup_{i=1}^m \psi_i(K_i)$$

is contained in A and satisfies

$$\mathcal{H}_d(D) > \mathcal{H}_d(A) - \delta.$$

Moreover, $\psi_i(K_i)$, $i = 1, \dots, m$, are pairwise disjoint. Since each set $\psi_i(K_i)$ is d-rectifiable, the set D is also d-rectifiable, and by Theorem 4.1,

$$\mathcal{M}_d(D) = \mathcal{H}_d(D) > \mathcal{H}_d(A) - \delta = \mathcal{M}_d(A) - \delta.$$

Let $h_N := C^2/(3N^{1/d})$, $\quad N \in \mathbb{N}$, and recall that $A(\epsilon)$ denotes the ϵ-neighborhood of a set A in $\mathbb{R}^p$. Then for every N sufficiently large,

$$\mathcal{L}_p\left(A(h_N) \setminus D(h_N)\right) = \mathcal{L}_p\left(A(h_N)\right) - \mathcal{L}_p\left(D(h_N)\right) \leq$$

$$\leq \beta_{p-d}\left(\mathcal{M}_d(A) + \delta\right) h_N^{p-d} - \beta_{p-d}\left(\mathcal{M}_d(D) - \delta\right) h_N^{p-d} \leq 3\delta\beta_{p-d} h_N^{p-d}.$$

Let $\widetilde{\eta}_{N,C} := \omega_{N,C} \setminus D(3h_N)$ and

$$F_N = \bigcup_{x\in\widetilde{\eta}_{N,C}} B(x, h_N), \quad N \in \mathbb{N}.$$

Then $F_N \subset A(h_N) \setminus D(h_N)$. Since for every $x, y \in \omega_{N,C}$, $x \neq y$, we have

$$|x - y| \geq CN^{-1/d} \geq C^2 N^{-1/d} = 3h_N,$$

the collection $\{B(x, h_N) : x \in \widetilde{\eta}_{N,C}\}$, is pairwise disjoint. Thus

$$\#\widetilde{\eta}_{N,C} = (\beta_p h_N^p)^{-1}\mathcal{L}_p(F_N) \leq (\beta_p h_N^p)^{-1}\mathcal{L}_p\left(A(h_N) \setminus D(h_N)\right) \leq$$

$$\leq 3\delta\beta_{p-d} h_N^{p-d} (\beta_p h_N^p)^{-1} = 3^{d+1}\beta_{p-d}\beta_p^{-1} C^{2d} N. \tag{46}$$

Setting $\eta_{N,C} := \omega_{N,C} \cap D(3h_N)$, it follows from (46), (45), and (43), that

$$\liminf_{N\to\infty} \frac{\#\eta_{N,C}}{N} \geq 1 - C^s h^{-1} g^w_{s,d}(A) - 3^{d+1}\beta_{p-d}\beta_p^{-1} C^{2d} = 1 - \alpha_C, \tag{47}$$

which completes Step 2.

For the next step, let $z : \eta_{N,C} \to D$ be a mapping, where $z(x)$, $x \in \eta_{N,C}$, is a point in D such that $|z(x) - x| < 3h_N$. Then

$$|z(x) - x| < C^2 N^{-1/d} \leq C\delta(\omega_{N,C}) \leq C\delta(\eta_{N,C}), \quad x \in \eta_{N,C},$$

and for every pair of distinct points $x, y \in \eta_{N,C}$, we have

$$|z(x) - z(y)| \geq |x - y| - |z(x) - x| - |z(y) - y| \geq$$

$$\geq |x - y| - 2C\delta(\eta_{N,C}) \geq (1 - 2C)\,|x - y| > 0,$$

which implies that z is an injective mapping. Similarly,

$$|z(x) - z(y)| \leq (1 + 2C)\,|x - y|\,, \quad x, y \in \eta_{N,C}, \quad x \neq y,$$

completing Step 3.

We now consider Step 4. Let $\xi_N := (1-2C)\sqrt{C_N}N^{-1/d}$ and $z_{N,C} := z(\eta_{N,C}) = \{z(x) : x \in \eta_{N,C}\}$. Then since w was assumed to be bounded, we have

$$\begin{aligned}
\Pi_s^w(\eta_{N,C}) :=& \sum_{\substack{x,y\in\eta_{N,C}\\ |x-y|>\sqrt{C_N}N^{-1/d}}} \frac{w(x,y)}{|y-x|^s} \leq \|w\|_\infty \sum_{\substack{x,y\in\eta_{N,C}\\ |x-y|>\sqrt{C_N}N^{-1/d}}} \frac{1}{|y-x|^s}\\
&\leq (1+2C)^s\|w\|_\infty \sum_{\substack{x,y\in\eta_{N,C}\\ |x-y|>\sqrt{C_N}N^{-1/d}}} \frac{1}{|z(x)-z(y)|^s}\\
&\leq (1+2C)^s\|w\|_\infty \sum_{\substack{x,y\in z_{N,C}\\ |x-y|>\xi_N}} \frac{1}{|y-x|^s}.
\end{aligned}$$

Let $G_i = \psi_i^{-1}(z_{N,C}) \cap K_i$, $i = 1, \ldots, m$. Then

$$\delta(G_i) \geq \frac{1-2C}{\lambda}\delta(\eta_{N,C}) \geq \theta_N := \frac{C(1-2C)}{\lambda N^{1/d}}$$

and since $\psi_i(K_i)$ are pairwise disjoint, $\sum_{i=1}^m (\#G_i) = \#\eta_{N,C}$. Since

$$\tau := \min_{1\leq i\neq j\leq m} \operatorname{dist}(\psi_i(K_i), \psi_j(K_j)) > 0,$$

and $G_i \subset \mathbb{R}^d$, $i = 1, \dots, m$, taking into account Lemma 5.2, we have, for N sufficiently large, with $\sigma_w^s := (1+2C)^s \|w\|_\infty$

$$\begin{aligned}
\Pi_s^w(\eta_{N,C}) &\le \sigma_w^s \left(\sum_{i=1}^m \sum_{\substack{x,y \in z_{N,C} \cap \psi_i(K_i) \\ |x-y| > \xi_N}} \frac{1}{|y-x|^s} + \sum_{\substack{x,y \in z_{N,C} \\ |x-y| \ge \tau}} \frac{1}{|y-x|^s} \right) \\
&\le \sigma_w^s \left(\lambda^s \sum_{i=1}^m \sum_{\substack{x,y \in z_{N,C} \cap \psi_i(K_i) \\ |y-x| > \xi_N}} \frac{1}{\left|\psi_i^{-1}(x) - \psi_i^{-1}(y)\right|^s} + \tau^{-s} N^2 \right) \\
&\le \sigma_w^s \left(\lambda^s \sum_{i=1}^m \sum_{x \in G_i} \sum_{\substack{y \in G_i \\ |y-x| > \xi_N/\lambda}} \frac{1}{|x-y|^s} + \tau^{-s} N^2 \right) \\
&\le \sigma_w^s \left(\lambda^s \sum_{i=1}^m \sum_{x \in G_i} \frac{d5^d}{\theta_N^s} \sum_{j = \left[\frac{\xi_N}{\lambda \theta_N}\right]}^{\infty} \frac{1}{j^{s-d+1}} + \tau^{-s} N^2 \right) \\
&= \sigma_w^s \left(\lambda^{2s} \sum_{i=1}^m \frac{d5^d (\# G_i) N^{s/d}}{C^s (1-2C)^s} \sum_{j = \left[\sqrt{C_N}/C\right]}^{\infty} \frac{1}{j^{s-d+1}} + \tau^{-s} N^2 \right) \\
&= \sigma_w^s \left(\lambda^{2s} \frac{d5^d (\# \eta_{N,C}) o(N^{s/d})}{C^s (1-2C)^s} + o(N^{1+s/d}) \right) \\
&= o(N^{1+s/d}), \qquad N \to \infty,
\end{aligned}$$

which completes Step 4.

