Asymptotics of k-nearest neighbor Riesz energies

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Dedicated to Ronald DeVore for his 80th birthday

Abstract

We obtain new asymptotic results about systems of N particles governed by Riesz interactions involving k-nearest neighbors of each particle as $N \to \infty$. These results include a generalization to weighted Riesz potentials with external field. Such interactions offer an appealing alternative to other approaches for reducing the computational complexity of an N-body interaction. We find the first-order term of the large N asymptotics and characterize the limiting distribution of the minimizers. We also obtain results about the Γ convergence of such interactions, and describe minimizers on the 1-dimensional flat torus in the absence of external field, for all N.

1 Introduction and main results

Energy minimization methods for generating non-structured grids on compact sets in $\mathbb{R}^p$ have been explored in, for example, [4, 13, 14]. For a given d-dimensional compact set $A \subset \mathbb{R}^p$, these techniques utilize the Riesz kernel $\|x - y\|^{-s}$ with $s > 0$ and minimize the following energy associated with an N point configuration $\omega_N = \{x_1, x_2, \ldots, x_N\} \subset A$:

$$E_s(\omega_N) := \sum_{i=1}^{N} \sum_{\substack{j=1 \\ j \neq i}}^{N} \|x - y\|^{-s}. \tag{1.1}$$

In the hypersingular case $s \geqslant d$, the poppy-seed bagel theorem [4, Thm 8.5.2] asserts under mild conditions on A that minimizing configurations ω_N^* for this energy converge in the weak-star sense to the uniform distribution with respect to d-dimensional Hausdorff measure. More generally, by incorporating a multiplicative weight [2] or an external field [15] in the above energy, one can generate configurations that converge to a prescribed density on A.

An obvious drawback to this method for discretizing manifolds is the $O(N^2)$ computational cost for evaluating the energy or its gradient. One approach [3] to reducing this cost involves radial truncation. Instead, here we analyze truncation of E_s to a fixed number k of nearest neighbors, as used heuristically in [25]. An advantage of this technique, in contrast to the radial truncation, is that memory and computational costs depend only on k and N (essentially kN) and not on ω_N. Furthermore, it leads to dimension-independent methods: optimization of an unweighted Riesz k-energy E_s^k, defined below, for a fixed $s > 0$ and $k \geqslant 1$ yields a uniform distribution on the underlying set A, irrespective of the Hausdorff dimension of A.

In addition to grid generation, repulsive interactions depending only on a certain number of nearest neighbors arise in many applications in physics, chemistry, and engineering [17, 18, 12, 22]. Inspired by these examples, in the sequel we introduce the Riesz interaction with a fixed number k of nearest neighbors, and obtain the asymptotics of the minima of the energy E_s^k, as well as the limiting distribution of asymptotic minimizers.

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An outline of our manuscript is the following. In subsections 1.1–1.5 we formulate the main results and explain notational conventions assumed for the rest of the paper. Section 2 gives some numerical illustrations of applying E_s^k to discretizing distributions, in particular on manifolds. In Section 3 we outline the proof strategy and discuss how choosing nearest neighbors in an interaction influences the geometry of its minimizers. The main proofs are contained in Section 4. Finally, Section 5 begins by investigating the special case of $A = \mathbb{T}$, the 1-dimensional flat torus, and finds the minimizers of unweighted E_s^k on $\mathbb{T}$; it also shows that the hypersingular full Riesz interaction E_s is in a sense limiting case of E_s^k when $k \to \infty$. This allows to establish some new results for the hypersingular interaction, namely, the asymptotics of the combined functional, equipped with both weight and external field. The discussion concludes with the proof of Γ-convergence of energies E_s^k on N-point configurations for $N \to \infty$.

1.1 Preliminaries

Throughout this paper, A shall denote a compact set in $\mathbb{R}^p$ with d-dimensional Hausdorff measure $\mathcal{H}_d(A) < \infty$. We refer to an N-tuple $\omega_N = (x_1, x_2, \ldots, x_N) \in A^N$ as an *N-point configuration* (note that this allows repeated points of A) and define the associated normalized counting measure (or empirical measure)

$$\nu(\omega_N) := \frac{1}{N} \sum_{x \in \omega_N} \delta_x. \tag{1.2}$$

Defined in this way, the space of N-point configurations ω_N inherits the topology from $(\mathbb{R}^p)^N$. We will occasionally need to apply set-theoretic operations to ω_N, such as removing or adding entries. For example, by an abuse notation we write $\omega_N \setminus \{x_2\} = (x_1, x_3, \ldots, x_N) \in A^{N-1}$. In the case of repeated entries in ω_N, only the first instance is removed. Similarly, $x \in \omega_N$ means that the point x is one of the entries of tuple ω_N; in this case $I(x; \omega_N)$ denotes its index in the tuple.

For $k, N \geqslant 1$ and $\omega_N \in A^N$, let $\mathcal{N}_k(x; \omega_N)$ stand for the multiset consisting of the k nearest neighbors of x from $\omega_N \setminus \{x\}$ (with respect to $\|\cdot\|$) where, in the event of ties, we select the points with the smaller indices in ω_N. When $N < k+1$, then we set $\mathcal{N}_k(x; \omega_N) = \omega_N \setminus \{x\}$. For instance, when $\omega_4 = (a, a, a, b)$ we have $\mathcal{N}_3(a; \omega_4) = \mathcal{N}_4(a; \omega_4) = \{a, a, b\}$. When it cannot cause confusion, we will omit the reference to the configuration and write simply $\mathcal{N}_k(x)$.

For an external field $V : A \to \mathbb{R}$, a multiplicative weight $w : A \times A \to [0, \infty]$, Riesz parameter $s > 0$, and $k, N \geqslant 1$, we define the *k-nearest neighbor Riesz s-energy (k-energy for short)* of an N-point configuration $\omega_N = (x_1, x_2, \ldots, x_N) \in A^N$ as follows:

$$E_s^k(\omega_N; w, V) := \sum_{x \in \omega_N} \sum_{y \in \mathcal{N}_k(x; \omega_N)} w(x, y) \|x - y\|^{-s} + N^{s/d} \sum_{x \in \omega_N} V(x), \qquad k, N \geqslant 1, \ s > 0. \tag{1.3}$$

We use the convention that a sum over the empty set is zero; i.e., for $N = 1$ we have $E_s^k((x_1); w, V) = V(x_1)$. For brevity we also write $E_s^k(\omega_N; w)$ for $E_s^k(\omega_N; w, 0)$ so that

$$E_s^k(\omega_N; w, V) = E_s^k(\omega_N; w) + N^{s/d} \sum_{x \in \omega_N} V(x).$$

We define the optimal value of the above energy as

$$\mathcal{E}_s^k(A, N; w, V) := \inf_{\omega_N \in A^N} E_s^k(\omega_N; w, V). \tag{1.4}$$

We say that a sequence $\{\omega_N\}$ of N-point configurations in A is *(k, s, w, V)-asymptotically optimal* if

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

As in [2], we require that w be a *CPD-weight*; that is, $w : A \times A \to [0, \infty]$ satisfies

(a) w is positive and continuous at $\mathcal{H}_d$-a.e. point of $\operatorname{diag}(A)$ in the sense of limits taken on $A \times A$;

(b) there is a neighborhood $G \supset \operatorname{diag}(A)$ (relative to $A \times A$) such that $\inf_G w > 0$;

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

Here CPD stands for *(almost) continuous and positive on the diagonal.* In fact, for our purposes a weaker version of (a) suffices, assuming (c) be strengthened to the boundedness of w on the entire $A \times A$; it will be discussed in Section 4.3. We shall refer to a weight that satisfies only (b)-(c) as a *PD-weight*, for *positive on the diagonal.*

We shall refer to a weight w as a *marginally radial weight on* A if it is of the form $w(x, y) = W(x, \|y - x\|)$ for some $W : A \times [0, \operatorname{diam}(A)] \to [0, \infty]$ and $W(x, \cdot)\| \cdot \|^{-s}$ is decreasing on $[0, \operatorname{diam}(A)]$ for each $x \in A$. Note that if w is a marginally radial weight on A, then the energy $\mathcal{E}_s^k(A, N; w, V)$ is independent of the chosen tie-breaking criterion so this energy is well-defined when ω_N is considered as a multiset. In Theorem 1.3 establishing that a sequence of near energy minimizers have optimal order of separation, we find it convenient to assume that w is a marginally radial weight since a point energy is monotonically decreasing as a function of nearest neighbor distances. In particular, this is used in the proof of Theorem 1.3 when a point energy is computed with respect to a subset of the entire configuration in which case the k-nearest neighbor distances can only increase when compared to those distance with respect to the complete configuration.

1.2 Asymptotics of k-energies

For the statement of our main results, we use the following definitions and notation: a set $A \subset \mathbb{R}^p$ is called *d-rectifiable* if for some compact $A_0 \subset \mathbb{R}^d$ and a Lipschitz map f there holds $A = f(A_0)$ and A is called *$(\mathcal{H}_d, d)$-rectifiable* if it is a union of countably many d-rectifiable sets together with a set of $\mathcal{H}_d$-measure zero (see [10]). The d-dimensional Lebesgue measure on $\mathbb{R}^d$ is denoted by $\mathcal{L}_d$ and the d-dimensional Hausdorff measure on $\mathbb{R}^p$ for $d \leqslant p$ is denoted by $\mathcal{H}_d$ and is normalized so as to coincide with L_d on isometric embeddings from $\mathbb{R}^d$ to $\mathbb{R}^p$. By $\| \cdot \|$ we usually denote the Euclidean norm in $\mathbb{R}^d$ and $\mathbb{R}^p$, but the arguments below apply to any fixed norms in these spaces. We recall that a sequence of measures μ_n, $n \geqslant 1$, supported on a compact set A converges weak-star to a measure μ on A if $\lim_{n\to\infty} \int f\, d\mu_n = \int f\, d\mu$ for all continuous $f : A \to \mathbb{R}$, in which case we write $\mu_n \xrightarrow{*} \mu$, $n \to \infty$.

Theorem 1.1. *Suppose $A \subset \mathbb{R}^p$ is a compact $(\mathcal{H}_d, d)$-rectifiable set, $s > 0$, and k is a positive integer. Then there is a constant $C_{s,d}^k$ such that $C_{s,d}^k > 0$ and such that for any lower semicontinuous external field V and CPD-weight w the following limit holds:*

$$\lim_{N\to\infty} \frac{\mathcal{E}_s^k(A, N; w, V)}{N^{1+s/d}} = C_{s,d}^k \int_A w(x, x)\rho(x)^{1+s/d}\, d\mathcal{H}_d(x) + \int_A V(x)\rho(x)\, d\mathcal{H}_d(x)$$

where

$$\rho(x) = \left(\frac{L_1 - V(x)}{C_{s,d}^k (1 + s/d) w(x, x)} \right)_+^{d/s}, \qquad (\cdot)_+ := \max\{0, \cdot\}, \tag{1.5}$$

with the constant L_1 chosen so that $\rho\, d\mathcal{H}_d$ is a probability measure on A.

Furthermore, if $w(x, x) + V(x)$ is finite on a subset of A of positive $\mathcal{H}_d$-measure and $\{\omega_N\}$ is a (k, s, w, V)-asymptotically optimal sequence of N-point configurations in A, then the corresponding normalized counting measures $\nu(\omega_N)$ converge weak-star to $\rho\, d\mathcal{H}_d$.

If $d = p$, note that Theorem 1.1 holds for any compact set $A \subset \mathbb{R}^p$. We remark that in the special case $A = q_d$, the unit cube in $\mathbb{R}^d$, $V = 0$, and $w = 1$, Theorem 1.1 gives

$$C_{s,d}^k = \lim_{N\to\infty} \frac{\mathcal{E}_s^k(q_d, N; 1, 0)}{N^{1+s/d}}. \tag{1.6}$$

Corollary 1.2. *Suppose $A \subset \mathbb{R}^p$ is a compact d-rectifiable set, $s > 0$, and k is a positive integer. Let $\rho : A \to [0, \infty)$ be upper semi-continuous and such that $\rho\, d\mathcal{H}_d$ is a probability measure on A. If $L_1 \in \mathbb{R}$, w is a CPD-weight on $A \times A$ and V is a lower semi-continuous external field on A such that*

$$\begin{aligned} \frac{L_1 - V(x)}{w(x,x)} &= C_{s,d}^k (1 + s/d)\rho(x)^{s/d}, \qquad \text{for } \rho(x) > 0, \\ V(x) &\geqslant L_1, \qquad \text{for } \rho(x) = 0, \end{aligned} \tag{1.7}$$

then $\nu(\omega_N) \xrightarrow{*} \rho\, d\mathcal{H}_d$ for any (k, s, w, V)-asymptotically optimal sequence $\{\omega_N\}$.

In particular, if $V = 0$ and

$$w(x, y) := (\rho(x) + \|x - y\|)^{-s/d}, \tag{1.8}$$

then $\nu(\omega_N) \xrightarrow{*} \rho\, d\mathcal{H}_d$ for any $(k, s, w, 0)$-asymptotically optimal sequence $\{\omega_N\}$.

When $0 < s < d$, it is known (e.g., see [4]) that E_s-energy minimizing configurations on a d-rectifiable set A converge weak-star to the s-equilibrium measure on A which, except for in rare cases such as spheres. A rather surprising consequence of the above theorem is even for .... Riesz kernel involving only interactions with the nearest neighbor! Of course, the knowledge of the $C_{s,d}^k$ constant is required, but its value can easily be approximated numerically and is stable with respect to the computation error. This justifies the application of gradient flow to nearest neighbor truncation of the Riesz energy as a means to obtain a prescribed distribution, a strategy previously used as a heuristic [25].

Let the quantity

$$\Delta(\omega_N) := \min_{1 \leqslant i < j \leqslant N} \|x_i - x_j\| \tag{1.9}$$

denote the minimal distance between entries of the configuration $\omega_N \in A^N$. We refer to $\Delta(\omega_N)$ as the *separation* of ω_N.

The following theorem will be necessary to compare the asymptotics of k-energies to those of the full hypersingular Riesz energies; it shows that for k-nearest neighbor interaction with $k \geqslant 1$, near-minimizers are spread over the set A with the best possible order of separation. In its statement, we say that w is *bounded on D, a subset of A* (as opposed to being bounded on a subset of $\subset A \times A$), if the values of $w(z, x)$ and $w(x, z)$ are bounded uniformly over z from D and x from A:

$$M_w := \sup\{w(x, z) : (x, z) \in (A \times D) \cup (D \times A)\} < \infty. \tag{1.10}$$

Theorem 1.3. *Suppose $s > 0$, $A \subset \mathbb{R}^p$ is compact, $\mathcal{H}_d(A) > 0$, $w(x, y) : A \times A \to [0, \infty)$ is a marginally radial PD-weight, and V a lower semicontinuous external field, both bounded on some $D \subset A$, $\mathcal{H}_d(D) > 0$. If $\{\omega_N\}_1^\infty$ is a sequence such that*

$$E_s^k(\omega_N; w, V) \leqslant \mathcal{E}_s^k(A, N; w, V) + RN^{s/d}, \qquad N \geqslant 1$$

then this sequence has the optimal order separation:

$$\Delta(\omega_N) \geqslant CN^{-1/d}, \qquad N \geqslant 1,$$

with $C = C(s, k, p, d, w, V, A, R)$. In addition, in the case $d = p$, the constant C can be made independent of the set A.

1.3 Relation to hypersingular Riesz energies

In this section we will clarify the relation between the Riesz k-energy discussed above and the full hypersingular Riesz energy $E_s(\omega_N; w, V)$ on $\mathbb{R}^d$, defined as

$$E_s(\omega_N; w, V) := \sum_{x \neq y \in \omega_N} w(x, y)\|x - y\|^{-s} + N^{s/d} \sum_{x \in \omega_N} V(x), \qquad N \geqslant 2,\ s > d. \tag{1.11}$$

Just as for E_s^k, we write

$$\mathcal{E}_s(A, N; w, V) := \inf_{\omega_N \subset A} E_s(\omega_N; w, V).$$

We will show that for $k \to \infty$, the asymptotics of $\mathcal{E}_s^k$ approach those for $\mathcal{E}_s$.

The asymptotics of energy (1.11) and behavior of its minimizers are known for the case of a constant weight [15]. Similarly, they are also known for a non-constant weight and absence of external field [2]. By the general approach outlined in Section 3.1, the results of [2] and [15] can be combined to obtain a result identical to Theorem 1.1, with the full sum of the hypersingular interaction with $s > d$. We reproduce this result indirectly, by relating the full interaction (1.11) to the energies E_s^k.

In the following theorem, we write

$$C_{s,d} := \lim_{N\to\infty} \frac{\mathcal{E}_s(q_d, N)}{N^{1+s/d}}, \qquad s > d,$$

where q_d is the d-dimensional unit cube. By definition, $C_{s,d} \geqslant C_{s,d}^k$, $k \geqslant 1$. We call a sequence of configurations ω_N, $N \geqslant 2$, *asymptotically optimal for* E_s, if

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

Theorem 1.4. *If $A \subset \mathbb{R}^p$ is an $(\mathcal{H}_d, d)$-rectifiable compact set, $s > d$, w is a CPD-weight, and V a lower semicontinuous external field, then*

$$\lim_{k\to\infty} C_{s,d}^k = C_{s,d}, \tag{1.12}$$

and

$$\begin{aligned}\lim_{k\to\infty}\lim_{N\to\infty} \frac{\mathcal{E}_s^k(A, N; w, V)}{N^{1+s/d}} &= \lim_{N\to\infty} \frac{\mathcal{E}_s(A, N; w, V)}{N^{1+s/d}} \\ &= C_{s,d}\int_A w(x,x)\rho(x)^{1+s/d}\, d\mathcal{H}_d(x) + \int_A V(x)\rho(x)\, d\mathcal{H}_d(x),\end{aligned} \tag{1.13}$$

where

$$\rho(x) = \left(\frac{L_1 - V(x)}{C_{s,d}(1 + s/d)w(x,x)}\right)_+^{d/s},$$

with the constant L_1 chosen so that $\rho\, d\mathcal{H}_d$ is a probability measure on A.

Furthermore, if $w(x,x) + V(x)$ is finite on a subset of A of positive $\mathcal{H}_d$-measure and $\{\omega_N\}$ is an asymptotically optimal sequence of N-point configurations in A for E_s, then the corresponding normalized counting measures $\nu(\omega_N)$ converge weak-star to $\rho\, d\mathcal{H}_d$.

We wish to emphasize that the last equality in (1.13) for the minimal full Riesz interaction energy is also new since it includes both a weight and an external field.

The value of $C_{d,d}$ is given by

$$C_{d,d} := \mathcal{H}_d(\mathbb{B}^d) = \frac{\pi^{d/2}}{\Gamma\left(d/2 + 1\right)}, \quad d \geqslant 1, \tag{1.14}$$

where Γ is the standard gamma function, [13]. Furthermore, for $d = 1$, $s > 1$ there holds

$$C_{s,1} = 2\zeta(s), \quad s > 1, \tag{1.15}$$

where ζ is the Riemann zeta function, see e.g. [19]. The *universal optimality* of E_8 and the Leech lattice means that they minimize all energies with completely monotonic kernels as functions of the distance over discrete sets with fixed density. Such optimality of these lattices was shown by Cohn, Kumar, Miller, Radchenko, and Viazovska [7], following the methods of Viazovska [23]. The Riesz kernel $1/r^s$ is completely monotonic (that is, its derivatives have alternating signs), and as a result, $C_{s,d}$, $d = 8, 24$, is related to the respective lattice as

$$C_{s,d} = |\Lambda_d|^{s/d} \zeta_{\Lambda_d}(s), \qquad s > d, \quad d = 8, 24. \tag{1.16}$$

Here Λ_d denotes either E_8 or the Leech lattice; $|\Lambda_d|$ stands for the volume of the fundamental cell of Λ_d, and ζ_{Λ_d} is the corresponding Epstein zeta-function. The exact value of $C_{s,d}$ is unknown for all the other pairs s, d. In dimensions $d = 2,\ 4$, the conjectured value is also given by the expression (1.16) with Λ_d, respectively, the hexagonal and D_4 lattices [6, Conj. 2]. It is easy to show [6, Prop. 1] that the conjectured values (1.16) are upper bounds for their respective $C_{s,d}$.

