Minimal Riesz energy point configurations for rectifiable d-dimensional manifolds

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Abstract

We investigate the energy of arrangements of N points on a rectifiable d-dimensional manifold $A \subset \mathbb{R}^{d'}$ that interact through the power law (Riesz) potential $V = 1/r^s$, where $s > 0$ and r is Euclidean distance in $\mathbb{R}^{d'}$. With $\mathcal{E}_s(A, N)$ denoting the *minimal* energy for such N-point configurations, we determine the asymptotic behavior (as $N \to \infty$) of $\mathcal{E}_s(A, N)$ for each fixed $s \geq d$. Moreover, if A has positive d-dimensional Hausdorff measure, we show that N-point configurations on A that minimize the s-energy are asymptotically uniformly distributed with respect to d-dimensional Hausdorff measure on A when $s \geq d$. Even for the unit sphere $S^d \subset \mathbb{R}^{d+1}$, these results are new.

Key words: Minimal discrete Riesz energy, Best-packing, Hausdorff measure, Rectifiable manifolds, Uniform distribution of points on a sphere, Power law potential
AMS Classification: Primary 11K41, 70F10, 28A78; Secondary 78A30, 52A40

1 Introduction

Determining N points on the unit sphere S^d in $\mathbb{R}^{d+1}$ that are in some sense uniformly distributed over its surface is a classical problem that has applications to such diverse fields as crystallography, electrostatics, viral morphology, molecular modeling, and global positioning. Various criteria (appropriate to

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[1] The research of this author was supported, in part, by the U. S. National Science Foundation under grant DMS-0296026.

the application) for the generation of such points include best-packing, minimization of energy (e.g., Coulomb potentials), spherical t-designs (cubature), maximization of volume of convex polyhedra with N vertices on S^d, etc.

A motivation for the present paper is the analysis of the asymptotic behavior (as $N \to \infty$) of optimal (and near optimal) N-point configurations that minimize the **Riesz s-energy**

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

over all N-point subsets $\{x_1, \ldots, x_N\}$ of S^d, where $s > 0$ is a fixed parameter and $|\cdot|$ denotes the Euclidean norm in $\mathbb{R}^{d+1}$. We remark that as $s \to \infty$, with N fixed, the s-energy (1) is increasingly dominated by the term(s) involving the smallest of pairwise distances and, in this sense, leads to the best-packing problem on S^d (cf. [3], [4]). We further note that for $s = 1$ and $d = 2$, the minimization of (1) is the classic Thomson problem (see e.g. [1], [2], [12], [17]).

In this paper we investigate the case when s is fixed, $s \geq d$, and $N \to \infty$. Significantly our results apply not only to the sphere, but to a class of rectifiable d-dimensional manifolds embedded in $\mathbb{R}^{d'}$. For such manifolds we determine, for $s \geq d$, the asymptotic behavior of the minimum Riesz s-energy as well as the asymptotic distribution of optimal and near optimal N-point configurations. Indeed we shall prove that the latter is given by d-dimensional Hausdorff measure on the manifold and that the minimum N-point Riesz s-energy over the manifold is asymptotically given by $C_s N^{1+s/d}$ when $s > d$ and by $C_d N^2 \log N$ when $s = d$. The essential feature of these results (see Theorems 2.1, 2.2, and 2.4) is not merely the order of growth of the minimum energy as $N \to \infty$, but rather the more delicate verification of the existence of the positive constants C_s for $s \geq d$; a fact which is new even for the case of the sphere S^d when $s > d$. Somewhat surprising is the fact that we can give an explicit formula for C_d (i.e., for the case $s = d$) in terms of its Hausdorff measure for any compact subset of a d-dimensional C^1-manifold in $\mathbb{R}^{d'}$ (see Theorem 2.4 and equation (8)).

We remark that for $0 < s < d$, standard potential theoretic arguments can be used for the analysis of the minimum energy points (cf. [9]). However, for $s \geq d$ such methods do not apply. Instead we exploit the scaling and translation properties of the energy function together with self-similarity and convexity arguments.

For the remainder of this section we introduce some needed notation and, by way of further background, we mention known related results for the sphere S^d. We devote the next section to the statement of our main results.