For the last step, we use the above estimates to obtain

$$\begin{aligned}
E_s^{v_N}(\omega_N) \ge E_s^{v_N}(\eta_{N,C}) &\ge \sum_{\substack{x,y \in \eta_{N,C},\ x \ne y \\ |x-y| \le \sqrt{C_N}/N^{1/d}}} \frac{\Phi\left(\frac{|x-y|}{r_N}\right) w(x,y)}{|x-y|^s} \\
&\ge \overline{\Phi}\left(\frac{1}{\sqrt{C_N}}\right) \sum_{\substack{x,y \in \eta_{N,C},\ x \ne y \\ |x-y| \le \sqrt{C_N}/N^{1/d}}} \frac{w(x,y)}{|x-y|^s} \\
&= \overline{\Phi}\left(\frac{1}{\sqrt{C_N}}\right) \left(E_s^w(\eta_{N,C}) - \Pi_s^w(\eta_{N,C})\right) \\
&\ge \overline{\Phi}\left(\frac{1}{\sqrt{C_N}}\right) \left(\mathcal{E}_s^w(A, \# \eta_{N,C}) + o(N^{1+s/d})\right), \quad N \to \infty.
\end{aligned} \tag{48}$$

Then, taking into account Theorem 2.1, relations (41) and (47) and the fact that $\lim_{t\to 0^+}\overline{\Phi}(t)=1$, we have

$$\begin{aligned}\underline{g}^{\mathbf{v}}_{s,d}(A) &= \liminf_{N\to\infty}\ \frac{\mathcal{E}_s^{v_N}(A,N)}{N^{1+s/d}} = \liminf_{N\to\infty}\frac{E_s^{v_N}(\omega_N)}{N^{1+s/d}}\\ &\geq \liminf_{N\to\infty}\frac{\overline{\Phi}\left(\frac{1}{\sqrt{C_N}}\right)\mathcal{E}_s^{w}(A,\#\eta_{N,C})}{N^{1+s/d}}\\ &\geq \lim_{N\to\infty}\frac{\mathcal{E}_s^{w}(A,\#\eta_{N,C})}{(\#\eta_{N,C})^{1+s/d}}\cdot\liminf_{N\to\infty}\left(\frac{\#\eta_{N,C}}{N}\right)^{1+s/d}\\ &\geq \frac{C_{s,d}}{\mathcal{H}_d^{s,w}(A)^{s/d}}\,(1-\alpha_C)^{1+s/d}.\end{aligned}$$

Letting $C\to 0$ gives $\underline{g}^{\mathbf{v}}_{s,d}(A)\geq C_{s,d}/\mathcal{H}_d^{s,w}(A)^{s/d}$, completing Step 5. Taking into account (39), we obtain relation (37) for the case of bounded CPD-weight w.

Unbounded weight. We now prove (37) for an arbitrary (not necessarily bounded) CPD-weight w on $A\times A$. Let

$$w^M(x,y) := \min\{w(x,y),M\},\quad x,y\in A,\quad M>0.$$

It is not difficult to see that w^M is also a CPD-weight function on $A\times A$. Let $\mathbf{u}=\{u_N\}$ denote the sequence of 'truncated' weights

$$u_N(x,y) := \Phi\left(\frac{|x-y|}{r_N}\right)w^M(x,y),\quad x,y\in A,\quad x\neq y,\quad N\in\mathbb{N}.$$

As shown above (37) holds for bounded CPD-weights, and hence, for every $M>0$, we have

$$\underline{g}^{\mathbf{v}}_{s,d}(A)\geq g^{\mathbf{u}}_{s,d}(A) = C_{s,d}\left(\int_A (w^M(x,x))^{-d/s}\mathrm{d}\mathcal{H}_d(x)\right)^{-s/d}.$$

Letting $M\to\infty$, we obtain from the Monotone Convergence Theorem that

$$\underline{g}^{\mathbf{v}}_{s,d}(A)\geq g^{w}_{s,d}(A) = C_{s,d}\left(\int_A (w(x,x))^{-d/s}\mathrm{d}\mathcal{H}_d(x)\right)^{-s/d} = \frac{C_{s,d}}{[\mathcal{H}_d^{s,w}(A)]^{s/d}}.$$

Together with (39), we get (37) for the case of an unbounded weight.

Remark. It is easy to see that (37) holds if r_N is only defined for a subsequence $\mathcal{N}\subset\mathbb{N}$, a fact that we shall use in the next part of the proof. In this case, we shall also use $g^{\mathbf{v}}_{s,d}(A)$ to denote the limit along this subsequence.

We next prove the limit distribution assertion in Proposition 5.1. Let $\{\omega_N\}$ be an asymptotically $(\mathbf{v},s)$-energy minimizing sequence of N-point configurations on A. It might appear to the reader that a simple argument would show that $\{\omega_N\}$ is also asymptotically (w,s)-energy minimizing so that the limiting distribution statement in Theorem 2.1 may be applied. However, the authors have not as yet found such an argument. Instead, we adapt methods in [10] and [4] to the varying weight case.

Let B be an arbitrary *almost clopen* subset of A, that is, the boundary $\partial_A B$ of B relative to A has $\mathcal{H}_d^{s,w}$-measure zero. Since B is an arbitrary almost clopen subset of A, the condition that ω_N is uniformly distributed with respect to $h_d^{s,w}$ is equivalent to

$$\lim_{N\to\infty} \frac{\#(\omega_N \cap B)}{N} = h_d^{s,w}(B). \tag{49}$$

By Lemma 4.3, both the closure $\overline{B}$ of B and the closure $\overline{D}$ of $D := A \setminus B$ are compact $(\mathcal{H}_d, d)$-rectifiable sets, for which the d-dimensional Minkowski content exists and coincides with the $\mathcal{H}_d$-measure.