1.4 Γ-convergence

For the hypersingular kernel, uniqueness of the limiting distribution of global minimizers is due to the displacement convexity, in the sense of McCann [21], of the limiting continuous functional (see equation (1.17) below), which can be obtained by treating E_s^k as defined on counting probability measures, and then passing to the Γ-limit. In the paper [16] we demonstrate that this property is common to all short-range interactions with scale-invariant minimizers. In the present discussion we will derive the Γ-limit of k-nearest neighbor energies, as a typical case of a short-range interaction.

We first recall the notion of Γ-convergence:

Definition 1.5 ([9])**.** Let X be a metric space. Suppose that functionals F, $F_N : X \to \mathbb{R}$, $N \geqslant 1$, satisfy

1^Γ. for every sequence $\{x_N\} \subset X$ such that $x_N \to x$, $N \to \infty$, there holds $\liminf_{N\to\infty} F_N(x_N) \geqslant F(x)$;

2^Γ. for every $x \in X$ there exists a sequence $\{x_N\} \subset X$ converging to it and such that $\lim_{n\to\infty} F_N(x_N) = F(x)$.

We shall then say that the sequence $\{F_N\}$ is Γ-*converging* to the functional F on X with the metric topology; in symbols, $\Gamma\text{-}\lim_{N\to\infty} F_N = F$.

In our setting, the underlying metric space $X = \mathcal{P}(A)$, the space of probability measures on A with a metric corresponding to the weak* topology; functionals $F_N(\mu)$ are given by $E_s^k(\omega_N; w, V)$ when $\mu = \nu(\omega_N)$ is a counting measure for some ω_N, see (1.2), and equal to $+\infty$ otherwise; see Theorem 1.6. To give the formal definitions, denote by $\mathcal{P}_N(A)$ the class of counting measures of N-point subsets of $A \subset \mathbb{R}^p$:

$$\mathcal{P}_N(A) := \left\{ \nu(\omega_N) : \omega_N \in A^N \right\}.$$

In the following result, $C_{s,d}^k$ is as in (1.6).

Theorem 1.6. *Suppose $A \subset \mathbb{R}^p$ is $(\mathcal{H}_d, d)$-rectifiable, w is a CPD-weight and V is a lower semicontinuous external field. Let a sequence of functionals on $\mathcal{P}(A)$ be given by*

$$\mathcal{F}_N(\mu; w, V) := \begin{cases} E_s^k(\omega_N; w, V), & \text{if } \mu = \nu(\omega_N) \in \mathcal{P}_N(A); \\ +\infty, & \text{otherwise,} \end{cases}$$

and

$$\mathcal{F}(\mu; w, V) := \begin{cases} C_{s,d}^k \int_A w(x,x)\rho(x)^{1+s/d} \, d\mathcal{H}_d(x) + \int_A V(x)\rho(x) \, d\mathcal{H}_d(x), & \text{if } \mu \ll \mathcal{H}_d, \\ +\infty, & \text{otherwise,} \end{cases} \tag{1.17}$$

where ρ is the Radon-Nikodym derivative of μ with respect to $\mathcal{H}_d$. Then

$$\Gamma\text{-}\lim_{N\to\infty} \frac{\mathcal{F}_N}{N^{1+s/d}} = \mathcal{F}$$

on $\mathcal{P}(\Omega)$ equipped with the weak-star topology.

Comparison of Theorem 1.6 with the classical results for 2-point interactions with integrable kernel reveals the difference in the asymptotic structures of energies for the long-range and short-range energies: limiting functionals of the former depend quadratically (through a double integral) on the limiting measure; on the other hand, in (1.17) we have single integrals.

1.5 Notational conventions

It is assumed that p, d are integer with $p \geqslant d > 0$. By $\|\cdot\|$ we denote fixed norms on $\mathbb{R}^d$ and $\mathbb{R}^p$, not necessarily Euclidean. Closed balls in the ambient space (either $\mathbb{R}^d$ or $\mathbb{R}^p$) with respect to these norms are denoted by $B(x, r)$; here x is the center of the ball, r stands for the radius. For $r > 0$, the closed r-neighborhood of a set A is denoted by $A_r = \bigcup_{x \in A} B(x, r)$. Notation v_d stands for the volume of the unit ball in $\mathbb{R}^d$.

A "cube" always refers to a closed cube with sides parallel to the coordinate axes. The unit cube in $\mathbb{R}^d$, centered at the origin, is denoted by $q_d = [-1/2, 1/2]^d$.

The d-dimensional Lebesgue and Hausdorff measure are denoted by $\mathcal{L}_d$ and $\mathcal{H}_d$; the latter is normalized so as to coincide with $\mathcal{L}_d$ on isometric embeddings from $\mathbb{R}^d$ to $\mathbb{R}^p$. Weak* convergence of a sequence of measures μ_n, $n \geqslant 1$, to μ is denoted by $\mu_n \xrightarrow{*} \mu$, $n \to \infty$. Notation $\mathcal{M}_d$ stands for the d-dimensional Minkowski content in $\mathbb{R}^p$.

The adjacency graph of ω_N, introduced in Section 3.1 and corresponding to the nearest neighbor relation, is denoted by $\Lambda_k(\omega_N)$. Notation $\prec_x$ stands for the ordering of points in ω_N by indices and distance to a given point $x \in \mathbb{R}^p$. The l-th element of $\omega_N \setminus \{x\}$ under the ordering $\prec_x$ is written as $(x; \omega_N)_l$ (note that the set difference here removes only the first occurrence of x in ω_N). Given $x \in \omega_N$, we write $I(x; \omega_N)$ for the (first) index of x as an entry of ω_N.

A bijective map $\psi : \mathbb{R}^d \to \mathbb{R}^p$ is said to be bi-Lipschitz with the constant $(1 + c)$, $c > 0$, if there holds

$$(1 + c)^{-1}\|x - y\| \leqslant \|\psi(x) - \psi(y)\| \leqslant (1 + c)\|x - y\|$$

for every pair $x, y \in \mathbb{R}^d$.

In cases when the multiplicative weight and/or external field are absent from our considerations, we write simply $E_s^k(\omega_N; w)$ and $E_s^k(\omega_N)$ in place of $E_s^k(\omega_N; w, 0)$ and $E_s^k(\omega_N; 1, 0)$, respectively. Finite positive constants that may depend on some arguments are denoted $C(\ldots)$; we can sometimes refer to different constants of this form in different parts of an equation, using the same symbol C.

2 Numerical aspects and experiments

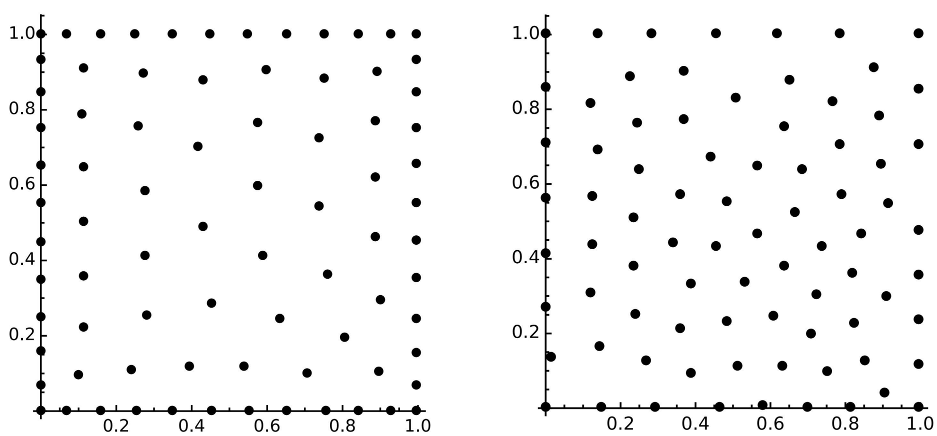

Figure 1: Left: approximate minimizer of the full Riesz interaction with $s = 1$; right: approximate minimizer of the k-nearest neighbor interaction with $k = 2$ and $s = 1$. In both images, $N = 80$.

The worst case complexity for constructing the k-nearest neighbor (k-nn) graph for an N-point configuration is $O(N \log N)$ floating point computations (FLOPS). Thus, the cost of evaluating E_s^k (or its gradient) is also $O(N \log N)$ compared with order N^2 FLOPS for the full interaction energy E_s. However, for sufficiently well-separated point configurations, the k-nn algorithm reduces to $O(kN)$ and thus the cost of one energy or gradient evaluation is also $O(kN)$.

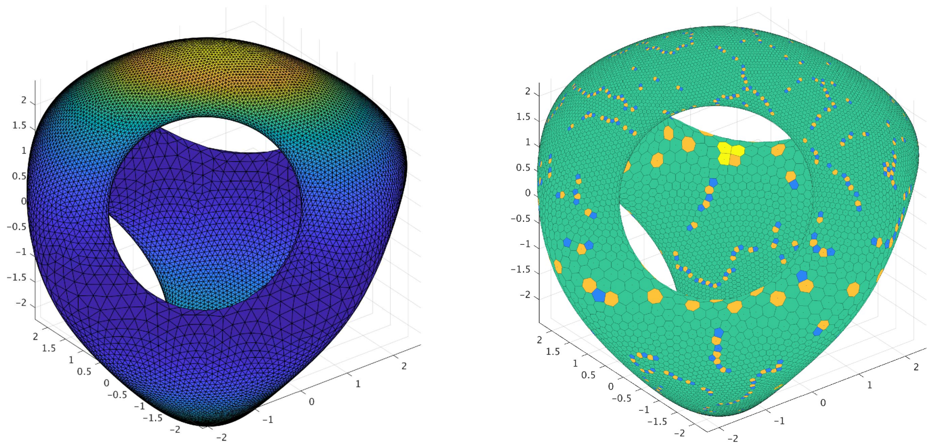

Figure 2: Approximate minimizing configuration of 20,000 points on a genus 3 surface in the $x_1x_2x_3$-cube $[-2, 2]^3$ for the energy E_s^k with $s = 4$, $k = 30$ and weight w chosen to give density ρ proportional to x_3^2 (external field $V = 0$). Left: Delaunay triangulation; right: Voronoi tessellation.

An interesting question is how the choice of k influences the speed of convergence of a given optimization algorithm such as gradient descent (we remark that E_s^k is not differentiable when there are ties for the k-th nearest neighbor). This issue is not explored here, but is left for future investigations.

In Figure 1, we show approximate energy minimizers for $N = 80$ points in the unit square for the full E_s energy (left) and E_s^k energy (right) with $s = 1$, $k = 2$, $w \equiv 1$, and $V \equiv 0$. Notice that the full kernel energy yields higher density distribution at the boundary of the square while, in accordance with Theorem 1.1, the points are more uniformly spaced when the interactions are restricted to the k-nearest neighbors. The two minimizers were computed using Mathematica's IPOPT interface and the built-in simulated annealing algorithm, respectively.

It has been demonstrated that the energies E_s^k can be used for efficient discretization of complicated surfaces, see [25, 24]. Here we illustrate the effectiveness of the algorithm in Figure 2 which shows an approximate minimizing configuration of $N = 20\,000$ points on an algebraic surface with $s = 4$, $k = 30$, $V \equiv 0$, and with a nonuniform weight. The left image shows the Delaunay triangulation of this configuration colored according to density where lighter colors reflect higher density. The right image, shows the Voronoi tessellation generated by the configuration where cells are colored according to their number of edges. Notice that the majority of cells are hexagons (light green).

3 Geometry of nearest neighbor interactions

3.1 Proof strategy and adjacency graph of nearest neighbors

Our strategy, as put forward in [16], is to show that unweighted functional E_s^k is a so-called short-range interaction, that is, it has the following four essential properties. Note that compared to paper [16], we strengthen and simplify the formulations, as appropriate for our context.

(i) Monotonicity: If $A \subset B \subset \mathbb{R}^p$, then, by definition,

$$\mathcal{E}_s^k(A, N) \geqslant \mathcal{E}_s^k(B, N), \qquad N \geqslant 1. \tag{3.1}$$

(ii) Asymptotics on cubes: For the unit cube $q_d \in \mathbb{R}^d$, the following limit exists and is positive and finite

$$C_{s,d}^k := \lim_{N\to\infty} \frac{\mathcal{E}_s^k(q_d, N)}{N^{1+s/d}}.$$

This fact will be established in Lemma 4.1.

(iii) Short-range property: The energy of a sequence of configurations contained in a pair (or finite collection) of disjoint compact sets is asymptotically the sum of energies on individual sets. Suppose $A_1, A_2 \subset \mathbb{R}^p$ are disjoint compact sets. If (ω_N) is a sequence of N-point configurations in $A_1 \cup A_2$ for $N \geqslant 2$, then

$$\lim_{N\to\infty} \frac{E_s^k(\omega_N \cap A_1) + E_s^k(\omega_N \cap A_2)}{E_s^k(\omega_N)} = 1. \tag{3.2}$$

The short-range property will be obtained in Lemma 4.4.

(iv) Stability: The minimum energy asymptotics is stable under small perturbations (in terms of Minkowski content) of the set; that is, for every compact $A \subset \mathbb{R}^p$ and $\varepsilon \in (0,1)$ there is some $\delta = \delta(\varepsilon, s, k, p, d, A) > 0$ such that for any compact $D \subset A$ satisfying $\mathcal{M}_d(D) \geqslant (1-\delta)\,\mathcal{M}_d(A)$, we have

$$\liminf_{N\to\infty} \frac{\mathcal{E}_s^k(A,N)}{N^{1+s/d}} \geqslant (1-\varepsilon) \liminf_{N\to\infty} \frac{\mathcal{E}_s^k(D,N)}{N^{1+s/d}}, \quad \limsup_{N\to\infty} \frac{\mathcal{E}_s^k(A,N)}{N^{1+s/d}} \geqslant (1-\varepsilon) \limsup_{N\to\infty} \frac{\mathcal{E}_s^k(D,N)}{N^{1+s/d}}. \tag{3.3}$$

In addition, for $p = d$, δ is independent of A. This result will be established in Lemma 4.5.

The above properties allow to extend the existence of asymptotics for $\mathcal{E}_s^k$ from cubes (shown in Section 4.1) to general compact subsets of $\mathbb{R}^d$ and subsequently, to $(\mathcal{H}_d, d)$-rectifiable subsets of $\mathbb{R}^p$, $p \geqslant d$. Once these properties have been established for the unweighted interaction E_s^k, existence of the asymptotics on compact sets in $\mathbb{R}^d$ follows. Finally, the statement of Theorem 1.1, applying to $(\mathcal{H}_d, d)$-rectifiable subsets of $\mathbb{R}^p$ is derived by approximating such sets with bi-Lipschitz parametrizations, an argument going back to Federer [10].

For some of the proofs in the sequel it will be useful to order the entries of $\omega_N \in (\mathbb{R}^p)^N$ by their distance to a given $x \in \mathbb{R}^p$; as was mentioned in Section 1, the interaction E_s^k selects points with smaller indices in the case of equal distance, so we will order lexicographically, first by distance, then by index. Formally, the order $\prec_x$ on entries of ω_N is defined like so:

$$y \prec_x z \qquad \overset{def}{\iff} \qquad \begin{array}{c} \|y-x\| < \|z-x\| \\ \text{or} \\ \|y-x\| = \|z-x\| \text{ and } I(y;\omega_N) < I(z;\omega_N), \end{array}$$

where as before, $I(y;\omega_N)$ is the index of the first occurrence of y as an entry of ω_N. The notation $\mathcal{N}_k(x;\omega_N)$ introduced above then stands for the multiset of the first k entries of $\omega_N \setminus \{x\}$ with respect to the ordering $\prec_x$. We further write $(x;\omega_N)_l$ for the l-th entry of $\omega_N \setminus x$ with respect to $\prec_x$, $1 \leqslant l \leqslant N-1$. In particular, distances $\|x - (x;\omega_N)_l\|$ are nondecreasing in l for a fixed x and ω_N.

Let

$$\Lambda_k(\omega_N) := \{(x,y) : x, y \in \omega_N,\ y \in \mathcal{N}_k(x;\omega_N)\},$$

the set of ordered pairs of entries of ω_N, corresponding to the relation "y is among the k nearest neighbors of x". Notice that this relation is not symmetric. In what follows, it will be occasionally convenient to think of $\Lambda_k(\omega_N)$ as the set of edges in the oriented graph $(\mathcal{V}, \mathcal{E}) = \big(\{x_i\}_1^N,\ \Lambda_k(\omega_N)\big)$ with $\{x_i\}_1^N$ being the multiset of entries from ω_N. Due to this, we will refer to Λ_k as the *adjacency graph* of ω_N.

3.2 Main geometric lemma and local properties of near-minimizers

Using $\Lambda_k(\omega_N)$, we can write

$$E_s^k(\omega_N; w, V) = \sum_{(x,y)\in\Lambda_k(\omega_N)} w(x,y)\|x-y\|^{-s} + N^{s/d} \sum_{x\in\omega_N} V(x), \qquad s \neq 0. \tag{3.4}$$

As before, the function w is assumed to be a CPD-weight on $A \times A$. The external field V is assumed to be lower semicontinuous on A (and therefore bounded below there).

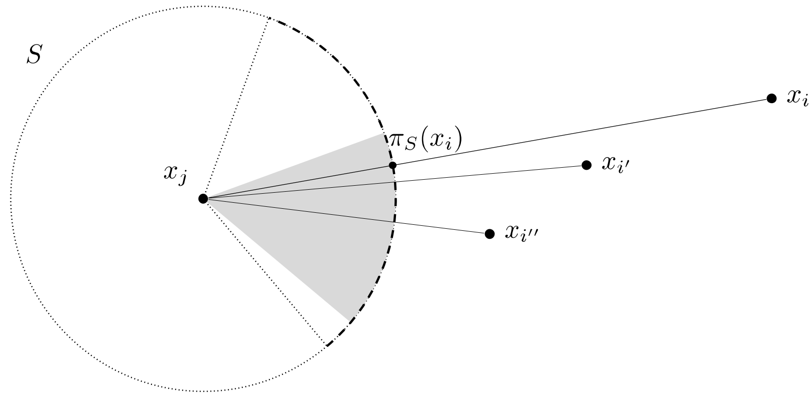

Figure 3: If the closed spherical cap of radius $\pi/3$ around projection $\pi_S(x_i)$ (dashed) contains the projection of $x_{i'}$, it follows $\|x_i - x_{i'}\| \leqslant \max\{\|x_j - x_i\|, \|x_j - x_{i'}\|\}$. Hence, as Lemma 3.1 shows, at most k points among $\{x \in \omega_N : x_j \in \mathcal{N}(x; \omega_N)\}$ can be projected into any given cap of angular radius $\pi/6$ (shaded).

Our eventual goal is to verify the properties from Section 3.1. It is easy to see that restricting interactions to k nearest neighbors guarantees that E_s^k is in a sense local. Without such restriction, the locality does not hold when $s < d$, as is well-known from classical potential theory. Since $s > 0$, the singular nature of the interaction on the diagonal results in that the pointwise separation is of the optimal order for near-minimizers, as will be shown in Theorem 1.3.

We will first obtain the following basic fact about the set $\Lambda_k(\omega_N)$.

Lemma 3.1. *Fix a configuration $\omega_N \in (\mathbb{R}^d)^N$ of N distinct points. For any $y \in \omega_N$, the number of points x in ω_N such that y is one of k nearest neighbors of x is bounded by $n(k,d)$, depending only on the number of neighbors k and the dimension d. That is,*

$$\#\{x \in \omega_N : y \in \mathcal{N}_k(x; \omega_N)\} \leqslant n(k,d).$$

This lemma can be interpreted is graph-theoretic terms as follows. Consider expression (3.4); the first sum involves terms $w(x,y)\|x-y\|^{-s}$ for oriented pairs $(x,y) \in \Lambda_k(\omega_N)$. By definition, the outgoing degree of every vertex in the graph $\big(\{x_i\}_1^N,\ \Lambda_k(\omega_N)\big)$ is k; the above lemma shows further that the maximal incoming degree in the graph is bounded by $n(k,d)$.

Proof. Fix $y = x_j \in \omega_N$ and denote $\omega_{N,j} = \{x \in \omega_N : x_j \in \mathcal{N}(x; \omega_N)\}$. Choose the radius $r_j > 0$ so that $B(x_j, r_j)$ does not contain any points from ω_N apart from x_j. Let π_S be the radial projection onto $S := \partial B(x_j, r_j)$ and consider the image of points in $\omega_{N,j}$ under this projection, see Figure 3. Suppose that a closed geodesic ball on S of radius $\pi/6$, denoted $B_S(z, \pi/6)$, $z \in S$, contains more than k elements of this image. Let

$$x_i = \arg\max\{\|x - y\| : x \in \omega_{N,j},\ \pi_S(x) \in B_S(z, \pi/6)\}.$$

Then $B_S(z, \pi/6) \subset B_S(\pi_S(x_i), \pi/3)$, implying that $B_S(\pi_S(x_i), \pi/3)$ contains k projections different from $\pi_S(x_i)$.