Throughout this paper, $\omega_N = \{x_1, \ldots, x_N\}$ denotes a set of N (possibly 0) distinct points in $\mathbb{R}^{d'}$. For each real $s > 0$ the s**-energy** of ω_N is given by

$$E_s(\omega_N) := \sum_{x \neq y \in \omega_N} \frac{1}{|x-y|^s} = \sum_{y \in \omega_N} \sum_{\substack{x \in \omega_N \\ x \neq y}} \frac{1}{|x-y|^s} \tag{2}$$

where, as above, $|\cdot|$ denotes Euclidean distance in $\mathbb{R}^{d'}$. For $A \subset \mathbb{R}^{d'}$ we define the N**-point minimal** s**-energy over** A by

$$\mathcal{E}_s(A, N) := \inf_{\omega_N \subset A} E_s(\omega_N). \tag{3}$$

By convention, the sum over an empty set of indices is taken to be zero and the infimum over an empty set is ∞. Hence, $\mathcal{E}_s(A,N) = \infty$ if N is greater than the cardinality of A and $E_s(\omega_N) = 0$ if $N = 0, 1$. It is clear that $\mathcal{E}_s(A,N) = \mathcal{E}_s(\bar{A}, N)$, where $\bar{A}$ denotes the closure of A and, furthermore, that $\mathcal{E}_s(A,N) = 0$ if A is unbounded. Hence, without loss of generality, we may restrict ourselves to the case that A is compact.

For the unit sphere $S^d \subset \mathbb{R}^{d+1}$, the asymptotic behavior (as $N \to \infty$) of $\mathcal{E}_s(S^d, N)$ is quite different for the three cases (*i*) $0 < s < d$; (*ii*) $s = d$; and (*iii*) $s > d$. The reason for this is that in case (*i*), the energy integral

$$I_s(\mu) := \iint_{S^d \times S^d} \frac{1}{|x-y|^s} \, d\mu(x) \, d\mu(y) \tag{4}$$

taken over all probability measures μ supported on S^d is *minimal* for normalized Lebesgue measure $\mathcal{H}_d(\cdot)|_{S^d} / \mathcal{H}_d(S^d)$ on S^d. However, for $s \geq d$, we have $I_s(\mu) = +\infty$ for all such measures μ. Roughly speaking, as the parameter s increases, there is a transition from the domination of global effects to the domination of more local (near-neighbors) influences, and this transition occurs precisely when $s = d$.

The following results are known for the above mentioned cases. In case (*i*), classical potential theory yields (cf. [9]):

Theorem 1.1 *If* $0 < s < d$*,*

$$\lim_{N \to \infty} \frac{\mathcal{E}_s(S^d, N)}{N^2} = I_s \left(\frac{\mathcal{H}_d(\cdot)|_{S^d}}{\mathcal{H}_d(S^d)} \right), \tag{5}$$

where I_s *is defined in (4). Moreover, any sequence of optimal* s*-energy configurations* $(\omega_N^*)_2^\infty \subset S^d$ *is asymptotically uniformly distributed in the sense that for the weak-star topology of measures,*

$$\frac{1}{N} \sum_{x \in \omega_N^*} \delta_x \longrightarrow \frac{\mathcal{H}_d(\cdot)|_{S^d}}{\mathcal{H}_d(S^d)} \qquad \text{as } N \to \infty, \tag{6}$$

where δ_x *denotes the unit point mass at* x*.*

For case (ii), we have from the results of Kuijlaars and Saff [8] and Götz and Saff [6] the following:

Theorem 1.2 *Let $\mathcal{B}^d := \bar{B}(0,1)$ denote closed unit ball in $\mathbb{R}^d$. For $s = d$,*

$$\lim_{N\to\infty} \frac{\mathcal{E}_d(S^d, N)}{N^2 \log N} = \frac{\mathcal{H}_d(\mathcal{B}^d)}{\mathcal{H}_d(S^d)} = \frac{1}{d} \frac{\Gamma(\frac{d+1}{2})}{\sqrt{\pi}\Gamma(\frac{d}{2})}, \tag{7}$$

and any sequence $(\omega_N^*) \subset S^d$ of optimal d-energy configurations satisfies (6).

(The reader is cautioned that the definition of energy used here differs by a factor of 2 from that in [8].)

Until now, results for $s > d$ have been less complete, describing only the order of growth of $\mathcal{E}_s(S^d, N)$. The following is proved in [8].

Theorem 1.3 *For $s > d$, there exist positive constants $c_1 = c_1(s,d)$, $c_2 = c_2(s,d)$ such that*

$$c_1 N^{1+s/d} \leq \mathcal{E}_s(S^d, N) \leq c_2 N^{1+s/d}, \qquad N \geq 2.$$

Natural questions that therefore arise for the case $s > d$ are:

(a) Does the limit
$$\lim_{N\to\infty} \frac{\mathcal{E}_s(S^d, N)}{N^{1+s/d}} \quad \text{exist?}$$
(b) If so, what is the limit?
(c) Are optimal s-energy configurations $\omega_N^* \subset S^d$ asymptotically uniformly distributed on S^d?