We consider the case $0 < \mathcal{H}_d^{s,w}(B) < \mathcal{H}_d^{s,w}(A)$ and leave the cases $\mathcal{H}_d^{s,w}(B) = 0$ or $\mathcal{H}_d^{s,w}(B) = \mathcal{H}_d^{s,w}(A)$ to the reader. Then both $\mathcal{H}_d^{s,w}(\overline{B})$ and $\mathcal{H}_d^{s,w}(\overline{D})$ are positive. Let $\mathcal{N} \subset \mathbb{N}$ be an infinite subset such that the limit

$$\alpha := \lim_{\mathcal{N}\ni N\to\infty} \frac{\#(\omega_N \cap B)}{N} \tag{50}$$

exists. Denote $N_B = \#(\omega_N \cap B)$ and $N_D = \#(\omega_N \setminus B)$. Then for every $N \in \mathcal{N}$, we have

$$E_s^{v_N}(\omega_N) \geq E_s^{v_N}(\omega_N \cap B) + E_s^{v_N}(\omega_N \setminus B) \geq \mathcal{E}_s^{v_N}(\overline{B}, N_B) + \mathcal{E}_s^{v_N}(\overline{D}, N_D).$$

If $\alpha \in (0,1]$, denote by $\mathcal{N}_1 \subset \mathcal{N}$ an infinite subset such that the sequence $\{\#(\omega_N \cap B)\}_{N\in\mathcal{N}_1}$ is strictly increasing. Let also $\mathcal{M}_1 = \{\#(\omega_N \cap B) : N \in \mathcal{N}_1\}$.

If $\alpha \in [0,1)$, we further let $\mathcal{N}_2 \subset \mathcal{N}_1$ (if $\alpha = 0$, let $\mathcal{N}_2 \subset \mathcal{N}$) be an infinite subset such that the sequence $\{\#(\omega_N \setminus B)\}_{N\in\mathcal{N}_2}$ is strictly increasing. Let also $\mathcal{M}_2 = \{\#(\omega_N \setminus B) : N \in \mathcal{N}_2\}$.

Denote by $n(M)$, $M \in \mathcal{M}_1$, the unique integer from $\mathcal{N}_1$ such that $\#(\omega_{n(M)} \cap B) = M$ and let $k(M)$, $M \in \mathcal{M}_2$ be the unique integer from $\mathcal{N}_2$ such that $\#(\omega_{k(M)} \setminus B) = M$. Note that if $\alpha \in (0,1]$, in view of assumption (50),

$$r_{n(M)} = \frac{C_{n(M)}}{n(M)^{1/d}} = \frac{\alpha^{1/d} C_{n(M)}}{M^{1/d}}(1 + o(1)), \quad \mathcal{M}_1 \ni M \to \infty,$$

where $C_{n(M)} \to \infty$, $\mathcal{M}_1 \ni M \to \infty$. Analogously, if $\alpha \in [0,1)$, we have

$$r_{k(M)} = \frac{C_{k(M)}}{k(M)^{1/d}} = \frac{(1-\alpha)^{1/d} C_{k(M)}}{M^{1/d}}(1 + o(1)), \quad \mathcal{M}_2 \ni M \to \infty,$$

where $C_{k(M)} \to \infty$, $\mathcal{M}_2 \ni M \to \infty$.

In view of relation (37), for any positive sequence $\{\kappa_N\}$ satisfying $\lim_{N\to\infty} \kappa_N N^{1/d} = \infty$, we have

$$g_{s,d}^{\mathbf{u}}(V) = g_{s,d}^{w}(V) = \frac{C_{s,d}}{[\mathcal{H}_d^{s,w}(V)]^{s/d}}, \quad (V = \overline{B} \text{ or } V = \overline{D}), \tag{51}$$

where $\mathbf{u} = \{u_N\}$ is given by $u_N(x,y) = \Phi\left(|x-y|/\kappa_N\right) w(x,y)$.

Suppose $\alpha \in (0,1)$. Applying relation (37) to the set A, using (51) with $\kappa_M = r_{n(M)}$ for $M \in \mathcal{M}_1$ (respectively, $\kappa_M = r_{k(M)}$ for $M \in \mathcal{M}_2$) and $V = \overline{B}$ (respectively, $\overline{D}$), and taking into account that $\mathcal{N}_2 \subset \mathcal{N}_1$, we obtain

$$\begin{aligned}
\frac{C_{s,d}}{[\mathcal{H}_d^{s,w}(A)]^{s/d}} &= \lim_{N\to\infty} \frac{E_s^{v_N}(\omega_N)}{N^{1+s/d}} = \lim_{\mathcal{N}_2 \ni N\to\infty} \frac{E_s^{v_N}(\omega_N)}{N^{1+s/d}} \\
&\geq \liminf_{\mathcal{N}_2 \ni N\to\infty} \frac{\mathcal{E}_s^{v_N}(\overline{B}, N_B)}{N_B^{1+s/d}} \cdot \left(\frac{N_B}{N}\right)^{1+s/d} \\
&\qquad + \liminf_{\mathcal{N}_2 \ni N\to\infty} \frac{\mathcal{E}_s^{v_N}(\overline{D}, N_D)}{N_D^{1+s/d}} \cdot \left(\frac{N_D}{N}\right)^{1+s/d} \\
&\geq \alpha^{1+s/d} \liminf_{\mathcal{N}_1 \ni N\to\infty} \frac{\mathcal{E}_s^{v_N}(\overline{B}, N_B)}{N_B^{1+s/d}} \\
&\qquad + (1-\alpha)^{1+s/d} \liminf_{\mathcal{N}_2 \ni N\to\infty} \frac{\mathcal{E}_s^{v_N}(\overline{D}, N_D)}{N_D^{1+s/d}} \\
&= \alpha^{1+s/d} \lim_{\mathcal{M}_1 \ni M\to\infty} \frac{\mathcal{E}_s^{v_{n(M)}}(\overline{B}, M)}{M^{1+s/d}} \\
&\qquad + (1-\alpha)^{1+s/d} \lim_{\mathcal{M}_2 \ni M\to\infty} \frac{\mathcal{E}_s^{v_{k(M)}}(\overline{D}, M)}{M^{1+s/d}} \\
&= C_{s,d}\left(\frac{\alpha^{1+s/d}}{\mathcal{H}_d^{s,w}(B)^{s/d}} + \frac{(1-\alpha)^{1+s/d}}{\mathcal{H}_d^{s,w}(D)^{s/d}}\right) =: F(\alpha).
\end{aligned}$$

We remark that if $\alpha = 0$ or $\alpha = 1$, then appropriate terms may be dropped and the final inequality still holds. Furthermore, it is not difficult to see that the minimum value of F on [0,1] is given by $C_{s,d}[\mathcal{H}_d^{s,w}(A)]^{-s/d}$ and occurs only at the point

$$\widetilde{\alpha} := \frac{\mathcal{H}_d^{s,w}(B)}{\mathcal{H}_d^{s,w}(B) + \mathcal{H}_d^{s,w}(D)} = h_d^{s,w}(B).$$

Hence, the above inequality shows $\alpha = \widetilde{\alpha}$. Since $\mathcal{N} \subset \mathbb{N}$ is arbitrary, we obtain (49), which completes the proof of Proposition 5.1.

□

We shall use the following corollary in the proof of Theorem 2.3.