On the other hand, for any $x_{i'} \in \omega_{N,j}$, from $\pi_S(x_{i'}) \in B_S(\pi_S(x_i), \pi/3)$ it follows $\angle x_i x_j x_{i'} < \pi/3$, so that

$$\|x_{i'} - x_i\| \leqslant \max\{\|x_j - x_i\|, \|x_j - x_{i'}\|\} = \|x_j - x_i\|,$$

since x_i was chosen the furthest from x_j. Thus, every other point projected into $B_S(\pi_S(x_i), \pi/3)$ is closer to x_i than x_j, and it must be $x_j \notin \mathcal{N}_k(x_i; \omega_N)$, a contradiction. By this argument, the constant $n(k,d)$ chosen as

$$n(k,d) := \max\left\{n : \exists \omega_n \subset \mathbb{S}^{d-1} \text{ such that } \#(B_S(z, \pi/6) \cap \omega_n) \leqslant k,\ \forall z \in \mathbb{S}^{d-1}\right\}$$

has the properties stated in the claim of the lemma. $\square$

We will also need a classical result from potential theory, due to Frostman.

Proposition 3.2 (Frostman's lemma [20, p. 112], [11])**.** *For any compact A with $\mathcal{H}_d(A) > 0$ there is a finite nontrivial Borel measure μ on $\mathbb{R}^p$ with support inside A such that*

$$\mu(B(x,r)) \leqslant r^d, \ x \in \mathbb{R}^p.$$

This statement is specifically used to obtain a lower bound on the optimal covering radius of the compact set A. Indeed, let the measure μ be as in Frostman's lemma. Given any collection $\omega_N = (x_i)_1^N \in A^N$, for the radius $r_0 = c_{\text{Fro}}(A)N^{-1/d} := (\mu(A)/2)^{1/d}N^{-1/d}$ and the set

$$D = A \setminus \bigcup_i B(x_i, r_0)$$

there holds $\mu(D) \geqslant \mu(A)/2$. In particular $D \neq \emptyset$, so that at least one point of A is distance r_0 away from the points in ω_N. It follows that the covering radius of A for any collection of N points $\omega_N \in A^N$ is at least $c_{\text{Fro}}(A)N^{-1/d}$. Observe also that for $d = p$, it suffices to use $\mu = v_d^{-1}\mathcal{L}_d$, and hence μ is independent of A in this case.

Proof of Theorem 1.3. Fix an $N > 2$. Since $s > 0$ and the product $w(x,y)\|x-y\|^{-s}$ is infinite on the diagonal of $A \times A$, assumptions of the theorem imply that all entries of ω_N are distinct. It will be convenient to assume that configuration $\omega_N = (x_1, \ldots, x_N)$ is numbered in such a way that minimal separation is attained for the pair x_1, x_2:

$$\Delta(\omega_N) = \|x_1 - x_2\| = c_N N^{-1/d}.$$

It will also be convenient to assume $V \geqslant 0$ on A; by lower semicontinuity this can be achieved by adding a sufficiently large constant to V, which does not change the behavior of minimizers.

We need to show $c_N \geqslant C(s,k,d,w,V,A,R) > 0, \ N \geqslant 1$. By definition, a PD-weight satisfies properties (b)-(c) of a CPD-weight; thus there exists a $\delta > 0$ such that $\{(x,z) : \|x-z\| \leqslant \delta\} \subset G$ for the neighborhood G as in the definition of CPD-weight. This implies

$$0 < m_w := \inf\{w(x,z) : \|x-z\| \leqslant \delta\}.$$

Let further M_w as in (1.10) – a finite quantity, due to the boundedness of w on D.

In view of boundedness of V on D, a set of positive $\mathcal{H}_d$-measure, and the discussion after Proposition 3.2, there exists a point $z \in D$, such that

$$\|z - x_i\| \geqslant c_{\text{Fro}} N^{-1/d}, \qquad i = 1, \ldots, N,$$

where $c_{\text{Fro}} := c(A,V,L) = (\mu(D)/2)^{1/d}$ is from Frostman's lemma for D. Let

$$\omega_N' = (z, x_2, \ldots, x_N),$$

the configuration obtained by replacing x_1 with z. If $\|x_1 - x_2\| = c_N N^{-1/d} \geqslant \delta$, $c_N \geqslant \delta$, and there is nothing to prove. Otherwise, suppose $c_N N^{-1/d} < \delta$ for some N. Since $E_s^k(\omega_N; w)$ is close to being optimal, replacing x_1 with z can lower the value of E_s^k by at most $RN^{s/d}$:

$$E_s^k(\omega_N'; w, V) - E_s^k(\omega_N; w, V) = E_s^k(\omega_N'; w) - E_s^k(\omega_N; w) + N^{s/d}(V(z) - V(x_1)) \geqslant -RN^{s/d},$$

so that, since $V(z) - V(x_1) \leqslant V(z) \leqslant L$,

$$E_s^k(\omega_N'; w) - E_s^k(\omega_N; w) \geqslant -(R+L)N^{s/d}. \tag{3.5}$$

Let us determine the terms remaining after cancellation in the left-hand side of this equation. Since

$$E_s^k(\omega_N'; w) - E_s^k(\omega_N; w) = \left(\sum_{(x,y)\in\Lambda_k(\omega_N')} - \sum_{(x,y)\in\Lambda_k(\omega_N)} \right) w(x,y)\|x-y\|^{-s},$$

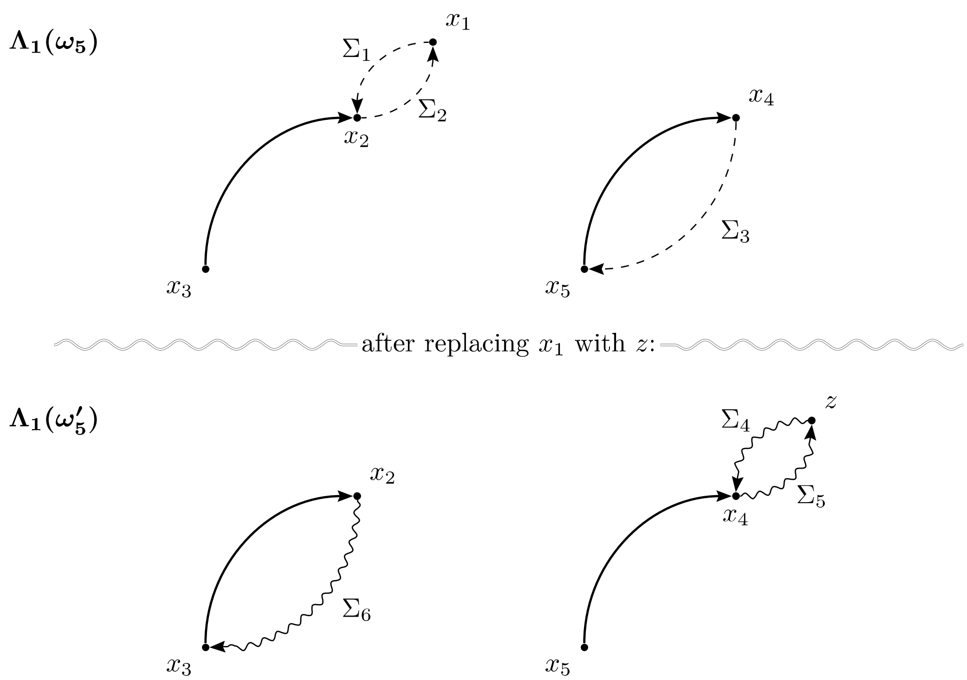

Figure 4: Elements of $\Lambda_1(\omega_5)$ compared to those in $\Lambda_1(\omega_5')$. Arrow from node x to node y means that pair (x, y) is present in the respective adjacency graph. Solid arrows show pairs present in both graphs; wavy arrows represent pairs appearing only in $\Lambda_1(\omega_5')$; dashed arrows those appearing only in $\Lambda_1(\omega_5)$. For this small example, each of Σ_m contains exactly one term/edge.

we can describe all the terms that occur only in $E_s^k(\omega_N; w)$, and therefore do not cancel out, as

$$\Sigma_1 + \Sigma_2 + \Sigma_3 := \left(\sum_{\substack{(x,y)\in\Lambda_k(\omega_N),\\ x=x_1}} + \sum_{\substack{(x,y)\in\Lambda_k(\omega_N),\\ y=x_1}} + \sum_{\substack{(x,y)\in\Lambda_k(\omega_N)\setminus\Lambda_k(\omega_N')\\ x,y\neq x_1}} \right) w(x,y)\|x-y\|^{-s}.$$

Likewise, the terms occurring only in $E_s^k(\omega_N'; w)$ are as follows:

$$\Sigma_4 + \Sigma_5 + \Sigma_6 := \left(\sum_{\substack{(x,y)\in\Lambda_k(\omega_N'),\\ x=z}} + \sum_{\substack{(x,y)\in\Lambda_k(\omega_N'),\\ y=z}} + \sum_{\substack{(x,y)\in\Lambda_k(\omega_N')\setminus\Lambda_k(\omega_N)\\ x,y\neq z}} \right) w(x,y)\|x-y\|^{-s}.$$

The term $\sum_3$ above arises due to the number of terms originating from each point being fixed at k, so any terms incoming into z must have had different terminating nodes in ω_N; similar logic applies to $\sum_6$. To summarize, there holds

$$E_s^k(\omega_N'; w) - E_s^k(\omega_N; w) = \Sigma_4 + \Sigma_5 + \Sigma_6 - \Sigma_1 - \Sigma_2 - \Sigma_3.$$

As an illustration, all the six sums Σ_m are present when point x_1 is replaced with z in the tuple $\omega_5 = (x_i)_1^5$, shown in Figure 4. In this figure, ordered pairs $(x, y) \in \Lambda_1$ for either tuple are represented as directed edges of a graph.

To finish the proof, we will need an upper bound on $\Sigma_6 - \Sigma_2$. To that end, note that each pair in Σ_6, that is,

$$(x, y) \in \Lambda_k(\omega_N') \setminus \Lambda_k(\omega_N) \quad \text{such that } x, y \neq z,$$

must be replacing a pair having the form (x, x_1) in $\Lambda_k(\omega_N)$, to keep the total number of outgoing edges from x equal to k. Grouping the new pairs in Σ_6 with the removed ones in Σ_2 by their starting node gives

$$\Sigma_6 - \Sigma_2 = \sum_{\substack{x:\ (x,x_1)\in\Lambda_k(\omega_N),\\ z\notin\mathcal{N}_k(x;\omega'_N)}} \left(\frac{w(x,(x;\omega_N)_{k+1})}{\|x-(x;\omega_N)_{k+1}\|^s} - \frac{w(x,x_1)}{\|x-x_1\|^s} \right) \leqslant 0,$$

since $\|x - x_1\| \leqslant \|x - (x;\omega_N)_{k+1}\|$, and w is marginally radial, so the expression $w(x,y)/\|x-y\|^{-s}$ is nonincreasing with the distance $\|x-y\|$ for every fixed x. We used here the notation $(x,\omega_N)_{k+1}$ for the $(k+1)$-st nearest neighbor to x in ω_N, as introduced in Section 3.1. Finally, equation (3.5) implies

$$\begin{aligned} -(R+L)N^{s/d} &\leqslant \Sigma_4 + \Sigma_5 + \Sigma_6 - \Sigma_1 - \Sigma_2 - \Sigma_3 \\ &\leqslant \Sigma_4 + \Sigma_5 + (\Sigma_6 - \Sigma_2) - \Sigma_1 \\ &\leqslant \sum_{x\in\mathcal{N}_k(z;\omega'_N)} \frac{w(z,x)}{\|z-x\|^s} + \sum_{x:z\in\mathcal{N}_k(x;\omega'_N)} \frac{w(x,z)}{\|x-z\|^s} - \frac{w(x_1,x_2)}{\|x_1-x_2\|^s} \\ &\leqslant \left(kM_w c_{\text{Fro}}^{-s} + n(k,p)M_w c_{\text{Fro}}^{-s} - m_w c_N^{-s}\right) N^{s/d}, \end{aligned}$$

where in the fourth inequality Lemma 3.1 is used to estimate the number of terms in the second sum.

This implies that whenever $c_N < \delta N^{1/d}$, there holds

$$c_N \geqslant \left(\frac{m_w}{(R+L)\, c_{\text{Fro}}^s + (k+n(k,p))M_w} \right)^{1/s} c_{\text{Fro}}, \tag{3.6}$$

as desired. ☐

Corollary 3.3. *Let $w \equiv 1$ and $p = d$; let also ω_N^* be such that $E_s^k(\omega_N^*) \leqslant \mathcal{E}_s^k(A,N) + 1$. Then equation* (3.6) *implies*

$$\Delta(\omega_N^*) \geqslant \left(\frac{1}{1+k+n(k,d)} \right)^{1/s} c_{\text{Fro}}\, N^{-1/d}, \qquad N \geqslant N_0(d, \mathcal{L}_d(A)),$$

where $c_{\text{Fro}} = c(d)\mathcal{L}_d(A)^{1/d}$, as in the discussion after Proposition 3.2.

Proof. It suffices to note that under such assumptions on ω_N^*, $L = 0$, $R \leqslant N^{-s/d}$, and $m_w = M_w = 1$ in equation (3.6). ☐

Corollary 3.4. *The proof of Theorem 1.3 shows that there holds an optimal covering result, at least for some sublevel set of $V + w$. In particular, when $V \equiv 0$, $w \equiv 1$ one has an optimal covering result: For a compact set $A \subset \mathbb{R}^d$ with $0 < \mathcal{H}_d(A) < \infty$, and a sequence of configurations $\{\omega_N^*\}_1^\infty$, such that*

$$E_s^k(\omega_N) \leqslant \mathcal{E}_s^k(A,N) + RN^{s/d}, \qquad N \geqslant 1,$$

for every $y \in A$ there holds

$$\operatorname{dist}(y, \omega_N) \leqslant C(s,k,d,A,R)\, N^{-1/d}.$$

Proof. It suffices to note that in the proof of the theorem, one obtains the inequality (3.6) between the covering radius at $z \in D$, equal to $c_{\text{Fro}} N^{-1/d}$, and the minimal separation, equal to $c_N N^{-1/d}$. Using $\mathcal{H}_d(A) < \infty$ and a standard volume argument, one easily obtains an upper bound of $C(A)N^{-1/d}$ on the optimal separation, at least for $p = d$. In the case $p > d$, one uses instead that Minkowski content $\mathcal{M}_d(A) < \infty$, to the same effect. In the sequel, we shall only need the optimal covering property for the unit cube in $\mathbb{R}^d$ in Section 4.1. It is not hard to see that the optimal covering holds on the L_1-sublevel set for V, with L_1 from the statement of Theorem 1.1, and not on any larger sublevel set. ☐

Existence of minimizers of E_s^k The above theorem concerns configurations with near-optimal value of energy. A natural question to ask is, under which assumptions on w the functional (3.4) attains its minimum on A^N; that is, whether E_s^k is lower semicontinuous. Recall that the topology on A^N is the product topology induced by the restriction of Euclidean metric to A. In the following proof it will be convenient to use l^∞ norm on A^N, so that distance between two configurations is

$$\rho(\omega'_N, \omega''_N) = \max_i \|x'_i - x''_i\|.$$

Lemma 3.5. *Let V, w be lower semicontinuous on A and $A \times A$, respectively. If w is a weight of the form*

$$w(x, y) = W(x, \|x - y\|), \tag{3.7}$$

with lower semicontinuous W, then $E_s^k(\omega_N; w, V)$ is lower semicontinuous on A^N for a fixed $N \geqslant 1$.

Remark 3.6. To see that w must indeed only depend on the distance $\|x - y\|$, let $d = 2$ and

$$\omega_3^{(n)} = \{x_1, x_2^{(n)}, x_3\} = \left\{(0,0),\ \left(0, 1 + 2^{-n}\right),\ (1,0)\right\}$$

be a sequence of 3-point configurations, converging to $\omega_3 = \{x_i\}_1^3 := \{(0,0),\ (0,1),\ (1,0)\}$. Let further w be continuous, symmetric, and such that

$$w((0,0),\ (0,1)) = 3, \qquad w((0,0),\ (1,0)) = 1.$$

Then

$$E_1^1(\omega_3^{(n)}) = 3\|x_2^{(n)}\|^{-1} + 2\|x_3\|^{-1} \to 5, \quad n \to \infty,$$

while

$$E_1^1(\omega_3) = 2 \cdot 3\|x_2\|^{-1} + \|x_3\|^{-1} = 7,$$

since the tie-breaking convention in E_1^1 prefers points with smaller indices (see page 2), thereby violating the lower semicontinuity.

Proof of Lemma 3.5. Fix a configuration $\omega_N^\circ = \{x_1^\circ, \ldots, x_N^\circ\}$. In this proof, points and indices related to ω_N° will be denoted by the $^\circ$ superscript. Objects related to a variable configuration ω_N, approaching ω_N° in the product topology, will not carry this superscript.

If $x_i^\circ = x_j^\circ$ for some $i \neq j$, $E_s^k(\omega_N^\circ; w, V) = +\infty$. Due to the lower semicontinuity and nonnegativity of $\|\cdot\|^{-s}$ and w, and lower semicontinuity of V, there holds

$$E_s^k(\omega_N; w, V) \to +\infty, \qquad \text{whenever } \omega_N \to \omega_N^\circ \text{ in } A^N.$$

Let now ω_N° consist of distinct points and $V \equiv 0$. Fix an $\varepsilon > 0$. Note that when $\omega_N = \{x_i\}_1^N$ is sufficiently close to ω_N° in the l^∞ metric on A^N, so that

$$\|x_i - x_i^\circ\| < \Delta(\omega_N^\circ)/3, \qquad 1 \leqslant i \leqslant N,$$

the value of $E_s^k(\omega_N)$ continuously depends on x_i. In addition, by lower semicontinuity of w, for a sufficiently small $\delta_1 = \delta(\varepsilon)$, one has

$$w(x_i, x_j)\|x_i - x_j\|^{-s} \geqslant w(x_i^\circ, x_j^\circ)\|x_i^\circ - x_j^\circ\|^{-s} - \frac{\varepsilon}{k}$$

whenever $r_{ij} := \|x_i - x_j\|$ and $r_{ij}^\circ := \|x_i^\circ - x_j^\circ\|$ differ by at most δ_1 for $1 \leqslant i, j \leqslant N$ (we used here the specific form of w).