In this paper we show as a corollary to our main results that questions (a) and (c) have affirmative answers. Question (b) remains open for $d \geq 2$. But more interesting is the fact that we can affirm (a) and (c) for a general class of d-dimensional rectifiable manifolds embedded in $\mathbb{R}^{d'}$ (cf. Theorem 2.4). And for such manifolds, in the case $s = d$, we give an explicit formula for $\lim_{N\to\infty} \mathcal{E}_d(A, N)/N^2 \log N$ for every $d \in \mathbb{N}$. For further background discussion, see [7,14–16].

2 Main Results

In this section we state our main results. Their proofs are given in the sections that follow. Let $\mathcal{H}_d$ denote d-dimensional Hausdorff measure in $\mathbb{R}^{d'}$ normalized so that a d-sided cube with side length 1 has $\mathcal{H}_d$-measure equal to 1. In the case $d' = d$, then $\mathcal{H}_d$ reduces to Lebesgue measure on $\mathbb{R}^d$.

Theorem 2.1 *Suppose $A \subset \mathbb{R}^d$ is compact. Then*

$$\lim_{N\to\infty} \frac{\mathcal{E}_d(A,N)}{N^2 \log N} = \frac{\mathcal{H}_d(\mathcal{B}^d)}{\mathcal{H}_d(A)}, \tag{8}$$

where $\mathcal{B}^d$ is the closed unit ball in $\mathbb{R}^d$. Furthermore, for $s > d$, the limit $\lim_{N\to\infty} \mathcal{E}_s(A,N)/N^{1+s/d}$ exists and is given by

$$\lim_{N\to\infty} \frac{\mathcal{E}_s(A,N)}{N^{1+s/d}} = \frac{C_{s,d}}{\mathcal{H}_d(A)^{s/d}}, \tag{9}$$

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

Remarks.

(i) From (9) it is clear that, for $s > d$,

$$C_{s,d} = \lim_{N\to\infty} \frac{\mathcal{E}_s(U^d,N)}{N^{1+s/d}}, \tag{10}$$

where $U^d := [0,1]^d$ is the unit cube in $\mathbb{R}^d$. We further remark that if $\mathcal{H}_d(A) = 0$, then the limits in (8) and (9) equal ∞.

(ii) Let $\bar{B}(a,\rho)$ denote the closed ball in $\mathbb{R}^d$ centered at a with radius ρ. Then the limit with $A = \bar{B}(a,\rho)$ in (8) is simply $1/\rho^d$.

Theorem 2.2 *Let $A \subset \mathbb{R}^d$ be compact with $\mathcal{H}_d(A) > 0$, and $\omega_N = \{x_{k,N}\}_{k=1}^N$ be a sequence of asymptotically optimal N-point configurations in A in the sense that for some $s > d$*

$$\lim_{N\to\infty} \frac{E_s(\omega_N)}{N^{1+s/d}} = \frac{C_{s,d}}{\mathcal{H}_d(A)^{s/d}}, \tag{11}$$

or

$$\lim_{N\to\infty} \frac{E_d(\omega_N)}{N^2 \log N} = \frac{\mathcal{H}_d(\mathcal{B}^d)}{\mathcal{H}_d(A)}. \tag{12}$$

Let δ_x denote the unit point mass in the point x. Then in the weak-star topology of measures we have

$$\frac{1}{N}\sum_{i=1}^N \delta_{x_{i,N}} \longrightarrow \frac{\mathcal{H}_d(\cdot)|_A}{\mathcal{H}_d(A)} \quad \text{as } N \to \infty. \tag{13}$$

Remark. The convergence assertion (13) is equivalent to each of the following assertions:

(i) For each f continuous on A,

$$\lim_{N\to\infty} \frac{1}{N}\sum_{i=1}^N f(x_{i,N}) = \frac{1}{\mathcal{H}_d(A)} \int_A f(x)\, d\mathcal{H}_d(x) \tag{14}$$

(ii) For every measurable set $B \subset A$ whose boundary relative to A has $\mathcal{H}_d$-measure zero, the cardinality $|B \cap \omega_N|$ satisfies

$$\frac{|B \cap \omega_N|}{N} \to \frac{\mathcal{H}_d(B)}{\mathcal{H}_d(A)} \quad \text{as } N \to \infty. \tag{15}$$

Theorem 2.3 *Let A be a compact set in $\mathbb{R}^d$ such that $\mathcal{H}_d(A) > 0$ and $\lambda_N^* = \{x_{1,N}^*, \ldots, x_{N,N}^*\} \subset A$ an optimal N point s-energy configuration for A. If $s \geq d$, there exists a positive constant $C = C(A, s, d)$ such that for every $N \geq 2$,*

$$\min_{i \neq j} |x_{i,N}^* - x_{j,N}^*| \geq \begin{cases} C/N^{1/d} & \text{for } s > d, \\ C/(N \log N)^{1/d} & \text{for } s = d. \end{cases} \tag{16}$$