Corollary 5.3. *Let $s > d$, $A \subset \mathbb{R}^p$, $p \geq d$, be a compact $(\mathcal{H}_d, d)$-rectifiable set with $\mathcal{H}_d(A) = \mathcal{M}_d(A) > 0$, w be a CPD-weight function on $A \times A$, and $\{r_N\}$ be a positive sequence satisfying (6). For any asymptotically (w,s)-energy minimizing sequence $\{\omega_N\}$ of point configurations on A such that $\#\omega_N = N$, there holds*

$$P_s^w(\omega_N, r_N) := \sum_{\substack{x,y\in\omega_N \\ |x-y|>r_N}} \frac{w(x,y)}{|x-y|^s} = o(N^{1+s/d}), \quad N \to \infty.$$

Proof. Let $\Phi_0 := \chi_{[0,1]}$ be the characteristic function of $[0,1]$ and let $\mathbf{v} = \{v_N\}$ be as in Proposition 5.1 with Φ replaced by Φ_0. Since $\{\omega_N\}$ is an asymptotically (w,s)-energy minimizing, it is also asymptotically $(\mathbf{v},s)$-energy minimizing. Observing that

$$E_s^w(\omega_N) = E_s^{v_N}(\omega_N) + P_s^w(\omega_N, r_N), \quad (N \in \mathbb{N})$$

and applying Proposition 5.1 completes the proof. □

6. Proof of Theorems 2.2 and 2.3.

We shall first prove Theorem 2.3 from which we will deduce Theorem 2.2.

Proof of Theorem 2.3. We first show that condition (12) implies that there is a positive sequence $\{r_N\}$ satisfying (6) such that

$$\lim_{N\to\infty} I^w(v_N, r_N) = \lim_{N\to\infty} S^w(v_N, r_N) = 1. \tag{52}$$

Indeed, for every $K \in \mathbb{N}$, one can choose a number $N_K \in \mathbb{N}$ such that

$$\left|I^w(v_N, KN^{-1/d}) - 1\right| < \frac{1}{K}, \quad \text{for every} \quad N > N_K,$$

and that $N_1 < N_2 < N_3 < \ldots$. Furthermore, we can increase each N_k so that $N_k > k^{d+1}$ and $\{N_k\}$ is still an increasing sequence. Define a sequence $\{C_N\}$ in the following way. Let $C_1, \ldots, C_{N_1}$ be arbitrary positive numbers and let $C_N := 1$ for $N_1 < N \leq N_2$, $C_N := 2$ for $N_2 < N \leq N_3$, ..., $C_N := m$ for $N_m < N \leq N_{m+1}$, ... Then since $N > N_{C_N}$ for every $N > N_1$, we have

$$\left|I^w(v_N, C_N N^{-1/d}) - 1\right| < \frac{1}{C_N}, \quad \text{for every} \quad N > N_1.$$

Since $C_N \to \infty$, $N \to \infty$, we have

$$\lim_{N\to\infty} I^w(v_N, \tau_N) = 1,$$

where $\tau_N := C_N N^{-1/d}$. Since $\tau_N = C_N N^{-1/d} < C_N N_{C_N}^{-1/d} < C_N^{-1/d}$, we have $\tau_N \to 0$ as $N \to \infty$. Analogously, one can show that there is a positive sequence $\{\kappa_N\}$ satisfying (6) such that $k_N \to 0$ as $N \to \infty$ and

$$\lim_{N\to\infty} S^w(v_N, \kappa_N) = 1.$$

Then $r_N := \min\{\tau_N, \kappa_N\}$, for $N \in \mathbb{N}$, satisfies (6), $r_N \to 0$ as $N \to \infty$, and

$$I^w(v_N, \tau_N) \leq I^w(v_N, r_N) \leq S^w(v_N, r_N) \leq S^w(v_N, \kappa_N),$$

which implies (52).

For $N \in \mathbb{N}$, and $x, y \in A$, we define $\mathbf{u}^0 = \{u_N^0\}$ by

$$u_N^0(x,y) := \Phi_0\left(\frac{|x-y|}{r_N}\right) w(x,y), \tag{53}$$

where we recall that $\Phi_0 = \chi_{[0,1]}$. It is not difficult to see that for any sequence $\{\omega_N\}$ of N-point configurations on A we have, for N sufficiently large, that

$$\begin{aligned} E_s^{v_N}(\omega_N) &\geq \sum_{\substack{x,y\in\omega_N \\ 0<|x-y|\leq r_N}} \frac{v_N(x,y)}{|x-y|^s} \geq I^w(v_N, r_N) \sum_{\substack{x,y\in\omega_N \\ 0<|x-y|\leq r_N}} \frac{w(x,y)}{|x-y|^s} \\ &= I^w(v_N, r_N) \sum_{\substack{x,y\in\omega_N \\ x\neq y}} \frac{u_N^0(x,y)}{|x-y|^s} \\ &= I^w(v_N, r_N) E_s^{u_N^0}(\omega_N) \geq I^w(v_N, r_N)\mathcal{E}_s^{u_N^0}(A, N). \end{aligned} \tag{54}$$

Let $\{\overline{\omega}_N\}$ be an asymptotically $(\mathbf{v}, s)$-energy minimizing sequence of N-point configurations on A. Then by (52) and Proposition 5.1,

$$\liminf_{N\to\infty} \frac{E_s^{v_N}(\overline{\omega}_N)}{N^{1+s/d}} \geq \lim_{N\to\infty} \frac{I^w(v_N, r_N)\mathcal{E}_s^{u_N^0}(A, N)}{N^{1+s/d}} = \frac{C_{s,d}}{[\mathcal{H}_d^{s,w}(A)]^{s/d}}. \tag{55}$$

On the other hand, if $\{\omega'_N\}$ is an asymptotically (w, s)-energy minimizing sequence of N-configurations on A, by Corollary 5.3, we obtain

$$\limsup_{N\to\infty} \frac{E_s^{v_N}(\overline{\omega}_N)}{N^{1+s/d}} = \limsup_{N\to\infty} \frac{\mathcal{E}_s^{v_N}(A, N)}{N^{1+s/d}} \leq \limsup_{N\to\infty} \frac{E_s^{v_N}(\omega'_N)}{N^{1+s/d}}.$$

Then by Corollary 5.3, we have

$$\begin{aligned} E_s^{v_N}(\omega'_N) &= \sum_{\substack{x,y\in\omega'_N \\ 0<|x-y|\leq r_N}} \frac{v_N(x,y)}{|x-y|^s} + \sum_{\substack{x,y\in\omega'_N \\ |x-y|>r_N}} \frac{v_N(x,y)}{|x-y|^s} \leq \\ &\leq S^w(v_N, r_N) \sum_{\substack{x,y\in\omega'_N \\ 0<|x-y|\leq r_N}} \frac{w(x,y)}{|x-y|^s} + C \sum_{\substack{x,y\in\omega'_N \\ |x-y|>r_N}} \frac{w(x,y)}{|x-y|^s} \leq \\ &\leq S^w(v_N, r_N)E_s^w(\omega'_N) + o(N^{1+s/d}), \quad N\to\infty. \end{aligned}$$

Thus from (52) and the fact that $\{\omega'_N\}$ is asymptotically (w, s)-energy minimizing, we obtain

$$\limsup_{N\to\infty} \frac{E_s^{v_N}(\overline{\omega}_N)}{N^{1+s/d}} \leq \lim_{N\to\infty} \frac{S^w(v_N, r_N)E_s^w(\omega'_N)}{N^{1+s/d}} = \frac{C_{s,d}}{[\mathcal{H}_d^{s,w}(A)]^{s/d}}.$$

Taking into account (55), it follows that

$$\lim_{N\to\infty} \frac{\mathcal{E}_s^{v_N}(A, N)}{N^{1+s/d}} = \lim_{N\to\infty} \frac{E_s^{v_N}(\overline{\omega}_N)}{N^{1+s/d}} = \frac{C_{s,d}}{[\mathcal{H}_d^{s,w}(A)]^{s/d}},$$

which proves (13).