We shall further need to show that the nearest neighbor structure $\Lambda_k(\omega_N)$ does not change much in a neighborhood of ω_N° – or more precisely, distances to the k nearest neighbors remain approximately the same, even if the points themselves may be different. Fix an index i. To obtain lower semicontinuity of $E_s^k(\omega_N; w)$, it suffices to verify the semicontinuity at ω_N° only for the sum

$$\sum_{x_j \in \mathcal{N}(x_i;\omega_N)} \|x_i - x_j\|^{-s}$$

as a function of configuration ω_N. Consider distances from x_i° to the other entries of ω_N°:

$$d_l := \|x_i^\circ - (x_i; \omega_N^\circ)_l\|, \qquad 1 \leqslant l \leqslant N.$$

By the definition of $(x_i; \omega_N^\circ)_l$, $d_{l+1} \geqslant d_l$. Let $\{D_l\}_1^K$ be the strictly increasing sequence of unique values among $\{d_l\}$, $K \leqslant N$. Partition the multiset of entries of ω_N° as

$$\bigsqcup_{l=1}^{K} J_l^\circ, \qquad J_l^\circ := \{y \in \omega_N^\circ : \|x_i^\circ - y\| = D_l\},$$

according to the unique distances to x_i°. Note that when a configuration $\omega_N = (x_1, \ldots, x_N) \in A^N$ is such that $\|x_i - x_i^\circ\| < \delta$, $1 \leqslant i \leqslant N$, with

$$\delta < \min\left[\delta_1,\ \min\left\{(D_{l+1} - D_l)/4\right\}_1^{K-1}\right],$$

there holds

$$\|x_i - x_{j_1}\| < \|x_i - x_{j_2}\|, \qquad x_{j_1}^\circ \in J_{l_1}^\circ,\ x_{j_2}^\circ \in J_{l_2}^\circ,\ l_1 < l_2.$$

That is, the entries of $\omega_N \setminus \{x_i\}$ can be collected into K groups, $\{J_l\}_1^K$, with any element of a group J_{l_1} closer to x_i than any element of another group J_{l_2} when $l_1 < l_2$. By construction,

$$\#J_l^\circ = \#J_l, \qquad 1 \leqslant l \leqslant K,$$

so there is a bijection between elements of corresponding groups. Observe also that for every pair of elements $y, z \in J_l$ and a pair $y^\circ, z^\circ \in J_l^\circ$, belonging to corresponding groups, there holds

$$\big|\, \|y - z\| - \|y^\circ - z^\circ\| \,\big| < 2\delta,$$

which by the definition of δ_1 gives

$$w(y,z)\|y - z\|^{-s} \geqslant w(y^\circ, z^\circ)\|y^\circ - z^\circ\|^{-s} - \frac{\varepsilon}{k}.$$

By the aforementioned bijection between corresponding groups J_l° and J_l, it implies

$$\sum_{x_j \in \mathcal{N}(x_i;\omega_N)} w(x_i, x_j)\|x_i - x_j\|^{-s} \geqslant \sum_{x_j \in \mathcal{N}(x_i^\circ;\omega_N^\circ)} w(x_i^\circ, x_j^\circ)\|x_i^\circ - x_j^\circ\|^{-s} - \varepsilon,$$

proving the lower semicontinuity of the point energy for a single x_i, and therefore lower semicontinuity of $E_s^k(\,\cdot\,; w) = E_s^k(\,\cdot\,; w, 0)$. Addition of an external field is only introducing another lower semicontinuous term, which completes the proof. □

Corollary 3.7. *Under the assumptions of Lemma 3.5, minimizing the k-energy for any $k \geqslant 1$ and $s > 0$ yields a separated configuration.*

4 Proofs of the main results

4.1 Asymptotics on cubes

Let us demonstrate how to establish the existence of asymptotics on cubes for the Riesz k-energy functionals, following the outline in Section 3.1. We shall need this fact only for the unweighted E_s^k – or, equivalently, for the constant weight w and zero external field V. In this section, the ambient space is $\mathbb{R}^d$.

Lemma 4.1. *For $s > 0$ and k, d positive integers, the following limit exists, and is positive and finite:*

$$C_{s,d}^{k} := \lim_{N\to\infty} \frac{\mathcal{E}_s^k(q_d, N)}{N^{1+s/d}}, \tag{4.1}$$

which is the constant appearing in (1.6).

Proof. Set

$$\underline{\mathfrak{L}} := \liminf_{N\to\infty} \frac{\mathcal{E}_s^k(A, N)}{N^{1+s/d}}.$$

Fix $\varepsilon > 0$ and let $\{\underline{\omega}_n\}_{n\in\underline{\mathscr{N}}}$ be a subsequence of n-point configurations in A for which

$$E_s^k(\underline{\omega}_n) < (\underline{\mathfrak{L}} + \varepsilon)n^{1+s/d}, \qquad n \in \underline{\mathscr{N}}.$$

We shall show that

$$\overline{\mathfrak{L}} := \limsup_{N\to\infty} \frac{\mathcal{E}_s^k(A, N)}{N^{1+s/d}},$$

equals $\underline{\mathfrak{L}}$ establishing the existence of the limit (4.1).

Fix $N > k$ and let $\{\overline{\omega}_N\}$ be an N-point configuration in A such that

$$E_s^k(\overline{\omega}_N) < \mathcal{E}_s^k(A, N) + 1. \tag{4.2}$$

Let $n \in \underline{\mathscr{N}}$ and L be the unique positive integer such that

$$n(L-1)^d \leqslant N < nL^d. \tag{4.3}$$

By Corollary 3.4, there is a positive constant $c(s, k, d)$ such that the distance to the k-th nearest neighbor in $\underline{\omega}_n$ is at most $c(s, k, d)n^{-1/d}$. Let

$$\gamma := 1 - c(s, k, d)n^{-1/d},$$

and consider the following configuration obtained by tiling q_d with copies of $\frac{\gamma}{L}\underline{\omega}_n$:

$$\omega := \bigcup_{\boldsymbol{i}\in (L\mathbb{Z})^d} \left(\frac{\gamma}{L}\underline{\omega}_n + \frac{\boldsymbol{i}}{L}\right),$$

where $L\mathbb{Z} := \{0, 1, \ldots, L-1\}$. We observe that with this choice of γ the k nearest neighbors in ω for every point in the subset $\frac{\gamma}{L}\underline{\omega}_n + \frac{\boldsymbol{i}}{L}$ also belong to this subset.

We next obtain an upper bound for $E_s^k(\overline{\omega}_N)$ using ω. By the scale invariance of E_s^k there holds

$$E_s^k\left(\frac{\gamma}{L}\underline{\omega}_n\right) = \left(\frac{L}{\gamma}\right)^s E_s^k(\underline{\omega}_n),$$

and so from (4.2) and (4.3), we have

$$\begin{aligned}\frac{E_s^k(\overline{\omega}_N)}{N^{1+s/d}} &\leqslant \frac{E_s^k(\omega)+1}{N^{1+s/d}} = \frac{L^d\left(\frac{L}{\gamma}\right)^s E_s^k(\underline{\omega}_n)+1}{N^{1+s/d}}\\ &\leqslant \frac{L^d\left(\frac{L}{\gamma}\right)^s E_s^k(\underline{\omega}_n)}{(n(L-1)^d)^{1+s/d}} + N^{-1-s/d}\\ &\leqslant \gamma^{-s}\left(\frac{L}{L-1}\right)^{s+d}(\underline{\mathfrak{L}}+\varepsilon) + N^{-1-s/d},\end{aligned} \tag{4.4}$$

where in the first equality we used that due to the choice of γ, no interactions between different tiles enter the sum for $E_s^k(\omega)$. Taking the limit superior as $N \to \infty$ in (4.4) for fixed n which implies $L \to \infty$, gives

$$\overline{\mathfrak{L}} \leqslant \gamma^{-s}(\underline{\mathfrak{L}} + \varepsilon).$$

Then taking $n \to \infty$, $n \in \mathscr{N}$, (in which case $\gamma \to 1$) shows that $\overline{\mathfrak{L}} \leqslant \underline{\mathfrak{L}} + \varepsilon$. Since ε is arbitrary, $\overline{\mathfrak{L}} \leqslant \underline{\mathfrak{L}}$ and so the limit $C^k_{s,d}$ in (4.1) exists in $[0, \infty]$.

It remains to show that $C^k_{s,d}$ is finite and positive. Notice that $\mathcal{E}^k_s(A, N) = O(N^{1+s/d})$ follows by placing the points in ω_N in the vertices of the cubic lattice which shows that $C^k_{s,d}$ is finite. To see that $C^k_{s,d}$ is positive, observe that for any configuration $\omega_N \subset [0,1]^d$ of N distinct points there holds

$$E^k_s(\omega_N) = \sum_{i=1}^{N} \sum_{y \in \mathcal{N}_k(x_i;\omega_N)} \|x_i - y\|^{-s} \geqslant \sum_{i=1}^{N} \|x_i - (x_i;\omega_N)_1\|^{-s} =: \sum_{i=1}^{N} r_i^{-s},$$

where as before we write $(x_i;\omega_N)_1$ for the nearest neighbor of x_i. Notice that the interiors of balls $B(x_i, r_i/2)$ are disjoint and contained in $[-\sqrt{2}, 1+\sqrt{2}]^d$, so $v_d \sum_i r_i^d \leqslant 2^{d/2}6^d$, where v_d denotes the volume of d-dimensional unit ball. In conjunction with Jensen's inequality this implies

$$\sum_{i=1}^{N} r_i^{-s} = \sum_{i=1}^{N} (r_i^d)^{-s/d} \geqslant N \left(\frac{1}{N} \sum_{i=1}^{N} r_i^d \right)^{-s/d} \geqslant N^{1+s/d} \, (2^{d/2}6^d/v_d)^{-s/d},$$

which is the desired lower bound. □

From scale- and translation-invariance of E^k_s, we obtain also the asymptotics for a general cube in $\mathbb{R}^d$.

Corollary 4.2. *For $s > 0$, k, d positive integers, and a cube $Q = x + aq_d \subset \mathbb{R}^d$ the following limit exists:*

$$\lim_{N\to\infty} \frac{\mathcal{E}^k_s(Q, N)}{N^{1+s/d}} = \frac{C^k_{s,d}}{a^s} = \frac{C^k_{s,d}}{\mathcal{H}_d(Q)^{s/d}}.$$

The lower bound on $\mathcal{E}^k_s$ derived in the proof of Lemma 4.1 relied on the condition $A = [0,1]^d$. To verify the short-range property, it will be necessary that $\mathcal{E}^k_s(A, N)$ grow to infinity with N, for which it suffices to assume that A is compact. In the following lemma we establish such growth for energy on compact sets.

Lemma 4.3. *Suppose $A \subset \mathbb{R}^d$ is a compact set, $k \geqslant 1$, and $s > 0$. Then*

$$\liminf_{N\to\infty} \frac{\mathcal{E}^k_s(A, N)}{N^{1+s/d}} \geqslant C(s,d)\,(\mathcal{L}_d(A))^{-s/d}.$$

Proof. Clearly, it is sufficient to assume $k = 1$. Fix an $\varepsilon > 0$. By Besicovitch's covering theorem [20, Theorem 2.7], for every sufficiently small $r > 0$ there exist a collection of balls $\{B_m\}_1^M := \{B(x_m, r)\}_{m=1}^M$ that cover A and satisfy

$$\sum_{m=1}^{M} v_d r^d = M v_d r^d \leqslant c(d) \mathcal{L}_d(A_r)$$

where as usual, A_r is the r-neighborhood of A. In fact, each point of $\mathbb{R}^d$ is contained in at most $c(d)$ among $\{B_m\}$. Let $\omega_N \in A^N$ be an arbitrary configuration of N points and denote by ω'_N the subset of its elements x, contained in some B_m that also contains at least one other element of ω_N. Then $\#(\omega_N \setminus \omega'_N) \leqslant M$. In addition, whenever B_m contains at least 2 elements of ω_N, for every such element $x \in \omega'_N \cap B_m$ there holds

$$r_x = \|x - (x;\omega_N)_1\| \leqslant 2r.$$

Note that the balls $\{B(x, r_x/2)\}_{x \in \omega_N}$ are disjoint, which gives

$$\sum_{x \in B(x_m, r)} v_d r_x^d \leqslant v_d (3r)^d,$$

Applying Jensen's inequality, one has

$$\begin{aligned}
E_s^k(\omega_N) &\geqslant \sum_{x\in\omega_N} r_x^{-s} \geqslant \sum_{x\in\omega'_N} r_x^{-s} = \sum_{x\in\omega'_N} (r_x^d)^{-s/d} \\
&\geqslant (N-M)\left(\frac{1}{N-M}\sum_{x\in\omega'_N} r_x^d\right)^{-s/d} \geqslant (N-M)^{1+s/d}(3^d M r^d)^{-s/d} \\
&\geqslant (N-M)^{1+s/d} C(s,d)(\mathcal{L}_d(A_r))^{-s/d}.
\end{aligned}$$

Since M is fixed, this gives further

$$\liminf_{N\to\infty} \frac{\mathcal{E}_s^k(A,N)}{N^{1+s/d}} \geqslant C(d)(\mathcal{L}_d(A_r))^{-s/d}.$$

By taking $r \downarrow 0$, the lemma follows. $\square$

We conclude this section with the proof of the short-range property for the functional E_s^k. The proof will use that $\mathcal{E}_s^k(A,N)$ grows to infinity, as we just established for all compact subsets of $\mathbb{R}^p$.

Lemma 4.4. *Let $A_1, A_2 \subset \mathbb{R}^p$ be disjoint compact sets. If $\{\omega_N\}$ is a sequence of N-point configurations in $A_1 \cup A_2$ for $N \geqslant 2$, then*

$$\lim_{N\to\infty} \frac{E_s^k(\omega_N\cap A_1) + E_s^k(\omega_N \cap A_2)}{E_s^k(\omega_N)} = 1. \tag{4.5}$$

Proof. Notice that for any $x \in \omega_N$,

$$\|x - (x;\omega_N)_l\| \leqslant \|x - (x;\omega_N\cap A_m)_l\|, \qquad 1 \leqslant l \leqslant k,\ m = 1,2.$$

As a result, there holds

$$\sum_{y\in\mathcal{N}_k(x;\omega_N)} \|x-y\|^{-s} \geqslant \sum_{y\in\mathcal{N}_k(x;\omega_N\cap A_m)} \|x-y\|^{-s}, \qquad x\in\omega_N,\ m=1,2,$$

which gives

$$E_s^k(\omega_N\cap A_1) + E_s^k(\omega_N\cap A_2) \leqslant E_s^k(\omega_N)$$

and

$$\limsup_{N\to\infty} \frac{E_s^k(\omega_N\cap A_1) + E_s^k(\omega_N \cap A_2)}{E_s^k(\omega_N)} \leqslant 1.$$

It remains to derive the converse estimate. Since A_1, A_2 are compact and disjoint, $\mathrm{dist}(A_1, A_2) = h > 0$. Pick an element $x \in \omega_N$; without loss of generality, $x \in A_1$. There are two possibilities: i) $(x;\omega_N)_k \in A_1$, in which case all the terms of the form

$$\sum_{y\in\mathcal{N}_k(x;\omega_N)} \|x-y\|^{-s}$$

are shared by the two sums $E_s^k(\omega_N\cap A_1) + E_s^k(\omega_N\cap A_2)$ and $E_s^k(\omega_N)$; ii) $(x;\omega_N)_k \in A_1$, in which case (see Section 3.1 for the adjacency graph notation)

$$\Lambda_k(\omega_N) \setminus [\Lambda_k(\omega_N\cap A_1) \cup \Lambda_k(\omega_N \cap A_2)] \supset \{(x,y) : y \in \mathcal{N}_k(x;\omega_N),\ y\in A_2\};$$

in other words, some of the edges connecting x to its nearest neighbors in ω_N are missing from the union of adjacency graphs $\bigcup_{m=1}^2 \Lambda_k(\omega_N\cap A_m)$. On the other hand, all the terms occurring in $E_s^k(\omega_N)$ but not in $E_s^k(\omega_N\cap A_1) + E_s^k(\omega_N\cap A_2)$ are precisely of this form, so collecting all the pairs with $x\in A_1$ into

$$G_1 := \bigcup_{x\in\omega_N\cap A_1} \{(x,y) : y\in\mathcal{N}_k(x;\omega_N),\ y\in A_2\}$$

and those with $x \in A_2$ into

$$G_2 := \bigcup_{x \in \omega_N \cap A_2} \{(x,y) : y \in \mathcal{N}_k(x;\omega_N),\ y \in A_1\},$$

we conclude

$$\Lambda_k(\omega_N) \setminus [\Lambda_k(\omega_N \cap A_1) \cup \Lambda_k(\omega_N \cap A_2)] = G_1 \cup G_2.$$

It follows

$$\begin{aligned}
E_s^k(\omega_N) &= \sum_{(x,y)\in\Lambda_k(\omega_N)} \|x-y\|^{-s} \\
&\leqslant \left(\sum_{(x,y)\in\Lambda_k(\omega_N\cap A_1)} + \sum_{(x,y)\in\Lambda_k(\omega_N\cap A_2)} + \sum_{(x,y)\in G_1} + \sum_{(x,y)\in G_2} \right) \|x-y\|^{-s} \\
&\leqslant E_s^k(\omega_N \cap A_1) + E_s^k(\omega_N \cap A_2) + Nk\, h^{-s}.
\end{aligned}$$

Here in the last inequality we used that $\|x-y\|^{-s} \leqslant h^{-s}$ for x, y placed in different A_m, and that the total number of edges in $\Lambda_k(\omega_N)$ is Nk. Using Lemma 4.3 with $p = d$, we conclude that $Nk\, h^{-s} = o(E_s^k(\omega_N))$, whence dividing the last display through by $E_s^k(\omega_N)$ and taking N to infinity yields

$$\liminf_{N\to\infty} \frac{E_s^k(\omega_N \cap A_1) + E_s^k(\omega_N \cap A_2)}{E_s^k(\omega_N)} \geqslant 1,$$

completing the proof of the lemma. □

4.2 Stability and poppy-seed bagel asymptotics for E_s^k

In this section we establish a set-stability result for E_s^k as described in (3.3). This lemma will play a key role in the proof of Theorem 4.7 which is the main goal of this section.

Lemma 4.5. *For a compact set $A \subset \mathbb{R}^p$ with $0 < \mathcal{M}_d(A) < \infty$, $s > 0$, and any $\varepsilon > 0$, there exists a $\delta = \delta(\varepsilon, s, k, p, d, A) > 0$ such that the inequalities*

$$\liminf_{N\to\infty} \frac{\mathcal{E}_s^k(A,N)}{N^{1+s/d}} \geqslant (1-\varepsilon) \liminf_{N\to\infty} \frac{\mathcal{E}_s^k(D,N)}{N^{1+s/d}}, \qquad \limsup_{N\to\infty} \frac{\mathcal{E}_s^k(A,N)}{N^{1+s/d}} \geqslant (1-\varepsilon) \limsup_{N\to\infty} \frac{\mathcal{E}_s^k(D,N)}{N^{1+s/d}}$$

hold whenever a compact set $D \subset A$ satisfies $\mathcal{M}_d(D) > (1-\delta)\mathcal{M}_d(A)$. In the case $d = p$, δ can be chosen independently of A.

Proof. Let ω_N^* be a sequence of configurations satisfying $E_s^k(\omega_N^*) < \mathcal{E}_s^k(A,N) + 1$, $N \geqslant 1$. According to Theorem 1.3, the separation for this sequence satisfies $\Delta(\omega_N^*) \geqslant CN^{-1/d}$ for $C = C(s,k,d,A)$.

The proof will consist in demonstrating a way to retract configurations from A to D without increasing the value of E_s^k on them too much. We will first show that most of $x_i \in \omega_N^*$ have a point from D close to them, for N sufficiently large. In this proof let us write $S(r) = S_r$ for the closed r-neighborhood of a set S; observe that $D(r) \subset A(r)$ for any $r > 0$.

Let $\delta \in (0,1)$ and $D \subset A$ be a compact set satisfying $\mathcal{M}_d(D) > (1-\delta)\mathcal{M}_d(A)$. Then for all sufficiently small $r > 0$, $\mathcal{L}_p[A(r)] - \mathcal{L}_p[D(r)] < v_{p-d} r^{p-d}\, 3\delta \mathcal{M}_d(A)$, by the definition of Minkowski content. In particular, for $N \geqslant N_0 = N_0(A,D,\delta)$ and any $0 < \gamma < C/4$ there holds

$$\mathcal{L}_p\left[A(\gamma N^{-1/d})\right] - \mathcal{L}_p\left[D(\gamma N^{-1/d})\right] < v_{p-d}\gamma^{p-d} N^{-(p-d)/d}\, 3\delta\mathcal{M}_d(A).$$

Thus the number of disjoint balls of radius $\gamma N^{-1/d}$ that can be contained in $A(\gamma N^{-1/d}) \setminus D(\gamma N^{-1/d})$ is at most

$$\frac{v_{p-d}\gamma^{p-d} N^{-(p-d)/d}\, 3\delta\mathcal{M}_d(A)}{v_p \gamma^p N^{-p/d}} = \delta\, c(p,d)\gamma^{-d} N \mathcal{M}_d(A).$$

It follows that for at least $N(1-\delta c(p,d)\gamma^{-d}\mathcal{M}_d(A))$ points in ω_N^*, a closest point in D is at most distance

$$2\gamma N^{-1/d}$$

away. Consider the subset $\{x_i'\}\subset\omega_N^*$ for which this is the case, and for each x_i' find a closest point in D. Denote the resulting set by ω. By the preceding discussion, it can be assumed

$$N_\omega := \#\omega = \left\lfloor N\left(1-\delta c(p,d)\gamma^{-d}\mathcal{M}_d(A)\right)\right\rfloor, \qquad N\geqslant N_0. \tag{4.6}$$

Consider a pair x_i', x_j'; let their nearest points in ω be y_i and y_j respectively. Since the separation between entries of ω_N^* is at least $CN^{-1/d}$, there holds

$$\|y_i-y_j\|\geqslant(1-2\gamma/C)\|x_i'-x_j'\|>0, \qquad i\neq j,$$

where we used that $2\gamma<C/2$. Due to the scaling properties of the kernel $\|x-y\|^{-s}$, this implies in turn

$$E_s^k(\omega_N^*)\geqslant(1-2\gamma/C)^sE_s^k(\omega).$$

By the estimate (4.6) on the cardinality N_ω, we have finally

$$\frac{E_s^k(\omega_N^*)}{N^{1+s/d}}\geqslant(1-2\gamma/C)^s\big(1-\delta c(p,d)\gamma^{-d}\mathcal{M}_d(A)\big)^{1+s/d}\cdot\frac{\mathcal{E}_s^k(D,N_\omega)}{N_\omega^{1+s/d}}, \qquad N\geqslant N_0.$$

Setting $\gamma=C\delta^{1/2d}$ gives

$$\frac{\mathcal{E}_s^k(A,N)+1}{N^{1+s/d}}\geqslant(1-2\delta^{1/2d})^s\Big(1-\sqrt{\delta}\,c(p,d)\mathcal{M}_d(A)/C^d\Big)^{1+s/d}\cdot\frac{\mathcal{E}_s^k(D,N_\omega)}{N_\omega^{1+s/d}}, \qquad N\geqslant N_0, \tag{4.7}$$

implying the claim of the lemma for lim inf and a suitably small δ.