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

$$|\phi(x) - \phi(y)| \leq L|x - y| \qquad \text{for } x, y \in T \tag{17}$$

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

$$(1/L)|x - y| \leq |\phi(x) - \phi(y)| \leq L|x - y| \qquad \text{for } x, y \in T. \tag{18}$$

We say that $A \subset \mathbb{R}^{d'}$ is a d**-rectifiable manifold** if A can be written as

$$A = \bigcup_{k=1}^{n} \phi_k(K_k) \tag{19}$$

where, for each $k = 1, \ldots, n$, $K_k \subset \mathbb{R}^d$ is compact and ϕ_k is bi-Lipschitz on an open set $G_k \supset K_k$. Obviously any compact subset of a d-rectifiable manifold is a d-rectifiable manifold.

Theorem 2.4 *Suppose $A \subset \mathbb{R}^{d'}$ is a d-rectifiable manifold and $s \geq d$. If $s = d$, we further suppose that A is a subset of a d-dimensional C^1-manifold. Then (8) and (9) hold. Furthermore, if $\mathcal{H}_d(A) > 0$, then (13) holds for any asymptotically minimal sequence of N point configurations ω_N for A satisfying (11) or (12). For the case when A is a bi-Lipschitz image of a single compact set in $\mathbb{R}^d$ and $\mathcal{H}_d(A) > 0$, the separation estimates of (16) hold for any optimal N-point s-energy configuration.*

Remark. Note that d' does not explicitly appear in (8) and (9) but arises only in the norms for the computation of the energy.

It is shown in [8] that, for the unit interval $U^1 = [0, 1]$,

$$\lim_{N \to \infty} \frac{\mathcal{E}_s(U^1, N)}{N^{1+s}} = 2\zeta(s) \qquad (s > 1), \tag{20}$$

where $\zeta(s)$ denotes the classical Riemann zeta function. Hence, using (10), we get $C_{s,1} = 2\zeta(s)$ for $s > 1$. Consequently, Theorem 2.4 gives the following.

Corollary 2.5 *Suppose A is a compact subset of a 1-rectifiable manifold in $\mathbb{R}^{d'}$ and $s > 1$. Then*

$$\lim_{N\to\infty} \frac{\mathcal{E}_s(A,N)}{N^{1+s}} = \frac{2\zeta(s)}{\mathcal{H}_1(A)^s}. \tag{21}$$

That Corollary 2.5 holds when A is a finite union of rectifiable Jordan arcs was shown in [10]. Since a Lipschitz mapping on an interval is absolutely continuous, but the converse is not necessarily true, the results in [10] hold in cases not covered by Corollary 2.5. On the other hand, Corollary 2.5 applies to 1-rectifiable manifolds that are not covered by the results in [10] such as, for example, when A is the bi-Lipschitz image of a Cantor subset of [0,1] having positive measure.

For the 2-sphere it is shown in [8] that for $s > 2$,

$$\limsup_{N\to\infty} \frac{\mathcal{E}_s(S^2,N)}{N^{1+s/2}} \leq \left(\frac{\sqrt{3}}{8\pi}\right)^{s/2} \zeta_L(s), \tag{22}$$

where $\zeta_L(s)$ is the zeta function for the hexagonal lattice L consisting of points of the form $m(1,0) + n(1/2, \sqrt{3}/2)$ for $m,n \in \mathbb{Z}$. Consequently (cf. (9)),

$$C_{s,2} \leq \left(\frac{\sqrt{3}}{2}\right)^{s/2} \zeta_L(s). \tag{23}$$

It is conjectured in [8] that equality holds in (22) which, if true, would imply that equality holds in (23).

An outline of the remainder of the paper is as follows. In Section 3 we establish some basic lemmas on the minimal s-energy of the union of two subsets of $\mathbb{R}^d$. Section 4 gives the proof of Theorem 2.1 for the special case when A is the unit cube in $\mathbb{R}^d$. In Section 5, we verify Theorems 2.1 and 2.2 for almost clopen sets in $\mathbb{R}^d$. Results on the separation of points in optimal energy configurations are established in Section 6. The proofs of Theorems 2.1 and 2.2 for general compact sets in $\mathbb{R}^d$ is presented in Section 7 and the proof of Theorem 2.4 appears in Section 8.

3 Basic Lemmas

In this section we establish several lemmas that are required for the proofs of our main results. First we establish that if $A \subset \mathbb{R}^d$ is bounded with nonempty interior, then $\mathcal{E}_s(A,N)$ grows as $N \to \infty$ with order $N^{1+s/d}$ for $s > d$ and $N^2 \log N$ for $s = d$.