To prove the assertion of Theorem 2.3 on the limiting distribution, we use (13) and (54) and obtain that

$$\frac{C_{s,d}}{[\mathcal{H}_d^{s,w}(A)]^{s/d}} = \lim_{N\to\infty} \frac{E_s^{v_N}(\overline{\omega}_N)}{N^{1+s/d}} \geq \limsup_{N\to\infty} \frac{I^w(v_N, r_N)E_s^{u_N^0}(\overline{\omega}_N)}{N^{1+s/d}} \geq$$

$$\geq \liminf_{N\to\infty} \frac{E_s^{u_N^0}(\overline{\omega}_N)}{N^{1+s/d}} \geq \lim_{N\to\infty} \frac{\mathcal{E}_s^{u_N^0}(A,N)}{N^{1+s/d}} = \frac{C_{s,d}}{[\mathcal{H}_d^{s,w}(A)]^{s/d}},$$

which implies that the sequence $\{\overline{\omega}_N\}$ is also asymptotically $(\mathbf{u}^0, s)$-energy minimizing. By Proposition 5.1, we obtain that the sequence $\{\overline{\omega}_N\}$ is asymptotically uniformly distributed with respect to the measure $\mathcal{H}_d^{s,w}$, which completes the proof of Theorem 2.3. □

We next provide the proof of Theorem 2.2.

Proof of Theorem 2.2. With v_N defined as in (7), the boundedness of the function Φ implies that (11) holds. We next verify that condition (12) is also satisfied. Let a be a positive constant and assume N is sufficiently large. If $(x, y) \in A \times A$ is such that $0 < |x - y| \leq aN^{-1/d}$, then

$$\frac{v_N(x,y)}{w(x,y)} = \Phi\left(\frac{|x-y|}{r_N}\right) \geq \overline{\Phi}\left(\frac{a}{N^{1/d} r_N}\right),$$

where the function $\overline{\Phi}$ is defined in (40). Hence,

$$I^w\left(v_N, aN^{-1/d}\right) \geq \overline{\Phi}\left(\frac{a}{N^{1/d} r_N}\right), \tag{56}$$

for every N sufficiently large. On the other hand, with

$$\widetilde{\Phi}(t) := \sup_{u\in(0,t]} \Phi(u), \quad t > 0,$$

we have for $(x, y) \in A \times A$, $0 < |x - y| \leq aN^{-1/d}$ that

$$\frac{v_N(x,y)}{w(x,y)} = \Phi\left(\frac{|x-y|}{r_N}\right) \leq \widetilde{\Phi}\left(\frac{a}{N^{1/d} r_N}\right).$$

Consequently, for every N sufficiently large, we have

$$S^w\left(v_N, aN^{-1/d}\right) \leq \widetilde{\Phi}\left(\frac{a}{N^{1/d} r_N}\right). \tag{57}$$

Since $\lim_{t\to 0^+} \overline{\Phi}(t) = \lim_{t\to 0^+} \widetilde{\Phi}(t) = 1$, letting $N \to \infty$ in (56) and (57), we obtain condition (12). Then applying Theorem 2.3 we obtain Theorem 2.2. □

7. Proof of Theorems 2.4 and 2.5

Throughout this section we shall assume that $A \subset \mathbb{R}^p$ is a compact set with $\mathcal{H}_d(A) > 0$. We first note that Frostman's lemma (cf. [14, Theorem 8.8]) implies that there is a Borel measure μ on $\mathbb{R}^p$ with support contained in A such that $0 < \mu(A) < \infty$ and

$$\mu(B(x,r)) \leq r^d, \quad x \in \mathbb{R}^p, \quad r > 0. \tag{58}$$

The proof of Theorem 2.4 follows arguments from [4], which in turn, use a technique from [12]. Also see [11]. We shall appeal to the following lemma whose proof follows standard arguments as in [12].

Lemma 7.1. *Let* $\omega = \{x_1, \ldots, x_N\}$ *be a point configuration on* A *with* μ *satisfying* (58), $r_0 := (\mu(A)/(2N))^{1/d}$,

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

and

$$U_i(\omega, x) := \sum_{j:j\neq i} \frac{1}{|x - x_j|^s}, \quad x \notin \omega \setminus \{x_i\}, \quad i = 1, \ldots, N.$$

Then for any $s > d$ *and* $N \in \mathbb{N}$,

$$\frac{1}{\mu(D_i)} \int_{D_i} U_i(\omega, x) \mathrm{d}\mu(x) \leq \frac{s}{(s-d)} \left(\frac{2N}{\mu(A)}\right)^{s/d}, \quad i = 1, \ldots, N.$$

Proof of Theorem 2.4. Denote by $\widetilde{x}_1, \ldots, \widetilde{x}_N$ the points in the (v_N, s)-energy minimizing configurations ω_N^s and let

$$U_{i,N}(x) := \sum_{j:j\neq i} \frac{v_N(\widetilde{x}_j, x)}{|x - \widetilde{x}_j|^s}, \quad x \in A, \quad i = 1, \ldots, N.$$

Let $M > 0$ be a number such that $v_N(x, y) \leq M$, $x, y \in A$, $N \in \mathbb{N}$. Then for every $i = 1, \ldots, N$, since ω_N^s is energy minimizing, we have

$$E_s^{v_N}(\omega_N^s \setminus \{\widetilde{x}_i\}) + 2U_{i,N}(\widetilde{x}_i) = E_s^{v_N}(\omega_N^s) \leq E_s^{v_N}((\omega_N^s \setminus \{\widetilde{x}_i\}) \cup \{x\}) =$$

$$= E_s^{v_N}(\omega_N^s \setminus \{\widetilde{x}_i\}) + 2U_{i,N}(x) \;\; x \in A, \;\; x \neq x_1, \ldots, x_N.$$

Hence,

$$U_{i,N}(\widetilde{x}_i) \leq U_{i,N}(x) = \sum_{j:j\neq i} \frac{v_N(\widetilde{x}_j, x)}{|\widetilde{x}_j - x|^s}$$

$$\leq \sum_{j:j\neq i} \frac{M}{|\widetilde{x}_j - x|^s}, \quad x \in A, \quad x \neq x_1, \ldots, x_N.$$

By Lemma 7.1, for $i = 1, \ldots, N$, we have

$$U_{i,N}(\widetilde{x}_i) \leq \frac{M}{\mu(D_i)} \int_{D_i} U_i(\omega_N^s, x) \mathrm{d}\mu(x) \leq \left(\frac{sM}{s-d}\right) \left(\frac{2N}{\mu(A)}\right)^{s/d}. \tag{59}$$