To prove the claim for lim sup, observe that following the above construction, given a cardinality $N\geqslant N_0$, one obtains cardinality

$$N_\omega=\Big\lfloor N\Big(1-\sqrt{\delta}\,c(p,d)\mathcal{M}_d(A)/C^d\Big)\Big\rfloor =: \lfloor N(1-c\sqrt{\delta})\rfloor,$$

for which inequality (4.7) holds. Here $c=c(s,k,p,d,A)$. Furthermore, the inequality (4.7) is also satisfied if N_ω is replaced with $N_\omega-1$. Since the image of the set $\{N : N\geqslant N_0\}$ under the mapping

$$n\mapsto\lfloor n(1-c\sqrt{\delta})\rfloor$$

contains $\{N : N\geqslant N_0\}$ for $\delta<(1/2c)^2$, for every given $N_\omega\geqslant k+1$, there exists a cardinality N, such that the inequality (4.7) holds with these particular values of N and N_ω. Now let $\mathscr{N}\subset\mathbb{N}$ be a sequence along which

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

is attained; taking $\mathscr{N}\ni N_\omega\to\infty$ in (4.7) completes the proof for lim sup.

Finally, for $d=p$, notice that by Corollary 3.3, $\mathcal{M}_d(A)/C^d=c(s,d,k)$ for sufficiently large N, so indeed δ in (4.7) is independent of A. This proves the last claim of the lemma. □

In the last auxiliary result before the main theorem of this section, we show that any functional equipped with the monotonicity, short-range, and stability properties from Section 3.1, and for which the asymptotics are known for all compact subsets of $\mathbb{R}^d$, also has asymptotics on $(\mathcal{H}_d,d)$-rectifiable subsets of $\mathbb{R}^p$, $p\geqslant d$. In addition, the formula for the asymptotics coincides with that on the compact subsets of $\mathbb{R}^d$. The precise statement follows; in it, we say that a functional acting on collections ω_N is *continuous under near-isometries*, if for any $\varepsilon>0$, there is a γ such that for every bi-Lipschitz map $\psi:\mathbb{R}^p\to\mathbb{R}^p$ with constant less then $(1+\gamma)$,

$$(1+\varepsilon)^{-1}\mathfrak{e}_N(\omega_N)\leqslant\mathfrak{e}_N(\psi(\omega_N))\leqslant(1+\varepsilon)\mathfrak{e}_N(\omega_N), \qquad f(c)\geqslant0,\ \lim_{c\downarrow0}f(c)=0.$$

Lemma 4.6. *Suppose $\mathfrak{e}_N : (\mathbb{R}^p)^N \to [0,\infty]$ is a sequence of functionals, continuous under near-isometries. For a compact $A \subset \mathbb{R}^p$, denote $\mathfrak{e}_N^*(A) := \inf_{\omega_N \subset A} \mathfrak{e}_N(\omega_N)$. Assume that $\mathfrak{e}_N$ have the following properties:*

1. *$\mathfrak{e}_N^*(A) \geqslant \mathfrak{e}_N^*(B)$ whenever $A \subset B \subset \mathbb{R}^p$ are compact sets.*
2. *Suppose $A_1, A_2 \subset \mathbb{R}^p$ are disjoint compact sets. If (ω_N) is a sequence of N-point configurations in $A_1 \cup A_2$ for $N \geqslant 2$, then*
$$\lim_{N\to\infty} \frac{\mathfrak{e}_{N_1}(\omega_N \cap A_1) + \mathfrak{e}_{N_2}(\omega_N \cap A_2)}{\mathfrak{e}_N(\omega_N)} = 1,$$
where N_m are the cardinalities of the intersections $\omega_N \cap A_m$, $m = 1, 2$.
3. *For every compact $A \subset \mathbb{R}^p$ and $\varepsilon \in (0,1)$ there is a $\delta > 0$ and $s > 0$ such that for any compact $D \subset A$ satisfying $\mathcal{M}_d(D) \geqslant (1-\delta(\varepsilon))\,\mathcal{M}_d(A)$, we have*
$$\liminf_{N\to\infty} \frac{\mathfrak{e}_N^*(A)}{N^{1+s/d}} \geqslant (1-\varepsilon) \liminf_{N\to\infty} \frac{\mathfrak{e}_N^*(D)}{N^{1+s/d}}.$$
4. *For every compact $A \subset \mathbb{R}^d$ and some $s > 0$,*
$$\lim_{N\to\infty} \frac{\mathfrak{e}_N^*(A)}{N^{1+s/d}} = \frac{C_{\mathfrak{e}}}{\mathcal{H}_d(A)^{s/d}}.$$

Then, for every $(\mathcal{H}_d, d)$-rectifiable compact set $A \subset \mathbb{R}^p$,
$$\lim_{N\to\infty} \frac{\mathfrak{e}_N^*(A)}{N^{1+s/d}} = \frac{C_{\mathfrak{e}}}{\mathcal{H}_d(A)^{s/d}}.$$

Proof. Fix an $\varepsilon > 0$ and let $\delta > 0$ be as in the stability assumption *3.* Without loss of generality, $0 < \delta < \varepsilon$. By a standard fact from geometric measure theory [10, Lemma 3.2.18], there exist bi-Lipschitz maps $\psi_m : \mathbb{R}^d \to \mathbb{R}^p$ with constant smaller then $(1+\gamma)$, and compact sets $K_m \subset \mathbb{R}^d$, $1 \leqslant m \leqslant M$ such that sets $\{\psi_m(K_m)\}$ are disjoint, contained in A, and
$$\mathcal{H}_d\left(A \setminus \bigcup_{m=1}^{M} \psi(K_m)\right) < \delta.$$
Without loss of generality, $0 < \gamma < \varepsilon$. Denoting $\tilde{A} := \bigcup_m \psi(K_m) \subset A$, we have from monotonicity assumption *1.*:
$$\limsup_{N\to\infty} \frac{\mathfrak{e}_N^*(A)}{N^{1+s/d}} \leqslant \limsup_{N\to\infty} \frac{\mathfrak{e}_N^*(\tilde{A})}{N^{1+s/d}}. \tag{4.8}$$
On the other hand, both A and $\tilde{A}$ are compact, $(\mathcal{H}_d, d)$-rectifiable, and $\mathcal{H}_d(A) = \mathcal{M}_d(A)$, $\mathcal{H}_d(\tilde{A}) = \mathcal{M}_d(\tilde{A})$, see [3, Lemma 4.3]; combined with the assumption on δ, this means the stability property *3.* applies, so that
$$\liminf_{N\to\infty} \frac{\mathfrak{e}_N^*(A)}{N^{1+s/d}} \geqslant (1-\varepsilon) \liminf_{N\to\infty} \frac{\mathfrak{e}_N^*(\tilde{A})}{N^{1+s/d}}. \tag{4.9}$$
By the last two displays, it suffices to derive the asymptotics of $\mathfrak{e}_N^*$ for $\tilde{A}$. This is where the short-range assumption *2.* comes into play.

Consider a sequence $\omega_N^* \subset \tilde{A}$, $N \geqslant 1$, such that $\mathfrak{e}_N(\omega_N^*) < \mathfrak{e}_N^*(\tilde{A}) + 1$. Let $A_m := \psi_m(K_m) \subset \tilde{A}$ and $N_m := \#(\omega_N^* \cap A_m)$. By passing to a subsequence, the following limits can be assumed to exist:
$$\beta_m := \lim_{N\to\infty} \frac{N_m}{N}, \qquad 1 \leqslant m \leqslant M.$$

Using assumption *2.*, the fact that A_m are disjoint, and the choice of ψ_m, we have

$$\begin{aligned}\liminf_{N\to\infty} \frac{\mathfrak{e}_N^*(A)+1}{N^{1+s/d}} &\geqslant \liminf_{N\to\infty} \frac{\mathfrak{e}_N(\omega_N^*)}{\sum_m \mathfrak{e}_{N_m}(\omega_N^*\cap A_m)} \cdot \frac{\sum_m \mathfrak{e}_{N_m}(\omega_N^*\cap A_m)}{N^{1+s/d}} \\ &= \liminf_{N\to\infty} \sum_m \left(\frac{N_m}{N}\right)^{1+s/d} \cdot \frac{\mathfrak{e}_{N_m}(\omega_N^*\cap A_m)}{N_m^{1+s/d}} \\ &\geqslant \sum_m \beta_m^{1+s/d} \cdot \liminf_{N\to\infty} \frac{\mathfrak{e}_{N_m}(\omega_N^*\cap A_m)}{N^{1+s/d}} \\ &\geqslant (1+\varepsilon)^{-1} \sum_m \beta_m^{1+s/d} \cdot \liminf_{N\to\infty} \frac{\mathfrak{e}_{N_m}(\psi_m^{-1}(\omega_N^*)\cap K_m)}{N^{1+s/d}},\end{aligned}$$

where the last inequality used that $\psi_m^{-1}(A_m) = K_m$ with a bi-Lipschitz constant $(1+\varepsilon)$. Using the asymptotics on subsets of $\mathbb{R}^d$ in assumption *4.*, we conclude further

$$\liminf_{N\to\infty} \frac{\mathcal{E}_s^k(\tilde{A},N)+1}{N^{1+s/d}} \geqslant (1+\varepsilon)^{-1} \sum_m \beta_m^{1+s/d} \cdot \frac{C_{\mathfrak{e}}}{\mathcal{H}_d(K_m)^{s/d}}. \tag{4.10}$$

Observe that the right-hand side of the previous display is minimal over nonnegative $\{\beta_m\}$ with $\sum_m \beta_m = 1$ when $\beta_m = \mathcal{H}_d(K_m)/\sum \mathcal{H}_d(K_m)$. As a result, to obtain an upper bound for the asymptotics, we choose N_m in such a way that $\sum_m N_m = N$, $N_m/N \to \mathcal{H}_d(K_m)/\sum_m \mathcal{H}_d(K_m)$, $N\to\infty$; then an upper bound on $\mathfrak{e}_N^*(\tilde{A})$ is obtained by taking the union of configurations $\omega_{N_m}^* \subset A_m$ for which $\mathfrak{e}_N(\omega_{N_m}^*) \leqslant \mathfrak{e}_N^*(A_m)+1$. Indeed, by the short-range assumption *2.* and the same argument as above applied to $\bigcup_m \omega_{N_m}^*$,

$$\begin{aligned}\limsup_{N\to\infty} \frac{\mathfrak{e}_N^*(\tilde{A})}{N^{1+s/d}} &\leqslant \sum_m \left(\frac{\mathcal{H}_d(K_m)}{\sum \mathcal{H}_d(K_m)}\right)^{1+s/d} \cdot \limsup_{N\to\infty} \frac{\mathfrak{e}_{N_m}^*(A_m)}{N^{1+s/d}} \\ &\leqslant \sum_m \left(\frac{\mathcal{H}_d(K_m)}{\sum \mathcal{H}_d(K_m)}\right)^{1+s/d} \cdot (1+\varepsilon) \limsup_{N\to\infty} \frac{\mathfrak{e}_{N_m}^*(K_m)}{N^{1+s/d}} \\ &= (1+\varepsilon)\cdot \frac{C_{\mathfrak{e}}}{\left(\sum_m \mathcal{H}_d(K_m)\right)^{s/d}} \leqslant (1+\varepsilon)^{1+s} \cdot \frac{C_{\mathfrak{e}}}{\left(\mathcal{H}_d(\tilde{A})\right)^{s/d}}.\end{aligned} \tag{4.11}$$

Here we again used that $\{\psi_m\}$ are bi-Lipschitz with the constant $(1+\gamma) \leqslant (1+\varepsilon)$. Finally, the substitution of (4.10)–(4.11) into (4.8)–(4.9) yields

$$(1-\varepsilon)(1+\varepsilon)^{-1} \frac{C_{\mathfrak{e}}}{(\mathcal{H}_d(A))^{s/d}} \leqslant \liminf_{N\to\infty} \frac{\mathfrak{e}_N^*(A)}{N^{1+s/d}} \leqslant \limsup_{N\to\infty} \frac{\mathfrak{e}_N^*(A)}{N^{1+s/d}} \leqslant (1+\varepsilon)^{1+s} \frac{C_{\mathfrak{e}}}{(\mathcal{H}_d(A)-\varepsilon)^{s/d}},$$

so that taking $\varepsilon \downarrow 0$ finishes the proof of the lemma. □

We are now in the position to prove our main theorem for the case with no weight or external field. Note that we have verified that E_s^k satisfies the properties formulated in Section 3.1, and is therefore an example of a *short-range interaction* [16].

Theorem 4.7. *Suppose $A \subset \mathbb{R}^p$ is a compact $(\mathcal{H}_d, d)$-rectifiable set with $\mathcal{M}_d(A) = \mathcal{H}_d(A)$, $s > 0$, $k \geqslant 1$, and $p \geqslant d$. Then*

$$\lim_{N\to\infty} \frac{\mathcal{E}_s^k(A,N)}{N^{1+s/d}} = \frac{C_{s,d}^k}{\mathcal{H}_d(A)^{s/d}}, \tag{4.12}$$

where the constant $C_{s,d}^k$ was introduced in (4.1).

Note that this is a special case of Theorem 1.1, in which $\rho(x) \equiv 1/\mathcal{H}_d(A)$. We obtain the result about limiting distribution in the general situation (with weight and external field) below, in Section 4.3.

Proof. This proof uses the approach developed in [16] for general short-range interactions. We proceed by establishing the asymptotics for unions of cubes, then for compact sets in $\mathbb{R}^d$ ($p = d$ case), before finally proving that (4.12) holds for compact $(\mathcal{H}_d, d)$-rectifiable sets A. Let $\mathcal{H}_d(A) > 0$ first.

We first consider the case $A = \bigcup_1^M Q_m$, a union of equal closed disjoint cubes. Fix a sequence ω_N^*, for which $E_s^k(\omega_N^*) < \mathcal{E}_s^k(A, N) + 1$. Passing to a subsequence if necessary, it can be assumed that the following limits exist

$$\beta_m := \lim_{N\to\infty} \frac{N_m}{N}, \qquad 1 \leqslant m \leqslant M,$$

where we set $N_m = \#(\omega_N^* \cap Q_m)$. On the one hand,

$$\begin{aligned}
\liminf_{N\to\infty} \frac{\mathcal{E}_s^k(A,N)+1}{N^{1+s/d}} &\geqslant \liminf_{N\to\infty} \frac{E_s^k(\omega_N^*)}{N^{1+s/d}} = \liminf_{N\to\infty} \frac{E_s^k(\omega_N^*)}{\sum_m E_s^k(\omega_N^* \cap Q_m)} \cdot \frac{\sum_m E_s^k(\omega_N^* \cap Q_m)}{N^{1+s/d}} \\
&\geqslant \sum_m \liminf_{N\to\infty} \frac{\mathcal{E}_s^k(Q_m, N_m)}{N^{1+s/d}} = \sum_m \beta_m^{1+s/d} \liminf_{N\to\infty} \frac{\mathcal{E}_s^k(Q_1, N_m)}{N_m^{1+s/d}} \\
&\geqslant \liminf_{N\to\infty} \frac{\mathcal{E}_s^k(Q_1, N)}{N^{1+s/d}} \cdot \sum_m \beta_m^{1+s/d} = \frac{C_{s,d}^k}{\mathcal{H}_d(Q_1)} \cdot \sum_m \beta_m^{1+s/d},
\end{aligned}$$

where we used the short-range property for E_s^k, Corollary 4.2, and that all the cubes Q_m are equal, hence the value of $\mathcal{E}_s^k(Q_m, N)$ is independent of m. On the other hand, given $\beta_m = 1/M$, $1 \leqslant m \leqslant M$, it suffices to place in Q_m a configuration $\omega_{N_m}^*$ of cardinality $N_m = \lfloor N/M \rfloor$ with $E_s^k(\omega_{N_m}^*) < \mathcal{E}_s^k(Q_m, N_m) + 1$ to obtain

$$\begin{aligned}
\limsup_{N\to\infty} \frac{\mathcal{E}_s^k(A,N)}{N^{1+s/d}} &\leqslant \limsup_{N\to\infty} \frac{E_s^k\left(\bigcup_m \omega_{N_m}^*\right)}{N^{1+s/d}} = \limsup_{N\to\infty} \frac{E_s^k\left(\bigcup_m \omega_{N_m}^*\right)}{\sum_m E_s^k(\omega_{N_m}^*)} \cdot \frac{\sum_m E_s^k(\omega_{N_m}^*)}{N^{1+s/d}} \\
&\leqslant \sum_m \limsup_{N\to\infty} \frac{E_s^k(\omega_{N_m}^*)}{N^{1+s/d}} = \sum_m \beta_m^{1+s/d} \limsup_{N\to\infty} \frac{E_s^k(\omega_{N_m}^*)}{N_m^{1+s/d}} \\
&= \limsup_{N\to\infty} \frac{\mathcal{E}_s^k(Q_1, N)}{N^{1+s/d}} \cdot \sum_m \beta_m^{1+s/d} = \frac{C_{s,d}^k}{\mathcal{H}_d(Q_1)} \cdot M^{-s/d}.
\end{aligned}$$

Since the minimum of $\sum_m \beta_m^{1+s/d}$ for nonnegative β_m with $\sum_m \beta_m = 1$ is obtained for $\beta_1 = \ldots = \beta_M = 1/M$, asymptotics for the union of M equal cubes is $M^{-s/d}$ times the asymptotics for one such cube, in agreement with (4.12).

The case of a union of closed equal cubes with disjoint interiors (but not necessarily disjoint) follows by an application of stability and monotonicity by approximating the cubes of the union from the inside with disjoint equal cubes. We shall omit the details and instead discuss obtaining (4.12) for general compact sets from unions of cubes with disjoint interiors. The omitted argument follows the same lines.

It suffices to assume $\mathcal{H}_d(A) > 0$, since otherwise A can be covered with a union of equal cubes of arbitrarily small measure, and monotonicity property directly implies that the limit from (4.12) is infinite. Now fix an $\varepsilon > 0$. For $\delta = \delta(\varepsilon, s, k, p, d)$ as in Lemma 4.5 (note that δ is set-independent!), let $J_\varepsilon \supset A$ be a finite union of closed equal dyadic cubes with disjoint interiors, such that $\mathcal{H}_d(A) > (1-\delta)\mathcal{H}_d(J_\varepsilon)$; then formula (4.12) applies to J_ε. Without loss of generality, $\delta \leqslant \varepsilon < 1$. On the one hand, monotonicity property together with asymptotics on J_ε give

$$\liminf_{N\to\infty} \frac{\mathcal{E}_s^k(A,N)}{N^{1+s/d}} \geqslant \lim_{N\to\infty} \frac{\mathcal{E}_s^k(J_\varepsilon, N)}{N^{1+s/d}} = \frac{C_{s,d}^k}{\mathcal{H}_d(J_\varepsilon)^{s/d}} \geqslant (1-\varepsilon)^{s/d} \frac{C_{s,d}^k}{\mathcal{H}_d(A)^{s/d}}.$$

On the other, by the choice of J_ε and stability property from Lemma 4.5 applied to the pair of sets $A \subset J_\varepsilon$,

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

which completes the proof when A is a general compact subset of $\mathbb{R}^d$.