Lemma 3.1 *Suppose $A \subset \mathbb{R}^d$ is a bounded set with nonempty interior. There exist positive constants C_0, C_1 (depending on A, s, and d, but not on N) such that, if $s > d$,*

$$C_0 N^{1+s/d} \leq \mathcal{E}_s(A,N) \leq C_1 N^{1+s/d} \qquad (N \geq 2) \tag{24}$$

and, if $s = d$,

$$C_0 N^2 \log N \leq \mathcal{E}_d(A,N) \leq C_1 N^2 \log N \qquad (N \geq 2). \tag{25}$$

Proof. We first consider $U^d = [0,1]^d$. Let $B(x,r)$ denote the open ball in $\mathbb{R}^d$ with center x and radius r. Then with $C = (1/2)^d \mathcal{H}_d(B(0,1))$ we have

$$\mathcal{H}_d(B(x,r) \cap U^d) \geq C r^d \tag{26}$$

for any $x \in U^d$ and $r < 1$.

For $N > 1$, let $\omega_N = \{x_1, \ldots, x_N\}$ be a collection of N distinct points in U^d and let

$$r_i := \min_{j \neq i} |x_i - x_j|.$$

Since $B(x_i, r_i/2) \cap B(x_j, r_j/2) = \emptyset$ for $1 \leq i \neq j \leq N$, we have

$$1 = \mathcal{H}_d(U^d) \geq \sum_{i=1}^N \mathcal{H}_d(B(x_i, r_i/2) \cap U^d) \geq \frac{C}{2^d} \sum_{i=1}^N r_i^d. \tag{27}$$

By the Cauchy-Schwarz inequality we have

$$N^2 = \left(\sum_{i=1}^N r_i^{d/2} r_i^{-d/2} \right)^2 \leq \sum_{i=1}^N r_i^d \sum_{i=1}^N r_i^{-d}, \tag{28}$$

which is known as the harmonic-arithmetic mean inequality. Thus

$$\begin{aligned} E_s(\omega_N) &\geq \sum_{i=1}^N \frac{1}{r_i^s} = N \sum_{i=1}^N \frac{1}{N} \left(\frac{1}{r_i^d} \right)^{s/d} \\ &\geq N \left(\sum_{i=1}^N \frac{1}{N} \frac{1}{r_i^d} \right)^{s/d} \geq N \left(\frac{N}{\sum_{i=1}^N r_i^d} \right)^{s/d}, \end{aligned} \tag{29}$$

where the next to the last inequality follows from Jensen's inequality (or Hölder's inequality) and the last inequality follows from (28). Since (29) holds for any collection ω_N of N distinct points in U^d, then using (27) we have

$$\mathcal{E}_s(U^d, N) \geq N^{1+s/d} C^{s/d} 2^{-s} \qquad (N > 2)$$

showing that the lower estimate in (24) holds for $A = U^d$ and with $C_0 = C^{s/d}2^{-s}$.

For $s = d$, the lower estimate in (25) is not so straightforward. For this case we shall apply the known result (7). The unit cube U^d in $\mathbb{R}^d$ can be projected onto a subset of S^d via the stereographic projection $\mathbb{P} : \mathbb{R}^d \to S^d$ defined by

$$\mathbb{P}(x) = (tx, 1 - t) \in \mathbb{R}^{d+1}, \qquad t = \frac{2}{|x|^2 + 1}. \tag{30}$$

It is easily verified (and well-known in the case $d = 2$) that for $x, y \in \mathbb{R}^d$, we have

$$|\mathbb{P}(x) - \mathbb{P}(y)| = \frac{2|x - y|}{\sqrt{1 + |x|^2}\sqrt{1 + |y|^2}}. \tag{31}$$

Consequently, for some positive constant C,

$$\mathcal{E}_d(U^d, N) \geq C\mathcal{E}_d(\mathbb{P}(U^d), N) \geq C\mathcal{E}_d(S^d, N),$$

and so the desired lower estimate follows from (7). (Later we shall show how (7) can be utilized to determine the precise asymptotic behavior of $\mathcal{E}_d(A, N)$ for d-rectifiable manifolds.)

For $N > 1$, let m be the positive integer such that $m^d \leq N < (m + 1)^d$. Let ω_N consist of N points selected from $U^d \cap \left(\mathbb{Z}^d/m\right)$. Then $x - y \in \mathbb{Z}^d/m$ for $x, y \in \omega_N$. For $\mathbf{k} = (k_1, \ldots, k_d) \in \mathbb{Z}^d$, set $\|\mathbf{k}\|_\infty = \max\{|k_i|, i = 1, \ldots, d\}$ and let $|\mathbf{k}|$ denote its Euclidean norm. Then

$$\begin{aligned} E_s(\omega_N) &= \sum_{x \neq y \in \omega_N} \frac{1}{|x - y|^s} \leq N m^s \sum_{1 \leq \|\mathbf{k}\|_\infty \leq m} \frac{1}{|\mathbf{k}|^s} \\ &\leq N^{1+s/d} \sum_{j=1}^{m} \sum_{\|\mathbf{k}\|_\infty = j} \frac{1}{j^s} = N^{1+s/d} \sum_{j=1}^{m} \frac{(2j+1)^d - (2j-1)^d}{j^s} \\ &\leq C N^{1+s/d} \sum_{j=1}^{[N^{1/d}]+1} \frac{1}{j^{1+s-d}}. \end{aligned}$$