Clearly, it is sufficient to only consider N such that $\delta(\omega_N^s) < a_0 N^{-1/d}$. For such N, let $\widetilde{x}_p, \widetilde{x}_q \in \omega_N^s$ satisfy $|\widetilde{x}_p - \widetilde{x}_q| = \delta(\omega_N^s)$. Then for every N sufficiently large, using (16) and (59), we obtain

$$\frac{\alpha_0}{\delta(\omega_N^s)^s} \leq \frac{v_N(\widetilde{x}_p, \widetilde{x}_q)}{|\widetilde{x}_p - \widetilde{x}_q|^s} \leq \sum_{j:j\neq p} \frac{v_N(\widetilde{x}_p, \widetilde{x}_j)}{|\widetilde{x}_p - \widetilde{x}_j|^s} = U_{p,N}(\widetilde{x}_p) \leq \left(\frac{sM}{s-d}\right) \left(\frac{2N}{\mu(A)}\right)^{s/d},$$

which implies the result. □

Proof of Theorem 2.5. We shall adapt an argument given in [11]. Let $\omega_N^s = \{x_1, \ldots, x_N\}$ be an N-point (v_N, s)-energy minimizing configuration for the compact set A and, for $y \in A$, consider the function

$$U(y) := \frac{1}{N}\sum_{i=1}^{N} \frac{v_N(y, x_i)}{|y - x_i|^s}. \tag{60}$$

For fixed $1 \leq j \leq N$, the function $U(y)$ can be decomposed as

$$U(y) = \frac{1}{N}\frac{v_N(y, x_j)}{|y - x_j|^s} + \frac{1}{N}\sum_{\substack{i=1\\ i\neq j}}^{N} \frac{v_N(y, x_i)}{|y - x_i|^s}, \tag{61}$$

and, since ω_N^s is a minimizing configuration on A, the point x_j minimizes the sum over $i \neq j$ on the right-hand side of equation (61). Thus for each fixed j and $y \in A$

$$U(y) \geq \frac{1}{N}\frac{v_N(y, x_j)}{|y - x_j|^s} + \frac{1}{N}\sum_{\substack{i=1\\ i\neq j}}^{N} \frac{v_N(x_j, x_i)}{|x_j - x_i|^s}. \tag{62}$$

Summing over j gives

$$NU(y) \geq \frac{1}{N}\sum_{j=1}^{N} \frac{v_N(y, x_j)}{|y - x_j|^s} + \frac{1}{N}\sum_{j=1}^{N}\sum_{\substack{i=1\\ i\neq j}}^{N} \frac{v_N(x_j, x_i)}{|x_j - x_i|^s} \tag{63}$$

$$= U(y) + \frac{1}{N}\mathcal{E}_s^{v_N}(A, N), \tag{64}$$

and thus

$$U(y) \geq \frac{1}{N(N-1)}\mathcal{E}_s^{v_N}(A, N) \geq \frac{\mathcal{E}_s^{v_N}(A, N)}{N^2} \qquad (y \in A). \tag{65}$$

Since A is compact, there exists a point $y^* \in A$ such that

$$\min_{1\leq i\leq N} |y^* - x_i| = \rho(\omega_N^s, A) =: \rho(\omega_N^s). \tag{66}$$

Then, by (13) in Theorem 2.3, there is a constant $C_1 > 0$ and some positive integer N_0 such that

$$\mathcal{E}_s^{v_N}(A, N) \geq C_1 N^{1+s/d} \qquad (N \geq N_0). \tag{67}$$

Since (65) holds for the point y^* of (66), we combine (65) with (67) to obtain

$$U(y^*) \geq \frac{\mathcal{E}_s^{v_N}(A, N)}{N^2} \geq C_1 N^{s/d-1} \qquad (N \geq N_0). \tag{68}$$

In addition, by equation (17) of Theorem 2.4, there is some $C_2 > 0$ such that $\delta(\omega_N^s) \geq C_2 N^{-1/d}$ for $N \geq 2$.

Let $\mathcal{N}$ consist of those $N \geq N_0$ such that

$$\rho(\omega_N^s) \geq \frac{C_2}{2} N^{-1/d}. \tag{69}$$

If $\mathcal{N}$ is empty (or finite) then we are done. Assuming that $\mathcal{N}$ is infinite, let $N \in \mathcal{N}$ be fixed. For $0 < \epsilon < 1/2$, let

$$r_0 = r_0(N, \epsilon) := \epsilon\, C_2 N^{-1/d}. \tag{70}$$

Note that any two of the relative balls $\tilde{B}(x_i, r_0) := \tilde{A} \cap B(x_i, r_0)$, for $1 \le i \le N$, do not intersect since $r_0 < \delta(\omega_N^s)/2$. For any $x \in \tilde{B}(x_i, r_0)$, inequalities (66) and (69) imply

$$\begin{aligned} |x - y^*| &\le |x - x_i| + |x_i - y^*| \le r_0 + |x_i - y^*| \\ &\le 2\epsilon\, \rho(\omega_N^s) + |x_i - y^*| \le (1 + 2\epsilon)|x_i - y^*|. \end{aligned} \tag{71}$$

Now let μ denote a d-regular measure on $\tilde{A}$ satisfying (18) with positive constants c_0, C_0. For fixed $1 \le i \le N$, using (71) and taking an average value on $\tilde{B}(x_i, r_0)$ we obtain

$$\begin{aligned} \frac{v_N(x_i, y^*)}{|x_i - y^*|^s} &\le \frac{C_3(1+2\epsilon)^s}{\mu(\tilde{B}(x_i, r_0))} \int_{\tilde{B}(x_i, r_0)} \frac{d\mu(x)}{|x - y^*|^s} \\ &\le \frac{C_3\,(1+2\epsilon)^s\, c_0}{r_0^d} \int_{\tilde{B}(x_i, r_0)} \frac{d\mu(x)}{|x - y^*|^s}, \end{aligned} \tag{72}$$

where C_3 denotes the uniform bound of the v_N on $A \times A$.