To obtain the desired result for $(\mathcal{H}_d, d)$-rectifiable $A \subset \mathbb{R}^p$ with $\mathcal{H}_d(A) > 0$, note that Lemma 4.6 applies to E_s^k in view of Lemmas 4.4 and 4.5. It thus remains to discuss the case $\mathcal{H}_d(A) = \mathcal{M}_d(A) = 0$. We can argue by contradiction: suppose

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

and let $\{n : n \in \mathscr{N}\}$ be the subsequence along which the lim inf is attained. Without loss of generality, $k = 1$. Let further ω_n^* be the sequence of configurations with $E_s^1(\omega_n^*) < \mathcal{E}_s^1(A,n) + 1$ for every $n \in \mathscr{N}$. It follows that for n_0 sufficiently large,

$$\sum_{x\in\omega_n} \|x - (x;\omega_n^*)_1\|^{-s} \leqslant 2Cn^{1+s/d}, \qquad n \geqslant n_0,$$

implying that for any $\gamma > 0$, the number of elements $x \in \omega_n^*$ such that $\|x - (x;\omega_n^*)_1\| < \gamma n^{-1/d}$ is at most $2C\gamma^s N$. Taking γ small enough gives at least $n(1 - 2C\gamma^s)$ elements $x \in \omega_n$ for which $\|x - (x;\omega_n^*)_1\| \geqslant \gamma n^{-1/d}$. Denote the set of such x by $\omega_n' \subset \omega_n$. It follows that the balls $\{B(x, \gamma n^{-1/d}) : x \in \omega_n'\}$ are disjoint, and so in view of

$$\bigcup_{x\in\omega_n'} B(x,\gamma n^{-1/d}) \subset A_{\gamma n^{-1/d}},$$

for any $\varepsilon > 0$ and all large enough $n_1 = n_1(\varepsilon)$ there holds

$$\#\omega_n' v_p(\gamma n^{-1/d})^p \leqslant (\mathcal{M}_d(A) + \varepsilon) v_{p-d}(\gamma n^{-1/d})^{p-d}, \qquad n \geqslant n_1.$$

Using that $\#\omega_n' \geqslant (1 - 2C\gamma^s)n$ and $\mathcal{M}_d(A) = 0$, from the last display we have

$$(1 - 2C\gamma^s) v_p \gamma^d \leqslant v_{p-d}\varepsilon,$$

which is the desired contradiction for sufficiently small $\varepsilon > 0$. This proves

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

□

4.3 Adding a multiplicative weight and external field

We will now extend the results of the previous section by introducing an external field and a weight, so that the problem at hand is optimization of the functional (1.3). An essential ingredient in the proof is the partitioning of the set A according to the values of V; similar ideas were used by the authors in [15].

First, some remarks about the positivity of weight w and external field V are in order.

Remark 4.8. Since V is assumed to be lower semicontinuous and A is compact, it follows that V is bounded below on A and, by adding a suitable constant, we may assume $V \geqslant 0$. Furthermore, by the definition of CPD-weight w, there exist positive numbers δ and w_0 such that for any pair $x, y \in A$ satisfying $\|x - y\| \leqslant \delta$ we have $w(x,y) \geqslant w_0$. Let $\{B_j\}_1^n$ be a covering of A with $n = n(\delta)$ balls of radius $\delta/2$. For $\omega_N \subset A$ and any ball B_j containing at least $k+1$ elements from ω_N, we have $\|x - y\| \leqslant \delta$ for $x \in \omega_N \cap B_j$ and $y \in \mathcal{N}_k(x, \omega_N)$. On the other hand, there are at most nk^2 pairs x, y with $x \in \omega_N \cap B_j$ and $y \in \mathcal{N}_k(x,\omega_N)$ satisfying $\|x - y\| > \delta$ since in such a case x must belong to a ball B_j with at most k elements. Defining $\widetilde{w} := \max\{w, w_0\}$, we then have

$$\lim_{N\to\infty} \frac{E_s^k(\omega_N, \widetilde{w}) - E_s^k(\omega_N, w)}{N^{1+s/d}} = 0,$$

since

$$0 \leqslant E_s^k(\omega_N, \widetilde{w}) - E_s^k(\omega_N, w) \leqslant \sum_{x\in\omega_N} \sum_{\substack{y\in\mathcal{N}_k(x;\omega_N),\\ \|x-y\|>\delta}} w_0\|x-y\|^{-s} \leqslant nk^2 w_0 \delta^{-s}.$$

Hence, for the purpose of asymptotics, it may be assumed $w \geqslant w_0$. We employ this fact in the following useful proposition.

Proposition 4.9. *Let the assumptions of Theorem 4.7 hold. If $\omega_N \in A^N$, $N \geqslant 1$, is a sequence of configurations for which*

$$\limsup_{N\to\infty} \frac{E_s^k(\omega_N; w)}{N^{1+s/d}} < +\infty,$$

then any cluster point of $\nu(\omega_N)$ is absolutely continuous with respect to $\mathcal{H}_d$.

Proof. As remarked above, we may assume $w \geqslant w_0 > 0$. Then $E_s^k(\omega_N; w) \geqslant w_0 E_s^k(\omega_N)$, and we may argue as in [15, Lemma 4.9]. □

Remark 4.10. The discussion in Remark 4.8 can also be used to estimate the terms in E_s^k for pairs (x, y) with a fixed positive separation. Namely, by property (c) of CPD-weight, for every $\delta > 0$ there exists a constant M_δ such that $\|x-y\| \geqslant \delta$ implies $0 \leqslant w(x, y) \leqslant M_\delta$. Using a covering of A with $n = n(\delta)$ balls of radius $\delta/2$ in the same way as in Remark 4.8, we conclude

$$0 \leqslant \sum_{x\in\omega_N} \sum_{\substack{y\in\mathcal{N}_k(x;\omega_N),\\ \|x-y\|>\delta}} w(x,y)\|x-y\|^{-s} \leqslant \sum_{x\in\omega_N} \sum_{\substack{y\in\mathcal{N}_k(x;\omega_N),\\ \|x-y\|>\delta}} M_\delta\|x-y\|^{-s} \leqslant nk^2 M_\delta \delta^{-s}. \tag{4.13}$$

Using the above observations we further derive an analog of the short-range property (3.2) for weighted interactions. For the purposes of the proof of the main theorem, it will be enough to establish an inequality corresponding to the local behavior of asymptotically optimal configurations. For the rest of the section, set

$$\mathbf{e}(\omega_N; S) := \sum_{\substack{(x,y)\in\Lambda_k(\omega_N),\\ x\in S}} \Big(w(x,y)\|x-y\|^{-s} + N^{s/d} V(x) \Big) \tag{4.14}$$

for the sum of terms in $E_s^k(\omega_N; w, V)$ corresponding to edges of $\Lambda_k(\omega_N)$, emanating from the entries $x \in \omega_N \cap S$ with $S \subset A$. Notice that as a function of set S, $\mathbf{e}(\omega_N; S)$ is a positive measure (as usual, $V \geqslant 0$ is assumed without loss of generality). Thus, for a sequence of configurations ω_N, $N \geqslant 1$, with $\limsup_N \mathbf{e}(\omega_N; A)/N^{1+s/d} < \infty$, up to passing to a subsequence there exists a weak* limit of measures $\mathbf{e}(\omega_N; \cdot\,)/N^{1+s/d}$, which will be denoted by λ.

Lemma 4.11. *Suppose $A \subset \mathbb{R}^p$ is a compact $(\mathcal{H}_d, d)$-rectifiable set with $\mathcal{M}_d(A) = \mathcal{H}_d(A)$, $\mathcal{H}_d(A) < \infty$, and let w be a CPD-weight and V a lower semicontinuous external field.*

Assume that ω_N^* is a sequence of asymptotically optimal configurations for $E_s^k(\cdot\,; w, V)$ on A, converging weak to the measure μ. Let $x_1, x_2 \in \operatorname{supp}\mu$ and $B_m := B(x_m, r_m)$, $m = 1, 2$, be disjoint and such that* $\max(\mathcal{H}_d, \mu, \lambda)[\partial B_m \cap A] = 0$. *In addition, let $w(x, y)$ be bounded when $x, y \in B(x_m, 2r_m)$.*

Then for any compact $S_m \subset A \cap B_m$, $m = 1, 2$, and $B = B_1 \cup B_2$,

$$\limsup_{N\to\infty} \frac{\mathbf{e}(\omega_N^*; B)}{N^{1+s/d}} \leqslant \min_{\alpha_1+\alpha_2=\mu(B)} \sum_{m=1,2} \left(\alpha_m^{1+s/d} \frac{\sup_{x,y\in S_m} w(x,y)}{\mathcal{H}_d(S_m)^{s/d}} + \alpha_m \sup_{x\in S_m} V(x) \right). \tag{4.15}$$

Proof. In view of the asymptotic optimality of ω_N^*, it suffices to present a sequence of configurations ω_N' with the energy asymptotics corresponding to the right-hand side in (4.15). Recall, asymptotic optimality means for any $\omega_N' \in A^N$ we have

$$\limsup_{N\to\infty} \frac{E_s^k(\omega_N^*; w, V)}{E_s^k(\omega_N'; w, V)} \leqslant 1.$$

Fix $\gamma \in (0,1)$ and $\alpha_1, \alpha_2 \geqslant 0$ such that $\alpha_1 + \alpha_2 = \mu(B)$. We further denote $\gamma B_m := B(x_m, \gamma r_m)$, $B := B_1 \cup B_2$, and $\gamma B := \gamma B_1 \cup \gamma B_2$. Let $n = \#(\omega_N^* \cap B)$, $n_1 := \min(\lfloor \alpha_1 N \rfloor, n)$, and $n_2 := n - n_1$ and note that $n_m/N \to \alpha_m$ as $N \to \infty$ for $m = 1, 2$, since $n/N \to \mu(B)$ by weak* convergence and the assumption that $\mu(\partial B \cap A) = 0$. Choosing an n_m-point configuration $\omega_{n_m} \subset S_m \cap \gamma B_m$ such that $E_s^k(\omega_{n_m}; w, V) \leqslant \mathcal{E}_s^k(A \cap \gamma B_m, n_m; w, V) + 1$ for $m = 1, 2$, let $\omega_n = \omega_{n_1} \cup \omega_{n_2}$ and define ω_N' by

$$\omega_N' := \omega_n \cup (\omega_N^* \cap (A \setminus B)). \tag{4.16}$$

By the definition of $\mathbf{e}$,

$$\begin{aligned} E_s^k(\omega_N^*; w, V) &= \mathbf{e}(\omega_N^*, B) + \mathbf{e}(\omega_N^*, A \setminus B), \\ E_s^k(\omega_N'; w, V) &= \mathbf{e}(\omega_N', B) + \mathbf{e}(\omega_N', A \setminus B). \end{aligned} \tag{4.17}$$

Let us now compare the asymptotics for $N \to \infty$ of $\mathbf{e}(\omega_N^*, A \setminus B)$ with that of $\mathbf{e}(\omega_N', A \setminus B)$. By (4.16), these sums differ only by the terms corresponding to pairs $(x, y) \in \Lambda_k(\omega_N^*)$ with $x \in \omega_N^* \setminus B$ and $y \in \omega_N^* \cap B$, which are replaced in $\Lambda_k(\omega_N')$ by pairs $x, y \in \omega_N' \setminus B$ for sufficiently large N, in view of the positive separation between γB and $A \setminus B$. Thus, we have

$$\mathbf{e}(\omega_N^*, A \setminus B) - \mathbf{e}(\omega_N', A \setminus B) = \sum_{\substack{x \in \omega_N \setminus B,\ (x,y) \in \Lambda_k(\omega_N^*), \\ y = (x;\, \omega_N^*)_i \in B}} \left(\frac{w(x,y)}{\|x-y\|^s} - \frac{w(x, (x; \omega_N')_i)}{\|x - (x; \omega_N')_i\|^s} \right). \tag{4.18}$$

Note, for any $r > 0$ we can decompose the sum in the right-hand side of (4.18) as

$$\Sigma_1 + \Sigma_2 := \left(\sum_{\substack{x \in \omega_N \setminus B_r,\ (x,y) \in \Lambda_k(\omega_N^*), \\ y = (x;\, \omega_N^*)_i \in B}} + \sum_{\substack{x \in \omega_N \cap B_r \setminus B,\ (x,y) \in \Lambda_k(\omega_N^*), \\ y = (x;\, \omega_N^*)_i \in B}} \right) \left(\frac{w(x,y)}{\|x-y\|^s} - \frac{w(x, (x; \omega_N')_i)}{\|x - (x; \omega_N')_i\|^s} \right).$$

By property (c) of CPD-weight, absolute value of the first sum Σ_1 is at most $2r^{-s} M_w(r) N k = o(N^{1+s/d})$. To estimate the second sum, let $r < \min(r_1, r_2)$, so w is bounded uniformly in $x, y \in B(x_m, 2r_m)$ by some constant $M_w > 0$. Note that since $\|x - (x; \omega_N')_i\| \geqslant \|x - (x; \omega_N^*)_i\|$, there holds

$$\frac{w(x, (x; \omega_N')_i)}{\|x - (x; \omega_N')_i\|^s} \Bigg/ \frac{w(x, (x; \omega_N^*)_i)}{\|x - (x; \omega_N^*)_i\|^s} \leqslant \frac{M_w}{w_0}, \qquad x \in \omega_N^* \setminus B,\ i \geqslant 1, \tag{4.19}$$

with w_0 from Remark 4.8. Using the definition of measure λ and (4.19), we have for N large enough

$$\Sigma_2 \leqslant N^{1+s/d} 2 \left(1 + \frac{M_w}{w_0} \right) \lambda(B_r \setminus B).$$

Observe that by our assumptions, for $r \downarrow 0$, $\lambda(B_r \setminus B) \to 0$, so the right-hand side can be made smaller than $\varepsilon N^{1+s/d}$ for any given $\varepsilon > 0$. It follows

$$|\mathbf{e}(\omega_N^*, A \setminus B) - \mathbf{e}(\omega_N', A \setminus B)| = o(N^{1+s/d}), \qquad N \to \infty.$$

Combined with equation (4.17), asymptotic optimality of ω_N^* now implies

$$\limsup_{N \to \infty} \frac{\mathbf{e}(\omega_N^*, B)}{N^{1+s/d}} \leqslant \liminf_{N \to \infty} \frac{\mathbf{e}(\omega_N', B)}{N^{1+s/d}}.$$

Writing $S_m^\gamma := S_m \cap \gamma B_m$, by the separation between γB and sets $A \setminus B$, and B_m being disjoint, we infer from the above inequality and Theorem 4.7:

$$\begin{aligned} \limsup_{N \to \infty} \frac{\mathbf{e}(\omega_N^*; B)}{N^{1+s/d}} &\leqslant \liminf_{N \to \infty} \sum_{m=1,2} \left(\frac{n_m}{N} \right)^{1+s/d} \frac{E_s^k(\omega_{n_m}; w, V)}{n_m^{1+s/d}} \\ &= \sum_{m=1,2} \alpha_m^{1+s/d} \frac{\sup_{x,y \in S^\gamma} w(x,y)}{\mathcal{H}_d(S^\gamma)^{s/d}} + \alpha_m \sup_{x \in S_m^\gamma} V(x). \end{aligned}$$

Taking $\gamma \uparrow 1$ gives (4.15), since $\mathcal{H}_d(\partial B \cap A) = 0$. $\square$

Before proving Theorem 1.1, let us discuss an alternative form of condition (a) in the definition of a CPD weight. It transpires from the proofs of Lemma 4.11 and Theorem 1.1 that in place of $\mathcal{H}_d$-a.e. continuity in condition (a) one can assume

(a′) w is bounded on $A \times A$ and lower semi-continuous (as a function on $A \times A$) at $\mathcal{H}_d$-a.e. point of the diagonal $\operatorname{diag}(A) := \{(x,x) : x \in A\}$, and such that for $\mathcal{H}_d$-a.e. $x \in A$ and any $\varepsilon > 0$ there is an $r'_x > 0$ such that for $0 < r < r'_x$ there exists a closed set $A_{x,r} \subset A \cap B(x,r)$ for which $\mathcal{H}_d(A_{x,r}) \geqslant (1-\varepsilon)\mathcal{H}_d[A \cap B(x,r)]$ and

$$w(y,z) \leqslant w(x,x) + \varepsilon, \qquad y, z \in A_{x,r}. \tag{4.20}$$

In particular, condition (a′) holds if w is symmetric and lower semicontinuous on $A \times A$ and $\mathcal{H}_d$-a.e. point of $\operatorname{diag}(A)$ is a Lebesgue point for $w(x,y)$ with respect to the measure $\mathcal{H}_d \otimes \mathcal{H}_d$ on $A \times A$. Another version of (a), not requiring boundedness on the diagonal, is as follows.

(a″) w is a marginally radial weight, lower semi-continuous at $\mathcal{H}_d$-a.e. $x \in \operatorname{diag}(A)$, and such that for $\mathcal{H}_d$-a.e. $x \in A$ and any $\varepsilon > 0$ there is an $r'_x > 0$ and a closed $A_{x,r} \subset A \cap B(x,r)$, $0 < r < r'_x$, as in property (a′).

Proof of Theorem 1.1. Let the assumptions of Theorem 1.1 hold. In view of Remark 4.8, we hereafter let $V \geqslant 0$ and suppose there is a $w_0 > 0$ such that $w \geqslant w_0$ on $A \times A$.

If $\mathcal{H}_d(A) = 0$, it follows from the latter assumption and Theorem 4.7 that

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

and so there is nothing to prove. Now let $\mathcal{H}_d(A) > 0$ and $w(x,x) + V(x) < \infty$ on a closed subset of A of positive $\mathcal{H}_d$-measure. Minimizing E_s^k on this subset gives an upper bound on $\mathcal{E}_s^k(A,N;w,V)$, implying that

$$\limsup_{N\to\infty} \frac{\mathcal{E}_s^k(A,N;w,V)}{N^{1+s/d}} < \infty. \tag{4.21}$$

Fix $0 < \varepsilon < w_0/3$. For $r > 0$, let $B_A(x,r) := A \cap B(x,r)$ denote the ball of radius r relative to A. By the (semi)continuity properties of V and w, for almost every $x \in A$ and a sufficiently small $r_x^{(1)}$, if $y, z \in B_A(x, r_x^{(1)})$ then (cases when e.g. $w(x,x) = +\infty$ satisfy the appropriate modifications of these inequalities)

$$|w(y,z) - w(x,x)| \leqslant \varepsilon \qquad V(y) \geqslant V(x) - \varepsilon. \tag{4.22}$$

Furthermore, the set A can be divided according to the values of V into subsets of the form

$$A_l := \{x \in A : l\varepsilon \leqslant V(x) < (l+1)\varepsilon\},$$

and we set $A_M := \{x \in A : M\varepsilon \leqslant V(x)\}$ with M chosen so that $\mathcal{H}_d(A_M) < \varepsilon$. Thus $A = \bigsqcup_0^M A_l$.

Applying the Lebesgue density theorem [20, Corollary 2.14] to each A_l gives that for $\mathcal{H}_d$-almost every $x \in A_l$ there exists some $r_x^{(2)} > 0$ such that for every $r < r_x^{(2)}$,

$$\mathcal{H}_d[A_l \cap B(x,r)] \geqslant (1-\varepsilon)\mathcal{H}_d[B_A(x,r)],$$

implying, since every $x \in A$ is in exactly one A_l, that for $\mathcal{H}_d$-a.e. $x \in A$ and $r < r_x^{(2)}$:

$$\mathcal{H}_d(\{y \in B_A(x,r) : V(y) \leqslant V(x) + \varepsilon\}) \geqslant (1-\varepsilon)\mathcal{H}_d[B_A(x,r)]. \tag{4.23}$$

Thus for $r < \min(r_x^{(1)}, r_x^{(2)})$ there is a closed set $A_{x,r} \subset B_A(x,r)$ satisfying

$$|w(y,z) - w(x,x)| \leqslant \varepsilon \qquad V(y) \leqslant V(x) + \varepsilon, \qquad y, z \in B_A(x,r), \tag{4.24}$$

and $\mathcal{H}_d[A_{x,r}] \geqslant (1-\varepsilon)\mathcal{H}_d[B_A(x,r)]$.