For $s > d$, the sum in the last inequality is bounded from above independently of N, while for $s = d$, it is bounded by a constant times $\log N$. Thus the estimates (24) and (25) hold for $A = U^d$.

More generally, if A is a bounded set with nonempty interior, then there exist $r, R > 0$ and $x_0, x_1 \in \mathbb{R}^d$ such that $rU^d + x_0 \subset A \subset RU^d + x_1$. Since $\mathcal{E}_s(\rho U^d + x, N) = \rho^{-s}\mathcal{E}_s(U^d, N)$ for any $\rho > 0$ and $x \in \mathbb{R}^d$, the estimates (24) and (25) follow for A. (For an alternative proof of the upper bound, see the proof of Theorem 2.3 in Section 6.) $\square$

Definition 1 *Let $\tau_{s,d} : \mathbb{N} \to \mathbb{R}$ be defined by*

$$\tau_{s,d}(N) = \begin{cases} N^{1+s/d} & \text{if } s > d \\ N^2 \log N & \text{if } s = d. \end{cases} \tag{32}$$

For $A \subset \mathbb{R}^{d'}$ and a positive integer N, define

$$\mathcal{G}_{s,d}(A, N) := \mathcal{E}_s(A, N)/\tau_{s,d}(N) \tag{33}$$

and let

$$\underline{g}_{s,d}(A) := \liminf_{N\to\infty} \mathcal{G}_{s,d}(A, N), \quad \overline{g}_{s,d}(A) := \limsup_{N\to\infty} \mathcal{G}_{s,d}(A, N).$$

We set

$$g_{s,d}(A) := \lim_{N\to\infty} \mathcal{G}_{s,d}(A, N)$$

when the limit (as an extended real number) exists.

If $A \subset \mathbb{R}^d$ is bounded and has nonempty interior, then by Lemma 3.1 there exist positive constants C_0, C_1 such that

$$C_0 \le \mathcal{G}_{s,d}(A, N) \le C_1$$

for $N \ge 2$. Hence, $\underline{g}_{s,d}(A)$ and $\overline{g}_{s,d}(A)$ are both positive and finite in this case.

Lemma 3.2 *Suppose $s \ge d$ and that A and B are bounded sets in $\mathbb{R}^{d'}$. Then*

$$\underline{g}_{s,d}(A \cup B) \ge \left(\underline{g}_{s,d}(A)^{-d/s} + \underline{g}_{s,d}(B)^{-d/s}\right)^{-s/d}. \tag{34}$$

Furthermore, if $\underline{g}_{s,d}(A) < \infty$ or if $\underline{g}_{s,d}(A) = \infty$ and $\underline{g}_{s,d}(B) < \infty$, and $\mathcal{N}$ is an infinite subset of $\mathbb{N}$ and $(\omega_N)_{N\in\mathcal{N}}$ is a sequence of sets $\omega_N \subset A \cup B$, $N \in \mathcal{N}$, such that

$$\lim_{\substack{N\to\infty \\ N\in\mathcal{N}}} \frac{E_s(\omega_N)}{\tau_{s,d}(N)} = \left(\underline{g}_{s,d}(A)^{-d/s} + \underline{g}_{s,d}(B)^{-d/s}\right)^{-s/d}, \tag{35}$$

then

$$\lim_{\substack{N\to\infty \\ N\in\mathcal{N}}} \frac{|\omega_N \cap A|}{N} = \frac{\underline{g}_{s,d}(B)^{d/s}}{\underline{g}_{s,d}(A)^{d/s} + \underline{g}_{s,d}(B)^{d/s}}. \tag{36}$$

Remark. If both $\underline{g}_{s,d}(A) < \infty$ and $\underline{g}_{s,d}(B) = \infty$, then the right-hand sides of (34) and (36) are understood to be $\underline{g}_{s,d}(A)$ and 1, respectively; while if $\underline{g}_{s,d}(A) = \underline{g}_{s,d}(B) = \infty$, then the right-hand side of (34) is understood to be ∞.