Inequality (69) and definition (70) imply $2\epsilon\rho(\omega_N^s) \ge r_0$ and thus, for $x \in \tilde{B}(x_i, r_0)$, we obtain

$$\begin{aligned} |x - y^*| &\ge |x_i - y^*| - |x - x_i| \ge |x_i - y^*| - r_0 \\ &\ge |x_i - y^*| - 2\epsilon\, \rho(\omega_N^s) \ge (1 - 2\epsilon)\rho(\omega_N^s). \end{aligned} \tag{73}$$

Inequality (73) implies

$$\bigcup_{i=1}^{N} \tilde{B}(x_i, r_0) \subset \tilde{A} \setminus \tilde{B}(y^*, (1 - 2\epsilon)\rho(\omega_N^s)),$$

and since the left-hand side is a disjoint union, averaging the inequalities of (72) we have

$$\begin{aligned} U(y^*) &\le \frac{C_3\,(1+2\epsilon)^s\, c_0}{N\, r_0^d} \sum_{i=1}^{N} \int_{\tilde{B}(x_i, r_0)} \frac{d\mu(x)}{|x - y^*|^s} \\ &\le \frac{C_3\,(1+2\epsilon)^s\, c_0}{N\, r_0^d} \int_{\tilde{A} \setminus \tilde{B}(y^*, (1-2\epsilon)\rho(\omega_N^s))} \frac{d\mu(x)}{|x - y^*|^s}. \end{aligned} \tag{74}$$

Next we use the standard conversion of the integral with respect to μ to an integral with respect to Lebesgue measure (see e.g. [14, Theorem 1.15]) to obtain

$$\begin{aligned} \int_{\tilde{A} \setminus \tilde{B}(y^*, (1-2\epsilon)\rho(\omega_N^s))} \frac{d\mu(x)}{|x - y^*|^s} &= \int_0^\infty \mu\{x \in \tilde{A} : t < \frac{1}{|x - y^*|^s} < \frac{1}{[(1-2\epsilon)\rho(\omega_N^s)]^s}\}\, dt \\ &\le C_0 \int_0^{((1-2\epsilon)\rho(\omega_N^s))^{-s}} t^{-d/s} dt \\ &= \frac{C_0}{(1 - d/s)(1 - 2\epsilon)^{s-d}} \rho(\omega_N^s)^{d-s}. \end{aligned} \tag{75}$$

Let $N \in \mathcal{N}$. Relations (70), (74) and (75) imply

$$U(y^*) \leq \left(\frac{C_0 C_3 (1+2\epsilon)^s c_0}{(1-d/s)(1-2\epsilon)^{s-d}\epsilon^d C_2^d} \right) \rho(\omega_N^s)^{d-s}. \tag{76}$$

Choosing $\epsilon = (2(2(s/d)-1))^{-1} < \frac{1}{2}$ minimizes the right hand side of inequality (76) for ϵ in $(0,1/2)$ giving

$$U(y^*) \leq \left[\frac{4^d C_0 C_3 c_0 s^d}{(1-d/s)^{s-d+1}(dC_2)^d} \right] \rho(\omega_N^s)^{d-s}. \tag{77}$$

Using (68) and (77), we then obtain

$$\rho(\omega_N^s) \leq \left[\frac{4^d C_0 C_3 c_0 s^d}{(1-d/s)^{s-d+1} C_1 (dC_2)^d} \right]^{1/(s-d)} N^{-1/d}, \tag{78}$$

for any $N \in \mathcal{N}$. If $N \geq N_0$ is not in $\mathcal{N}$, then $\rho(\omega_N^s) < \frac{C_2}{2} N^{-1/d}$ and thus (19) holds. □

8. Proof of statements from Section 3

Proof of Proposition 3.1. Denote $a := \delta(\omega_N)/2$. For any distinct points $y_1, y_2 \in \omega_N$, we have $B(y_1, a) \cap B(y_2, a) = \emptyset$. Let μ be a d-regular measure on A satisfying (18) with constants c_0 and C_0, for every point $x \in \omega_N$. Then we have

$$\begin{aligned} \#(\omega_N \cap B(x,\delta_N)) \cdot c_0^{-1} a^d &\leq \sum_{y \in \omega_N \cap B(x,\delta_N)} \mu\left(A \cap B(y,a)\right) \\ &= \mu\left(\bigcup_{y \in \omega_N \cap B(x,\delta_N)} A \cap B(y,a) \right) \\ &\leq \mu\left(A \cap B\left(x, \delta_N + a\right)\right) \leq C_0 (\delta_N + a)^d. \end{aligned}$$

Taking into account relation (33) and the fact that $\delta_N N^{1/d} = C_N$, we have

$$\begin{aligned} Z(\omega_N, \delta_N) &\leq N \max_{x \in \omega_N} \#(\omega_N \cap B(x,\delta_N)) \\ &\leq C_0 c_0 N \left(\frac{2\delta_N}{\delta(\omega_N)} + 1 \right)^d = O(NC_N^d), \quad N \to \infty, \end{aligned}$$

which completes the proof of Proposition 3.1. □

Proof of Proposition 3.2. From the estimate

$$\begin{aligned} E_s(\omega) &\geq \sum_{x \in \omega} \sum_{\substack{y \in \omega \\ 0<|y-x|\leq \delta}} \frac{1}{|y-x|^s} \\ &\geq \sum_{x \in \omega} \delta^{-s} \#\{y \in \omega : 0 < |y-x| \leq \delta\} = \delta^{-s}(Z(\omega,\delta)). \end{aligned}$$

Then we have $Z(\omega,\delta) \leq \delta^s E_s(\omega)$. To prove the second part of the proposition, we write

$$Z(\omega_N, r_N) \leq C_N^s \frac{E_s(\omega_N)}{N^{s/d}} = O(NC_N^s), \quad N \to \infty.$$

Proposition 3.2 is proved.

□

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References

[1] J. Benedetto, M. Fickus, Finite normalized tight frames, *Adv. Comput. Math.* **18** (2003), 357–385.
[2] J. L. Bentley, D. F. Stanat, and E. H. Williams, The complexity of finding fixed-radius near neighbors, *Inform. Proc. Lett.*, **6**(6) (1977), 209–212.
[3] S.V. Borodachov, D. P. Hardin, E.B. Saff, Asymptotics of best-packing on rectifiable sets, *Proc. Amer. Math. Soc.*, **135** (2007), 2369–2380.
[4] S.V. Borodachov, D.P. Hardin, E.B. Saff, Asymptotics for discrete weighted minimal Riesz energy problems on rectifiable sets, *Trans. Amer. Math. Soc.*, **360** (2008), 1559-1580.
[5] M. Bowick, D.R. Nelson, A. Travesset, Interacting topological defects in frozen topographies, *Phys. Rev. B* **62** (2000), 8738–8751.
[6] J.S. Brauchart, D.P. Hardin, E.B. Saff, The next-order term for optimal Riesz and logarithmic energy asymptotics on the sphere, *Contemp. Math.*, **578** (2012), 31–61.
[7] B. Chazelle, An improved algorithm for the fixed-radius neighbor problem, *Inform. Proc. Lett.*, **16** (1983), 193–198.
[8] J.H. Conway, N.J.A. Sloane, *Sphere Packings, Lattices and Groups,* Springer Verlag, New York: 3rd ed., 1999.
[9] H. Federer, *Geometric Measure Theory*, Springer-Verlag, 1969.
[10] D.P. Hardin, E.B. Saff, Minimal Riesz energy point configurations for rectifiable d-dimensional manifolds, *Adv. Math.*, **193** (2005), no. 1, 174–204.
[11] D. P. Hardin, E. B. Saff, and J. T. Whitehouse, Quasi-uniformity of minimal weighted energy points, *J. Complexity* **28** (2012), 177-191.
[12] A.B.J. Kuijlaars, E.B. Saff, Asymptotics for minimal discrete energy on the sphere, *Trans. Amer. Math. Soc.* **350** (1998), no. 2, 523–538.
[13] A. Martinez-Finkelshtein, V. Maymeskul, E. A. Rakhmanov, and E.B. Saff, Asymptotics for minimal discrete Riesz energy on curves in R^d, *Canad. J. Math.*, **56** (2004), 529–552.
[14] P. Mattila, *Geometry of Sets and Measures in Euclidean Space*, Cambridge University Press, 1995.
[15] T.W. Melnyk, O. Knop, and W. R. Smith, Extremal arrangements of points and unit charges on a sphere: equilibrium configurations revisited, *Canad. J. Chem.* **55**, (1977), 1745–1761.
[16] I.H. Sloan, R.S. Womersley, Extremal systems of points and numerical integration on the sphere, *Adv. Comp. Math.* **21** (2004), 102–125.