Let $\omega_N^* \in A^N$, $N = 1, 2, 3, \ldots$, be a (k, s, w, V)-asymptotically optimal sequence and let μ denote a cluster point of the normalized counting measures $\nu(\omega_N^*)$. From (4.21), the assumption $w \geqslant w_0$, and Proposition 4.9, it follows that $\mu \ll \mathcal{H}_d$. In addition, both μ and $\mathcal{H}_d$ are Radon measures since A is a complete metric space [1, Theorem 7.1.7]. The differentiation theorem for Radon measures [20, Theorem 2.12] implies that for $\mathcal{H}_d$-a.e. $x \in A$ there exists an $r_x^{(3)} > 0$ such that whenever $r < r_x^{(3)}$, we have

$$\tag{4.25} \begin{gathered} \left| \frac{\mu[B(x,r)]}{\mathcal{H}_d[B_A(x,r)]} - \frac{d\mu}{d\mathcal{H}_d}(x) \right| < \varepsilon, \qquad \text{and} \\ 1-\varepsilon < \frac{\mu[B(x,r)]}{\mathcal{H}_d[B_A(x,r)]} \Big/ \frac{d\mu}{d\mathcal{H}_d}(x) < 1+\varepsilon, \qquad \frac{d\mu}{d\mathcal{H}_d}(x) > 0. \end{gathered}$$

Setting for $\mathcal{H}_d$-a.e. $x \in A$ the quantity $r_x := \min\{r_x^{(1)}, r_x^{(2)}, r_x^{(3)}\}$, it follows that the properties (4.20) and (4.22)–(4.25) hold for $\mathcal{H}_d$-a.e. $x \in A$ and closed balls $B(x,r)$ of radius $r < r_x$. Denote the set of such x by $\tilde{A}$.

In the next part of the proof we shall derive two-sided estimates for the sum of terms in E_s^k corresponding to $(x,y) \in \Lambda_k(\omega_N^*)$, such that x is within a small distance from a pair of fixed points $x_1, x_2 \in \tilde{A}$. This will allow to derive estimates for the densities $d\mu/d\mathcal{H}_d(x_m)$, $m = 1, 2$. Fix a pair of elements $x_1 \neq x_2 \in \tilde{A} \cap \operatorname{supp} \mu$. We will consider two sequences of balls relative to A: $B_j^{(m)} = B_A(x_m, r_j^{(m)})$, $m = 1, 2$, with vanishing radii $r_j^{(m)} \downarrow 0$. Without loss of generality, $r_j^{(m)} \leqslant \min(r_{x_1}, r_{x_2})$ and $B_j^{(m)}$ are positive distance apart. Since $\mathcal{H}_d(A) < \infty$, the sequences of radii $r_j^{(m)}$ can further be chosen to satisfy $\mathcal{H}_d(\partial B_j^{(m)} \cap A) = 0$, $m = 1, 2$, since at most a countable number of possible $r_j^{(m)}$ have a positive value of $\mathcal{H}_d(\partial B_j \cap A)$; likewise, we chose them so that $\lambda(\partial B_j^{(m)} \cap A)$ for the energy measure λ, introduced before Lemma 4.11, associated to the sequence ω_N^*.

The absolute continuity of μ with respect to $\mathcal{H}_d$ implies that $\mu(\partial B_j^{(m)} \cap A) = 0$ for each j, m and by the weak-star convergence of $\nu(\omega_N^*)$ to μ we have

$$\tag{4.26} \lim_{N\to\infty} \frac{\#(\omega_N^* \cap B_j^{(m)})}{N} = \mu(B_j^{(m)}) =: \beta_j^{(m)}, \qquad m = 1, 2, \; j \geqslant 1.$$

We shall further estimate the asymptotics of $\mathbf{e}(\omega_N^*; B_j)/N^{1+s/d}$, defined in (4.14), for the set $B_j := B_j^{(1)} \cup B_j^{(2)}$. With $w_m := w(x_m, x_m)$, $V_m := V(x_m)$, remark that for $x, y \in B_j^{(m)}$ we have $w(x,y) \geqslant w_m - \varepsilon$ and $V(x) \geqslant V_m - \varepsilon$. Pick a $\gamma \in (0,1)$ and write $\gamma B_j^{(m)}$ for the ball $B_A(x_m,\ \gamma r_j^{(m)})$ relative to A; also, let $\gamma B_j = \bigcup_m \gamma B_j^{(m)}$. Observing that by (4.13), for j fixed,

$$\Sigma_j^{(m)} := \sum_{x \in \omega_N^* \cap \gamma B_j^{(m)}} \sum_{y \in \mathcal{N}_k(x; \omega_N^*) \setminus B_j^{(m)}} w(x,y) \|x-y\|^{-s} \leqslant n(\delta)\, k^2 M_\delta \delta^{-s} = o(N^{1+s/d}),$$

where $\delta = (1-\gamma) \min_m r_j^{(m)}$ and M_δ as in Remark 4.10, we obtain the following lower estimate for $\mathbf{e}(\omega_N^*; B_j)$ for a fixed γ:

$$\tag{4.27} \begin{aligned} \liminf_{N\to\infty} \frac{\mathbf{e}(\omega_N^*; B_j)}{N^{1+s/d}} &\geqslant \liminf_{N\to\infty} \frac{\mathbf{e}(\omega_N^*; \gamma B_j)}{N^{1+s/d}} \\ &\geqslant \sum_{m=1,2} \liminf_{N\to\infty} N^{-(1+s/d)} \left(E_s^k(\omega_N^* \cap \gamma B_j^{(m)}; w_m - \varepsilon, V_m) - \Sigma_j^{(m)} \right) \\ &\geqslant \sum_{m=1,2} \liminf_{N\to\infty} \frac{E_s^k(\omega_N^* \cap \gamma B_j^{(m)}; w_m - \varepsilon, V_m)}{N^{1+s/d}}, \end{aligned}$$

where the last inequality is due to the distance to nearest neighbors non-decreasing when passing from a configuration to its subconfiguration. Using Theorem 4.7 and (4.26), we then deduce that

$$
\begin{aligned}
\liminf_{N\to\infty} \frac{\mathbf{e}(\omega_N^*; B_j)}{N^{1+s/d}} &\geqslant \lim_{\gamma\uparrow 1} \sum_{m=1,2} \liminf_{N\to\infty} \frac{E_s^k(\omega_N^* \cap \gamma B_j^{(m)}; w_m-\varepsilon, V_m-\varepsilon)}{N^{1+s/d}} \\
&\geqslant \lim_{\gamma\uparrow 1} \sum_{m=1,2} \liminf_{N\to\infty} \frac{E_s^k(\omega_N^* \cap \gamma B_j^{(m)}; w_m-\varepsilon, V_m-\varepsilon)}{\#(\omega_N^* \cap \gamma B_j^{(m)})^{1+s/d}} \left(\frac{\#(\omega_N^* \cap \gamma B_j^{(m)})}{N}\right)^{1+s/d} \\
&\geqslant \sum_{m=1,2} \left(\beta_j^{(m)} (w_m-\varepsilon) \cdot \frac{C_{s,d}^k {\beta_j^{(m)}}^{s/d}}{\mathcal{H}_d(B_j)^{s/d}} + \beta_j^{(m)}(V_m-\varepsilon) \right) \\
&\geqslant \sum_{m=1,2} \left(\beta_j^{(m)} (w_m-\varepsilon) \cdot C_{s,d}^k \left(\frac{d\mu}{d\mathcal{H}_d}(x_m) - \varepsilon\right)^{s/d} + \beta_j^{(m)}(V_m-\varepsilon) \right).
\end{aligned} \tag{4.28}
$$

By Lemma 4.11, we also have an upper estimate on the asymptotics in the left-hand side above. Recall, by (4.24) and the choice of r_x, for each $B_j^{(m)}$ there exists a closed subset $S_j^{(m)} \subset B_j^{(m)}$ satisfying $\mathcal{H}_d(S_j^{(m)}) \geqslant (1-\varepsilon)\mathcal{H}_d[B_j^{(m)}]$, for which $w(y,z) \leqslant w_m + \varepsilon$ and $V(y) \leqslant V_m + \varepsilon$ whenever $y, z \in S_j^{(m)}$. Applying Lemma 4.11 with sets $S_j^{(m)}$ gives for any pair of positive numbers $\alpha_j^{(m)}$, $m = 1, 2$, with $\sum_m \alpha_j^{(m)} = \sum_m \beta_j^{(m)}$:

$$
\begin{aligned}
\limsup_{N\to\infty} \frac{\mathbf{e}(\omega_N^*; B_j)}{N^{1+s/d}} &\leqslant \sum_{m=1,2} \left((w_m+\varepsilon) \cdot \frac{C_{s,d}^k (\alpha_j^{(m)})^{1+s/d}}{\mathcal{H}_d(S_j^{(m)})^{s/d}} + \alpha_j^{(m)}(V_m+\varepsilon) \right) \\
&\leqslant \sum_{m=1,2} \left(\frac{w_m+\varepsilon}{(1-\varepsilon)^{s/d}} \cdot \frac{C_{s,d}^k (\alpha_j^{(m)})^{1+s/d}}{\mathcal{H}_d(B_j^{(m)})^{s/d}} + \alpha_j^{(m)}(V_m+\varepsilon) \right)
\end{aligned} \tag{4.29}
$$

where we used (4.25). Note that for the above to hold, we do not need $w_m + V_m$ to be finite. For instance, suppose $w_1 + V_1 < +\infty = w_2 + V_2$; then the above inequality is trivial unless $\alpha_j^{(2)} = 0$, in which case we apply the argument of Lemma 4.11 to the ball $B_j^{(1)}$ only.

Inequality (4.29) holds if the values $\alpha_j^{(m)} = \tilde\alpha_j^{(m)}$ are chosen to minimize the right-hand side over positive $\alpha_j^{(m)}$, $m = 1, 2$, with $\sum_m \alpha_j^{(m)} = \sum_m \beta_j^{(m)}$. Using Lagrange multipliers, we see that such $\tilde\alpha_j^{(m)}$ must satisfy

$$
\frac{V_2 - V_1}{C_{s,d}^k (1+s/d)} = w_1 \left(\frac{\tilde\alpha_j^{(1)}}{(1-\varepsilon)\mathcal{H}_d(B_j^{(1)})} \right)^{s/d} - w_2 \left(\frac{\tilde\alpha_j^{(2)}}{(1-\varepsilon)\mathcal{H}_d(B_j^{(2)})} \right)^{s/d}.
$$

Note that the left-hand side in the above equation is independent of $\mathcal{H}_d(B_j^{(1)})/\mathcal{H}_d(B_j^{(2)})$. As a result, limit of the right-hand side for $j \to \infty$ is also independent of this ratio. This fact will be essential in completing the proof.

Observe that equations (4.28)-(4.29) hold for any pair of sufficiently small radii $r_j^{(m)}$. To obtain estimates for the density $d\mu/d\mathcal{H}_d$, divide (4.28) and (4.29) through by $\mathcal{H}_d(B_j)$ and take $j \to \infty$. Without loss of generality, the limit $\lim_{j\to\infty} \mathcal{H}_d(B_j^{(m)})/\mathcal{H}_d(B_j) = \gamma_m$ exists; otherwise we pass to a suitable subsequence. We have from (4.28)-(4.29) and optimality of $\tilde{\alpha}_j^{(m)}$,

$$\begin{aligned}
&\sum_{m=1,2} \gamma_m \left(C_{s,d}^k (w_m - \varepsilon)(\rho_m - \varepsilon)^{1+s/d} + (\rho_m - \varepsilon)(V_m - \varepsilon) \right) \\
&\leqslant \sum_{m=1,2} \gamma_m \frac{\tilde{\alpha}_j^{(m)}}{\mathcal{H}_d(B_j^{(m)})} \left(\frac{w_m + \varepsilon}{(1-\varepsilon)^{s/d}} \cdot \frac{C_{s,d}^k (\tilde{\alpha}_j^{(m)})^{s/d}}{\mathcal{H}_d(B_j^{(m)})^{s/d}} + (V_m + \varepsilon) \right) \\
&\leqslant \sum_{m=1,2} \gamma_m \left(C_{s,d}^k \frac{w_m + \varepsilon}{(1-\varepsilon)^{s/d}} (\rho_m + \varepsilon)^{1+s/d} + (\rho_m + \varepsilon)(V_m + \varepsilon) \right)
\end{aligned} \tag{4.30}$$

Here $\rho_m = d\mu/d\mathcal{H}_d(x_m)$, $m = 1, 2$. Since the above holds for every fixed $\varepsilon > 0$, after one takes $\varepsilon \downarrow 0$, the inequalities turn into equalities:

$$\begin{aligned}
&\sum_{m=1,2} \gamma_m \left(C_{s,d}^k w_m \rho_m^{1+s/d} + \rho_m V_m \right) \\
&= \sum_{m=1,2} \gamma_m \alpha_m \left(C_{s,d} w_m \cdot \alpha_m^{s/d} + V_m \right),
\end{aligned} \tag{4.31}$$

where we denote $\alpha_m := \lim_{N\to\infty} \tilde{\alpha}_j^{(m)}/\mathcal{H}_d(B_j^{(m)})$; we ensure these limits exist by passing to a subsequence. Recall that the ratios $\tilde{\alpha}_j^{(m)}/\mathcal{H}_d(B_j^{(m)})$ do not depend on the ratio $\mathcal{H}_d(B_j^{(1)})/\mathcal{H}_d(B_j^{(2)})$. On the other hand, the double estimate (4.30) holds for any pair of sufficiently small radii $r_j^{(m)}$. This allows us to vary the two radii independently, to produce sequences of balls B_i^1 and B_i^2, centered around x_1 and x_2 respectively, for which the limiting ratios (γ_1, γ_2) are $(1, 0)$ and (0,1). For such sequences, equation (4.31) gives

$$\rho_m = \lim_{j\to\infty} \frac{\tilde{\alpha}_j^{(m)}}{\mathcal{H}_d(B_j^{(m)})}, \qquad m = 1, 2,$$

whence we conclude the equation

$$\frac{V_2 - V_1}{C_{s,d}^k (1 + s/d)} = w_1 \rho_1^{s/d} - w_2 \rho_2^{s/d}$$

holds for $\mathcal{H}_d$-a.e. pair x_1, x_2. In particular, $w(x,x)\rho(x)^{s/d} + V_1/(C_{s,d}^k(1+s/d)) = const =: L_1 < \infty$ $\mathcal{H}_d$-a.e., since we can pick x_1 among the points for which $w(x_1,x_1) + V(x_1) < \infty$ and $\rho(x_1) < \infty$. Combined with the condition $\int \rho(x)\, d\mathcal{H}_d(x) = 1$ that $\rho = d\mu/d\mathcal{H}_d$ must satisfy as the density of a probability measure, this yields (1.5).

In the remaining part of the proof we derive the formula for the asymptotics of minimizers of E_s^k on A. To begin, note that when $w(x,x) + V(x) = +\infty$ for $\mathcal{H}_d$-a.e. $x \in A$, lower semicontinuity implies the equality for all $x \in A$. Arguing as in (4.28), we immediately have that the asymptotics with respect to $N^{1+s/d}$ are infinite. It suffices to assume for the rest of this proof that $w(x,x) + V(x) < \infty$ on a set of positive $\mathcal{H}_d$-measure.

By the above argument, $w(x,x)\rho(x)^{s/d} + V(x)$ is bounded on $\operatorname{supp}\mu$ by L_1; hence, $w\rho^{1+s/d} \in L^1(A, \mathcal{H}_d)$; similarly, $V\rho \in L^1(A, \mathcal{H}_d)$. As a result, $\mathcal{H}_d$-a.e. point in A is a Lebesgue point for functions $w\rho^{1+s/d}$ and $V\rho$, and the measure $\mathcal{H}_d$: for any fixed $\varepsilon > 0$, at $\mathcal{H}_d$-a.e. $x \in A$ there exists a small enough $r > 0$ such that

$$\begin{aligned}
\left| w(x,x)\rho(x)^{1+s/d} \cdot \mathcal{H}_d[B_A(x,r)] - \int_{B_A(x,r)} w(y,y)\rho(y)^{1+s/d}\, d\mathcal{H}_d(y) \right| &\leqslant \varepsilon \mathcal{H}_d[B_A(x,r)], \\
\left| V(x)\rho(x) \cdot \mathcal{H}_d[B_A(x,r)] - \int_{B_A(x,r)} V(y)\rho(y)\, d\mathcal{H}_d(y) \right| &\leqslant \varepsilon \mathcal{H}_d[B_A(x,r)].
\end{aligned} \tag{4.32}$$

To obtain the expression for optimal asymptotics, we argue in the same way as in (4.28), to derive for every $\varepsilon > 0$ the following inequalities satisfied at μ-a.e. $x \in A$, with $r < r_{x,\varepsilon}$ sufficiently small:

$$\begin{aligned}\liminf_{N\to\infty} \frac{\mathbf{e}(\omega_N^*; B_x)}{N^{1+s/d}} &\geqslant \mu(B_x)\left(C_{s,d}^k(w(x,x)-\varepsilon)\cdot((1-\varepsilon)\rho(x))^{s/d} + (V(x)-\varepsilon)\right)\\ &\geqslant (1-\varepsilon)^{1+s/d}\int_{B_x}\left(C_{s,d}^k w(x,x)\rho^{s/d} + V(x)\right)d\mu(x) - \varepsilon\mu(B_x)\left(C_{s,d}^k\rho(x,x)^{s/d}+1\right),\end{aligned}$$

where $B_x := B_A(x,r)$. Using the Vitali covering theorem for the Radon measure $\mathcal{H}_d$, we can cover $\mathcal{H}_d$-a.e. of A with a countable collection of such disjoint B_x; since

$$\begin{aligned}\liminf_{N\to\infty}\frac{E_s^k(\omega_N^*; w, V)}{N^{1+s/d}} &\geqslant \liminf_{N\to\infty}\sum_j \frac{\mathbf{e}(\omega_N^*; B_{x_j})}{N^{1+s/d}}\\ &\geqslant (1-\varepsilon)^{s/d}\int_A\left(C_{s,d}^k w(x,x)\rho(x)^{s/d} + V\right)d\mu(x) - c\varepsilon\end{aligned}$$

for a suitable constant c (we used that $\rho^{s/d}$ is bounded because $w \geqslant w_0$), it remains to show that $C_{s,d}^k \int w\rho^{1+s/d}\, d\mathcal{H}_d + \int V\rho\, d\mathcal{H}_d$ is also an upper bound for the asymptotics.

Such upper bound follows by placing optimal configurations of cardinalities $\lfloor\mu(B_{x_j})N\rfloor$ into the sets $S_{x_j} \subset B_A(x_j, \gamma r_{x_j,\varepsilon})$, defined in the same way as $S_j^{(m)}$ above, for $\gamma \in (0,1)$. Indeed, for any finite collection of disjoint closed balls B_m with $\mathcal{H}_d(\partial B_m \cap A) = 0$ by placing the minimizers in a suitable closed subset $S_m \subset B_m$ satisfying (4.22), (4.24), with $\mathcal{H}_d(S_m) \geqslant (1-\varepsilon)\mathcal{H}_d(B_m)$:

$$\omega_N := \bigcup_m \omega_{N_m}, \qquad E_s^k(\omega_{N_m}; w, V) \leqslant \mathcal{E}_s^k(N_m, S_m; w, V) + 1, \quad N_m = \lceil \mu(B_m)N\rceil$$

arguing as in the right-hand side of (4.30) one has

$$\begin{aligned}\limsup_{N\to\infty}\frac{E_s^k(\omega_N^*; w, V)}{N^{1+s/d}} &\leqslant \limsup_{N\to\infty}\frac{E_s^k(\omega_N; w, V)}{N^{1+s/d}}\\ &\leqslant \sum_{m=1}^M\left(C_{s,d}^k\frac{w_m+\varepsilon}{(1-\varepsilon)^{s/d}}((1+\varepsilon)\rho_m)^{1+s/d} + (1+\varepsilon)\rho_m(V_m+\varepsilon)\right)\mathcal{H}_d(B_m),\end{aligned}$$

where as usual, we write w_m and V_m for the values of the respective functions at the centers of B_m, and $B = \bigcup_m B_m$. Choosing the centers of B_m in $\operatorname{supp}\mu$ and such that $\mu(B) > 1-\varepsilon$, and using (4.32) gives

$$\limsup_{N\to\infty}\frac{E_s^k(\omega_N^*; w, V)}{N^{1+s/d}} \leqslant \frac{(1+\varepsilon)^{s/d}}{(1-\varepsilon)^{1+s/d}}\left(C_{s,d}^k\int_B\left((w(x,x)+\varepsilon)\rho(x)^{s/d}+V\right)d\mu(x) + \varepsilon c\right),$$

where it is used again that $\rho^{s/d}$ is bounded on $\operatorname{supp}\mu$. This finishes the proof of the theorem. □

5 Connections to other short-range interactions

5.1 Convex kernels on the circle

When $d = \dim_H A = 1$, we can compute explicitly the values of $C_{s,1}^k$ for any $s > 0$ and $k \geqslant 1$. Moreover, we will show that on the periodized interval $[0,1]$, the minimizers of the energy E_φ^k defined below are equally spaced, for any convex decreasing function of distance φ. Equivalently, minimizers of such energies on $\mathbb{S}^1$ with embedded distance are equally spaced points for any convex decreasing kernel.