Proof. Both $\underline{g}_{s,d}(A)$ and $\underline{g}_{s,d}(B)$ are positive since A and B are bounded. First we assume that $\underline{g}_{s,d}(A)$ and $\underline{g}_{s,d}(B)$ are finite. Suppose, for $N \in \mathbb{N}$, that ω_N

is a set of N distinct points in $A \cup B$. Let $\omega_N^A = \omega_N \cap A$ and $\omega_N^B = \omega_N \setminus \omega_N^A$. Then

$$E_s(\omega_N) = E_s(\omega_N^A) + E_s(\omega_N^B) + 2 \sum_{a \in \omega_N^A, b \in \omega_N^B} \frac{1}{|a-b|^s} \geq E_s(\omega_N^A) + E_s(\omega_N^B) \quad (37)$$

and hence

$$\mathcal{E}_s(A \cup B, N) \geq \min_{N_A + N_B = N} \left(\mathcal{E}_s(A, N_A) + \mathcal{E}_s(B, N_B) \right), \quad (38)$$

where N_A and N_B are nonnegative integers. First suppose $s > d$. Then we have

$$\begin{aligned}
&\underline{g}_{s,d}(A \cup B) \\
&\quad \geq \liminf_{N\to\infty} \min_{N_A+N_B=N} \left[\frac{\mathcal{E}_s(A, N_A)}{N_A^{1+s/d}} \left(\frac{N_A}{N}\right)^{1+s/d} + \frac{\mathcal{E}_s(B, N_B)}{N_B^{1+s/d}} \left(\frac{N_B}{N}\right)^{1+s/d} \right] \\
&\quad \geq \liminf_{N\to\infty} \min_{N_A+N_B=N} \left[\underline{g}_{s,d}(A) \left(\frac{N_A}{N}\right)^{1+s/d} + \underline{g}_{s,d}(B) \left(\frac{N_B}{N}\right)^{1+s/d} \right] \quad (39) \\
&\quad \geq \min_{0\leq\alpha\leq 1} \left[\underline{g}_{s,d}(A) \alpha^{1+s/d} + \underline{g}_{s,d}(B) (1-\alpha)^{1+s/d} \right].
\end{aligned}$$

(Note: In the case $N_A = 0$ we set $\frac{\mathcal{E}_s(A,N_A)}{N_A^{1+s/d}} \left(\frac{N_A}{N}\right)^{1+s/d} = \frac{\mathcal{E}_s(A,N_A)}{N^{1+s/d}} = 0$. The case $N_B = 0$ is handled similarly.) Let

$$F(\alpha) := \underline{g}_{s,d}(A) \alpha^{1+s/d} + \underline{g}_{s,d}(B) (1-\alpha)^{1+s/d} \qquad (0 \leq \alpha \leq 1). \quad (40)$$

The reader may verify using elementary calculus that F has a unique minimum value $F(\alpha^*) = \left(\underline{g}_{s,d}(A)^{-d/s} + \underline{g}_{s,d}(B)^{-d/s} \right)^{-s/d}$, where

$$\alpha^* = \underline{g}_{s,d}(B)^{d/s} / \left(\underline{g}_{s,d}(A)^{d/s} + \underline{g}_{s,d}(B)^{d/s} \right).$$

This proves (34) when $s > d$.

Now suppose $(\omega_N)_{N\in\mathcal{N}}$ is a sequence of sets $\omega_N \subset A \cup B$, $N \in \mathcal{N}$, such that (35) holds. We may rewrite (37) in the form

$$\frac{E_s(\omega_N)}{N^{1+s/d}} \geq \frac{E_s(\omega_N^A)}{N_A^{1+s/d}} \left(\frac{N_A}{N}\right)^{1+s/d} + \frac{E_s(\omega_N^B)}{N_B^{1+s/d}} \left(\frac{N_B}{N}\right)^{1+s/d} \qquad (N \in \mathcal{N}), \quad (41)$$

and hence, if β is any limit point of the sequence N_A/N, $N \in \mathcal{N}$, we get from (35) that $F(\alpha^*) \geq F(\beta)$. Consequently, $\beta = \alpha^*$, which is equivalent to (36) in the case $s > d$.

We leave to the reader the remaining cases where at least one of $\underline{g}_{s,d}(A)$ and $\underline{g}_{s,d}(B)$ is infinite. It is helpful to regard separately the cases when N_B remains bounded or when $N_B \to \infty$ as $N \to \infty$.

The $s = d$ case of both (34) and (36) follows in a similar manner and is left as well for the reader. □

For $A, B \subset \mathbb{R}^{d'}$, let $\operatorname{dist}(A, B) := \inf_{a\in A,\, b\in B} |a - b|$.