Appendix A. Proof of Proposition 2.7.

Denote

$$\operatorname{dist}((x,y),(x_0,y_0)) = \sqrt{|x-x_0|^2 + |y-y_0|^2}$$

and let

$$Q_\delta(x_0) = \{(x,y) \in A \times A \setminus D(A) : 0 < \operatorname{dist}((x,y),(x_0,x_0)) \leq \delta\}.$$

Since w is a CPD weight, there is a number $\kappa > 0$ such that $w(x,y) > 0$, $|x-y| < \kappa$. The inequality $\operatorname{dist}((x,y),(x_0,x_0)) \leq \delta$ implies that $|x-y| < 2\delta$. Assume first that

$I^w(v_N, \alpha_N) > 0$. Taking into account (22), we will have

$$\begin{aligned} L(v_N, x_0) &= \lim_{\delta\to 0} \sup_{(x,y)\in Q_\delta(x_0)} v_N(x,y) \\ &\geq \lim_{\delta\to 0} \sup_{(x,y)\in Q_\delta(x_0)} I^w(v_N, 2\delta) w(x,y) \\ &\geq \liminf_{\delta\to 0} I^w(v_N, 2\delta) \cdot \lim_{\delta\to 0} \sup_{(x,y)\in Q_\delta(x_0)} w(x,y) \\ &\geq I^w(v_N, \alpha_N) L(w, x_0). \end{aligned}$$

For every x_0 such that $L(w, x_0) = \infty$, the above estimate implies that $L(v_N, x_0) = \infty$, $N > N_0$, where N_0 does not depend on x_0. By the agreement, $L(v_N, x_0)/L(w, x_0) = 1$ for $N > N_0$ and every such $x_0 \in A$. Assuming now that $L(w, x_0) < \infty$, we similarly obtain

$$\begin{aligned} L(v_N, x_0) &= \lim_{\delta\to 0} \sup_{(x,y)\in Q_\delta(x_0)} v_N(x,y) \\ &\leq \lim_{\delta\to 0} \sup_{(x,y)\in Q_\delta(x_0)} S^w(v_N, 2\delta) w(x,y) \\ &\leq \limsup_{\delta\to 0} S^w(v_N, 2\delta) \cdot \lim_{\delta\to 0} \sup_{(x,y)\in Q_\delta(x_0)} w(x,y) \\ &\leq S^w(v_N, \alpha_N) L(w, x_0). \end{aligned}$$

Property (b) of a CPD-weight also implies that $L(w, x_0) \geq \kappa > 0$. Consequently,

$$I^w(v_N, \alpha_N) \leq \frac{L(v_N, x_0)}{L(w, x_0)} \leq S^w(v_N, \alpha_N)$$

for every $x_0 \in A$ with $L(w, x_0) < \infty$. Since quantities $I^w(v_N, \alpha_N)$ and $S^w(v_N, \alpha_N)$ do not depend on x_0, taking into account (22) and the fact that $L(v_N, x_0)/L(w, x_0) = 1$, $N > N_0$, if $L(w, x_0) = \infty$, we obtain uniform convergence in (23). Using an analogous argument one can establish the second equality in (23).

Assume now that the weight w is continuous on $D(A)$ and (22) holds. Then w is bounded by two positive constants on $D(A)$. Since $L(w, x_0) = l(w, x_0) = w(x_0, x_0)$, relations (23) imply relations (24).

To establish the converse statement, notice that for every $m \in \mathbb{N}$, there is a positive integer N_m such that for $N > N_m$ and $x_0 \in A$,

$$|L(v_N, x_0) - w(x_0, x_0)| \leq \frac{1}{m} \quad \text{and} \quad |l(v_N, x_0) - w(x_0, x_0)| \leq \frac{1}{m}.$$

Moreover, the sequence $\{N_m\}$ can be chosen to be increasing. Then

$$\begin{aligned} &\lim_{\delta\to 0} \sup_{(x,y)\in Q_\delta(x_0)} (v_N(x,y) - w(x,y)) \\ &\leq \lim_{\delta\to 0} \sup_{(x,y)\in Q_\delta(x_0)} v_N(x,y) - \lim_{\delta\to 0} \inf_{(x,y)\in Q_\delta(x_0)} w(x,y) \\ &= L(v_N, x_0) - w(x_0, x_0) \leq \frac{1}{m}, \quad x_0 \in A, \quad N > N_m. \end{aligned}$$

In view of property (b) of a CPD-weight, there are positive numbers h and κ such that $w(x,y) > h$ for $|x-y| < \kappa$. Let $\beta_N^m = \beta_N^m(x_0) < \kappa/\sqrt{2}$ be such that

$$\sup_{(x,y)\in Q_{\beta_N^m}(x_0)} (v_N(x,y) - w(x,y)) < \frac{2}{m}.$$

The collection of open balls $\{B((x,x),\beta_N^m(x))\}_{x\in A}$ has a finite subcollection $\{B((x_i,x_i),\beta_N^m(x_i))\}$ whose union $U_{m,N}$ covers the compact set $D(A)$. Let $\alpha_N^m := \operatorname{dist}(D(A),(A\times A)\setminus U_{m,N}) > 0$. Since

$$Q_{m,N} := \{(x,y)\in A\times A : 0 < |x-y| \le \alpha_N^m\} \subset U_{m,N},$$

for every $N > N_m$, we have

$$\sup_{(x,y)\in Q_{m,N}} (v_N(x,y) - w(x,y))$$

$$\le \max_i \sup_{(x,y)\in Q_{\beta_N^m}(x_i)} (v_N(x,y) - w(x,y)) \le \frac{2}{m}.$$

Consequently, since $|x-y| < \kappa$ for any $x,y \in Q_{m,N}$, we have

$$S^w(v_N,\frac{\alpha_N^m}{2}) = \sup_{(x,y)\in Q_{m,N}} \frac{v_N(x,y)}{w(x,y)} \le 1 + \frac{2}{hm}, \quad N > N_m.$$

Letting $\gamma_N := \alpha_N^m/2$, $N_m < N \le N_{m+1}$, $m\in\mathbb{N}$, we will have

$$\limsup_{N\to\infty} S^w(v_N,\gamma_N) \le 1.$$

Using the second equality in (24), one can obtain that

$$\liminf_{N\to\infty} I^w(v_N,\gamma'_N) \ge 1,$$

where $\{\gamma'_N\}$ is some positive and bounded sequence. Then for any positive sequence $\alpha_N = o(\min\{\gamma_N,\gamma'_N\})$, relation (22) still holds which completes the proof of Proposition 2.7.

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