Theorem 5.1. *Let $A = \mathbb{S}^1$ with the distance $\vartheta = s/2\pi$ for the arc length s, and assume that $g(x,y) = \varphi(\vartheta(x,y))$ for a convex decreasing $\varphi : [0,1/2) \to [0,\infty]$. For any $N \geqslant 1$ and $k \geqslant 1$, the energy*

$$E_\varphi^k(\omega_N) := \sum_{x\in\omega_N}\sum_{y\in\mathcal{N}_k(x;\omega_N)}\varphi\left(\vartheta(x,y)\right).$$

is minimized by every set ω_N^* consisting of N equally spaced points.

Proof. Consider an arbitrary set ω_N of N distinct points in A. It suffices to show that its energy is at least the one of ω_N^*, as defined above. We will assume that the entries of $\omega_N = (x_1, \dots, x_N)$ are enumerated clockwise, so that for example x_1 and x_3 are adjacent to the point x_2, etc. We will also use indices of x_i modulo N, so for any x_i the two adjacent points in the above ordering are given by x_{i-1} and x_{i+1}.

Consider the following sets of k indices

$$I_{i,k} := \left\{ i - \left\lfloor \frac{k}{2} \right\rfloor, i - \left\lfloor \frac{k}{2} \right\rfloor + 1, \dots, i-1, i+1, \dots, i + \left\lceil \frac{k}{2} \right\rceil - 1, i + \left\lceil \frac{k}{2} \right\rceil \right\}.$$

Let $y_1^{(i)}, \dots, y_k^{(i)}$ be the entries $x_j \in \omega_N$ with $j \in I_{i,k}$, ordered by the nondecreasing distance from x_i to $y_j^{(i)}$. Then there holds

$$\vartheta(x_i, (x_i; \omega_N)_j) \leqslant \vartheta(x_i, y_j^{(i)}),$$

where as before, $(x_i; \omega_N)_j)$ is the j-th nearest entry of ω_N to x_i. This inequality follows from $\vartheta(x_i, y_l^{(i)}) \leqslant \vartheta(x_i, y_j^{(i)})$ for $l \leqslant j$, so there are at least $j-1$ entries of ω_N that are closer to x_i than $y_j^{(i)}$. By the monotonicity of φ, then

$$\sum_{y \in \mathcal{N}_k(x_i; \omega_N)} \varphi\left(\vartheta(x_i, y)\right) \geqslant \sum_{j=1}^{k} \varphi\left(\vartheta(x_i, y_j^{(i)})\right), \qquad 1 \leqslant i \leqslant N. \tag{5.1}$$

Now observe that for any set of N distinct points $\omega_N \subset A$,

$$\sum_{i=1}^{N} \vartheta(x_i, x_{i+1}) = 1.$$

Indeed, the above sum contains the distances between adjacent points, which add up to the length of A. Similarly, one has

$$\sum_{i=1}^{N} \vartheta(x_i, x_{i+l}) = \sum_{i=1}^{N} \sum_{j=1}^{l} \vartheta(x_{i+j-\operatorname{sgn} l}, x_{i+j}) = l, \tag{5.2}$$

whenever $2|l| \leqslant N$.

In view of (5.1), (5.2), convexity of φ, and that without loss of generality $k \leqslant N-1$, we obtain

$$\begin{aligned}
E_\varphi^k(\omega_N) &= \sum_{i=1}^{N} \sum_{y \in \mathcal{N}_k(x_i;\omega_N)} \varphi\left(\vartheta(x_i, y)\right) \geqslant \sum_{i=1}^{N} \sum_{j=1}^{k} \varphi\left(\vartheta(x_i, y_j^{(i)})\right) \\
&= \sum_{\substack{j=-\lfloor k/2 \rfloor \\ j \neq 0}}^{\lceil k/2 \rceil} \sum_{i=1}^{N} \varphi\left(\vartheta(x_i, x_{i+j})\right) \geqslant \sum_{\substack{j=-\lfloor k/2 \rfloor \\ j \neq 0}}^{\lceil k/2 \rceil} N \varphi\left(\frac{1}{N} \sum_{i=1}^{N} \left(\vartheta(x_i, x_{i+j})\right)\right) \\
&= N \sum_{\substack{j=-\lfloor k/2 \rfloor \\ j \neq 0}}^{\lceil k/2 \rceil} \varphi\left(\frac{l}{N}\right) = E_\varphi^k(\omega_N^*).
\end{aligned}$$

In the second line of the above equation we used Jensen inequality. Here, as defined in the statement of the theorem, ω_N^* consists of N equally spaced points in $A = \mathbb{S}^1$. $\square$

Corollary 5.2. *The value of the constant* $C_{s,1}^k$ *is given by*

$$C_{s,1}^k = \sum_{\substack{l=-\lfloor k/2 \rfloor \\ l \neq 0}}^{\lceil k/2 \rceil} \frac{1}{|l|^s}.$$

Proof. The unit circle $\mathbb{S}^1$ with the metric ϑ above can be identified with the periodized unit interval $[0,1)$ equipped with the natural distance. Due to the short-range properties of Riesz k-energies E_s^k (with convex decreasing $\varphi(r) = 1/r^s$), the asymptotics of the minimal energy for set $A' = [0,1)$ with this distance coincide with the asymptotics for $A = [0,1] \subset \mathbb{R}$ with the Euclidean distance. ☐

5.2 Relation of k-energies with $s > d$ to full hypersingular Riesz energies

As explained above, we obtain the result about hypersingular case $s > d$ by passing to the limit $k \to \infty$ in E_s^k. To do that, we will need the following lemma, which has been established in a slightly different form in [3, Lem. 5.2]. Recall that $\Delta(\omega_N) = \min_{1 \leqslant i < j \leqslant N} \|x_i - x_j\|$ stands for the separation of the configuration ω_N.

Lemma 5.3. *Let $A \subset \mathbb{R}^d$ be a compact set. Let further $\omega_N \subset A$ be a sequence of configurations satisfying $\Delta(\omega_N) \geqslant c_0 N^{-1/d}$, $N \geqslant 2$, and w a bounded weight function on $A \times A$. Then there holds*

$$\limsup_{N\to\infty} \frac{1}{N^{1+s/d}} \sum_{x\in\omega_N} \sum_{y \notin \mathcal{N}_k(x;\omega_N)} w(x,y)\|x-y\|^{-s} \leqslant c(k,s,d),$$

with $c(k,s,d) \to 0$, $k \to \infty$.

Proof. Fix a point $x \in \omega_N$. Denote $2h_N := c_0 N^{-1/d}$ for brevity. For an $m \geqslant 1$, let

$$L_m = \{y \in \omega_N : mh_N < \|y - x\| \leqslant (m+1)h_N\}.$$

There holds $\mathcal{H}_d[B(x_i, r)] = c'_d r^d$ for any $r > 0$, whence $\mathcal{H}_d[B(x_i, r+t) \setminus B(x_i, r)] \leqslant c''_d t(r+t)^{d-1}$, $t \geqslant 0$ for some positive constants c'_d, c''_d. Since the distance between any two points in ω_N is at least $2h_N$, the interiors of balls $B(x_j, h_N)$ for $1 \leqslant j \leqslant N$ must be pairwise disjoint. This allows to estimate $\#L_m$ by volume considerations: since

$$\bigcup_{y\in L_m} B(y, h_N) \subset \left[B\left(x, (m+2)h\right) \setminus B\left(x, (m-1)h\right)\right],$$

there holds $c'_d h_N^d \cdot \#L_m \leqslant 3c''_d h_N((m+2)h_N)^{d-1}$, which gives

$$\#L_m \leqslant c_d m^{d-1}.$$

Summing up the pairwise energies over spherical layers around x, one obtains further

$$\sum_{y\in\omega_N} \|y-x\|^{-s} = \sum_{m=1}^{\infty} \sum_{y\in L_m} \|y-x\|^{-s} \leqslant \sum_{m=1}^{\infty} \frac{c_d m^{d-1}}{(mh_N)^s} = \frac{c_d N^{s/d}}{c_0^s} \sum_{m=1}^{\infty} \frac{1}{m^{s-d+1}}.$$

This implies for $k \geqslant \sum_{m=1}^{M-1} c_d m^{d-1} \geqslant \sum_1^{M-1} \#L_m$,

$$\frac{1}{N^{1+s/d}} \sum_{x\in\omega_N} \sum_{y\notin\mathcal{N}_k(x;\omega_N)} \|x-y\|^{-s} \leqslant c_d c_0^{-s} \sum_{m=M}^{\infty} \frac{1}{m^{s-d+1}},$$

which converges to 0 for $k \to \infty$, and thus gives the desired statement. Observe that the convergence is uniform over all configurations with $\Delta(\omega_N) \geqslant c_0 N^{-1/d}$ ☐

Lemma 5.4. *Suppose $A \subset \mathbb{R}^d$ is a compact set, w, V are bounded and satisfy the assumptions of Theorem 1.3; assume also a sequence k_n, $n \geqslant 1$, satisfies $k_n \to \infty$, $n \to \infty$. Then*

$$\mathcal{E}_s^{k_n}(A, N; w, V) \Big/ \mathcal{E}_s(A, N; w, V) \longrightarrow 1, \qquad N \to \infty, n \to \infty.$$

Proof. Let $\omega_N^* = \{x_1^*, \dots, x_N^*\}$ be such that

$$E_s^{k_n}(\omega_N^*; w, V) \leqslant \mathcal{E}_s^{k_n}(\omega_N; w, V) + 1, \qquad N \geqslant 2.$$

Similarly, let $\omega_N' = \{x_1', \dots, x_N'\}$ be the sequence minimizing E_s:

$$E_s(\omega_N'; w, V) \leqslant \mathcal{E}_s(A, N; w, V) + 1, \qquad N \geqslant 2.$$

By the construction of ω_N^* and ω_N', for every N there holds,

$$E_s^{k_n}(\omega_N^*; w, V) \leqslant E_s^{k_n}(\omega_N'; w, V) + 1 \leqslant E_s(\omega_N'; w, V) + 1 \leqslant E_s(\omega_N^*; w, V) + 2.$$

On the other hand, since ω_N^* is separated by Theorem 1.3, using Lemma 5.3 the difference of the left- and right-hand side of the above display can be estimated as

$$\begin{aligned} &E_s(\omega_N^*; w, V) - E_s^{k_n}(\omega_N^*; w, V) \\ &\qquad \leqslant \sum_{x \in \omega_N} \sum_{y \notin \mathcal{N}_{k_n}(x; \omega_N)} w(x, y) \|x - y\|^{-s} = c(k, s, d) N^{1+s/d}, \end{aligned}$$

where $c(k, s, d) \to 0$, $k \to \infty$, and we used the boundedness of w. This completes the proof of the lemma. □

Proof of Theorem 1.4. If $w(x, x) + V(x)$ is not bounded on a subset of A of positive $\mathcal{H}_d$-measure, the optimal asymptotics of E_s^1 are infinite by Theorem 1.1, and since $E_s \geqslant E_s^1$, there is nothing to prove.

First assume w, V are bounded on the entire A and w marginally radial. For a compact $A \subset \mathbb{R}^d$, constant weight w, and $V = 0$, the first claim of the theorem (1.13) follows from Lemma 5.4. The asymptotics and limiting density of asymptotic minimizers of E_s are then obtained by passing to the limit in Theorem 1.1 and the dominated convergence theorem. To extend the result to a compact $(\mathcal{H}_d, d)$-rectifiable $A \subset \mathbb{R}^p$, we then apply Lemma 4.6 to the functionals E_s^k and E_s. Note that the short-range property and stability for E_s for $s > d$ are well-known [4, Section 8.6.2]. Finally, the case of general weight and external field follows by extending the asymptotics of E_s^k and E_s following the argument given in the proof of Theorem 1.1 and pointwise convergence in the resulting integral functionals expressing the asymptotics.

The case of unbounded w, V, where w is still assumed marginally radial, is obtained by using the truncated weights $w_h := w \cdot \mathbb{1}_{w \leqslant h}$ and external fields $V_h := V \cdot \mathbb{1}_{V \leqslant h}$, and that, on the one hand,

$$\mathcal{E}_s(A, N; w_h, V_h) \leqslant \mathcal{E}_s(A, N; w, V), \qquad \mathcal{E}_s^k(A, N; w_h, V_h) \leqslant \mathcal{E}_s^k(A, N; w, V),$$

and on the other, that for $h \uparrow +\infty$, the integrals expressing the respective asymptotics converge to their analogs with w, V, by the monotone convergence theorem.

Finally, to obtain the claim of the theorem for non-marginally radial weights, observe that the asymptotics of E_s^k, E_s do not depend on the off-diagonal values of w; thus, choosing $\tilde{w}$ to be a marginally radial weight with the same values as w on $\operatorname{diag}(A)$ results in

$$\lim_{k\to\infty} \lim_{N\to\infty} \frac{\mathcal{E}_s^k(A, N; w, V)}{N^{1+s/d}} = \lim_{k\to\infty} \lim_{N\to\infty} \frac{\mathcal{E}_s^k(A, N; \tilde{w}, V)}{N^{1+s/d}} = \lim_{N\to\infty} \frac{\mathcal{E}_s(A, N; \tilde{w}, V)}{N^{1+s/d}} = \lim_{N\to\infty} \frac{\mathcal{E}_s(A, N; w, V)}{N^{1+s/d}},$$

and we have the desired statement. □

5.3 Proof of Γ-convergence

For a compact A we denoted by $\mathcal{P}(A)$ the space of probability measures supported on A. It is a compact metrizable space. As explained in the introduction, we discuss the properties of short-range interactions on discrete configurations ω_N, by viewing them as acting on the normalized counting measures $\nu(\omega_N)$.

The sequence introduced in $\mathbf{2}^\Gamma$ is called a *recovery sequence* at the point x. Usefulness of Γ-convergence for energy minimization consists in that, together with compactness of X, it guarantees that minimizers of F_N converge to those of F. Moreover, F_N need not attain its minimizer, but this is the case for F on compact sets, due to lower semicontinuity. Namely, the following properties hold.

Proposition 5.5 ([5], [8]). *If a sequence of functionals $\{F_N\}$ on a compact metric space X Γ-converges to F, then*

1. *F is lower semicontinuous and $\min F = \lim_{N\to\infty} \inf F_N$*
2. *if $\{x_N\}$ is a sequence of (global) minimizers of F_N, converging to an $x \in X$, then x is a (global) minimizer for F.*

If F_N is a constant sequence, Γ-$\lim F$ is the lower semicontinuous envelope of F; i.e., the supremum of lower semicontinuous functions bounded by F above.

Proof of Theorem 1.6. To verify the property $\mathbf{1}^\Gamma$ of the definition of Γ-convergence, suppose a sequence $\{\mu_N\} \subset \mathcal{P}(A)$ weak* converges to $\mu \in \mathcal{P}(A)$. Observe that if

$$\liminf_{N\to\infty} \frac{1}{N^{1+s/d}} \mathcal{F}_N(\mu_N; w, V) = +\infty \geqslant \mathcal{F}(\mu; w, V),$$

the inequality in $\mathbf{1}^\Gamma$ holds trivially. It therefore suffices to assume that the limit in the last equation is finite. In particular, $\{\mu_N\}$ must contain a subsequence comprising only elements from $\mathcal{P}_N(A)$, so without loss of generality we suppose that μ_N, $N \geqslant 1$, is a sequence of discrete measures converging to $\mu \in \mathcal{P}(A)$, such that the following limit exists and is finite:

$$\lim_{N\to\infty} \frac{1}{N^{1+s/d}} \mathcal{F}_N(\mu_N; w, V),$$

so that it will suffice to show its value is at least $\mathcal{F}(\mu; w, V)$. By Corollary 1.1, finiteness of the asymptotics implies that μ must be absolutely continuous with respect to $\mathcal{H}_d$.

The rest of the proof can be obtained by a modification of that of Theorem 1.1. Indeed, let ω_N be the sequence of N-point configurations corresponding to the measures μ_N, and denote $\rho := d\mu/d\mathcal{H}_d$. First, let ρ, w, V be bounded on A; then also $w\rho^{1+s/d}$, V are bounded, hence in $L^1(A, \mathcal{H}_d)$, and equations (4.32) apply. Since the argument resulting in (4.28) did not use optimality of the sequence of configurations, it applies to the ω_N; thus, we have for $\mathcal{H}_d$-a.e. $x \in A$, setting $B_x := B_A(x, r)$ with $r < r_{x,\varepsilon}$ sufficiently small:

$$\begin{aligned}\liminf_{N\to\infty} \frac{\mathbf{e}(\omega_N; B_x)}{N^{1+s/d}} &\geqslant \mu(B_x) \left(C^k_{s,d}(w(x,x) - \varepsilon) \cdot ((1-\varepsilon)\rho(x))^{s/d} + (V(x) - \varepsilon) \right) \\ &\geqslant (1-\varepsilon)^{1+s/d} \int_{B_x} \left(C^k_{s,d} w(x,x) \rho^{s/d} + V(x) \right) d\mu(x) - \varepsilon \mu(B_x) \left(C^k_{s,d} \rho(x,x)^{s/d} + 1 \right),\end{aligned}$$

Applying Vitali covering theorem to A, we conclude as in the proof of Theorem 1.1:

$$\begin{aligned}\liminf_{N\to\infty} \frac{E^k_s(\omega_N; w, V)}{N^{1+s/d}} &\geqslant \liminf_{N\to\infty} \sum_j \frac{\mathbf{e}(\omega^*_N; B_{x_j})}{N^{1+s/d}} \\ &\geqslant (1-\varepsilon)^{s/d} \int_A \left(C^k_{s,d} w(x,x) \rho(x)^{s/d} + V \right) d\mu(x) - c\varepsilon.\end{aligned}$$

This completes the proof of $\mathbf{1}^\Gamma$ for bounded densities ρ and w, V. The case of unbounded ρ and/or w, V follows by applying the previous lower bound to the probability measures

$$\mu_h(E) := \frac{\int_{E \cap \{\rho \leqslant h\}} \rho(x)\, d\mathcal{H}_d(x)}{\int_{\{\rho \leqslant h\}} \rho(x)\, d\mathcal{H}_d(x)},$$

and the monotone convergence $\rho \cdot \mathbb{1}_{\rho \leqslant h} \uparrow \rho$, $h \to \infty$; similarly, weights $w_h := w \cdot \mathbb{1}_{w \leqslant h}$ and external fields $V_h := V \cdot \mathbb{1}_{V \leqslant h}$, with the respective monotone convergences. This proves $\mathbf{1}^\Gamma$.

To present a recovery sequence, we again invoke the argument from Theorem 1.1. In the case of a bounded ρ, constructing a sequence of piecewise minimizers ω_N as in that proof gives

$$\limsup_{N\to\infty} \frac{E^k_s(\omega_N; w, V)}{N^{1+s/d}} \leqslant \frac{(1+\varepsilon)^{s/d}}{(1-\varepsilon)^{1+s/d}} \left(C^k_{s,d} \int_B \left((w(x,x) + \varepsilon) \rho(x)^{s/d} + V \right) d\mu(x) + \varepsilon c \right),$$

where B is a union of disjoint closed balls with $\mu(B) > (1-\varepsilon)$. In the case of unbounded ρ, we construct recovery sequences for μ_h as above, and then take a diagonal sequence. $\square$

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