Lemma 3.3 *Suppose A and B are bounded sets in $\mathbb{R}^{d'}$ such that* $\operatorname{dist}(A, B) > 0$. *Then*

$$\overline{g}_{s,d}(A \cup B) \le \left(\overline{g}_{s,d}(A)^{-d/s} + \overline{g}_{s,d}(B)^{-d/s}\right)^{-s/d}. \tag{42}$$

Proof. If $\overline{g}_{s,d}(A)$ or $\overline{g}_{s,d}(B)$ equal zero then $\overline{g}_{s,d}(A \cup B) = 0$ and so (42) holds (note that the right hand side of (42) is understood to be zero in this case).

Now suppose $\overline{g}_{s,d}(A)$ and $\overline{g}_{s,d}(B)$ are both positive. Let $\delta = \operatorname{dist}(A, B)$ and suppose $N \in \mathbb{N}$. Let $N_A = [\alpha^* N]$ where $\alpha^* = \overline{g}_{s,d}(B)^{d/s} / \left(\overline{g}_{s,d}(A)^{d/s} + \overline{g}_{s,d}(B)^{d/s}\right)$ and let $N_B = N - N_A$. Then

$$\begin{aligned} \mathcal{E}_s(A \cup B, N) &\le \mathcal{E}_s(A, N_A) + \mathcal{E}_s(B, N_B) + 2\delta^{-s} N_A N_B \\ &\le \mathcal{E}_s(A, N_A) + \mathcal{E}_s(B, N_B) + 2\delta^{-s} N^2, \end{aligned}$$

and hence

$$\mathcal{G}_{s,d}(A \cup B, N) \le \frac{\mathcal{E}_s(A, N_A)}{\tau_{s,d}(N_A)} \frac{\tau_{s,d}(N_A)}{\tau_{s,d}(N)} + \frac{\mathcal{E}_s(B, N_B)}{\tau_{s,d}(N_B)} \frac{\tau_{s,d}(N_B)}{\tau_{s,d}(N)} + 2\delta^{-s} \frac{N^2}{\tau_{s,d}(N)}.$$

Observe that $\lim_{N\to\infty} \tau_{s,d}(N_A)/\tau_{s,d}(N) = (\alpha^*)^{1+s/d}$, $\lim_{N\to\infty} \tau_{s,d}(N_B)/\tau_{s,d}(N) = (1-\alpha^*)^{1+s/d}$, and $\lim_{N\to\infty} N^2/\tau_{s,d}(N) = 0$. Thus we have

$$\begin{aligned} \overline{g}_{s,d}(A \cup B) &\le \overline{g}_{s,d}(A)(\alpha^*)^{1+s/d} + \overline{g}_{s,d}(B)(1-\alpha^*)^{1+s/d} \\ &= \left(\overline{g}_{s,d}(A)^{-d/s} + \overline{g}_{s,d}(B)^{-d/s}\right)^{-s/d}. \end{aligned}$$

□

We say that a set $A \subset \mathbb{R}^d$ is **scalable** if A is closed and if for each $\epsilon > 0$ there is some bi-Lipschitz mapping $h : A \to A^\circ$ with constant $(1+\epsilon)$ where A° denotes the interior of A. For example, a compact, convex set with nonempty interior is scalable since, for $\epsilon > 0$, one may choose $h(x) = (1+\epsilon)^{-1}(x + \epsilon u)$ for any fixed u in the interior of A. Similarly, a star-like set is scalable.

Corollary 3.4 *Suppose $s \ge d$ and A and B are compact subsets of $\mathbb{R}^d$ with disjoint interiors such that $g_{s,d}(A)$ and $g_{s,d}(B)$ both exist and A is scalable. Then $g_{s,d}(A \cup B)$ exists and*

$$g_{s,d}(A \cup B) = \left(g_{s,d}(A)^{-d/s} + g_{s,d}(B)^{-d/s}\right)^{-s/d}. \tag{43}$$

Proof. Let $0 < \epsilon < 1$. Since A is scalable, there is some bi-Lipschitz mapping h with constant $(1+\epsilon)$ such that $h(A) \subset A^\circ$ and, hence, $\mathrm{dist}(h(A), B) \geq \mathrm{dist}(h(A), A^c) > 0$. Then Lemmas 3.2 and 3.3 imply

$$\begin{aligned}\left(g_{s,d}(A)^{-d/s} + g_{s,d}(B)^{-d/s}\right)^{-s/d} &\leq \underline{g}_{s,d}(A \cup B) \\ &\leq \overline{g}_{s,d}(A \cup B) \leq \overline{g}_{s,d}(h(A) \cup B) \\ &\leq \left(\overline{g}_{s,d}(h(A))^{-d/s} + g_{s,d}(B)^{-d/s}\right)^{-s/d}.\end{aligned}$$

Since $\overline{g}_{s,d}(h(A)) \leq (1+\epsilon)^s g_{s,d}(A)$, on letting $\epsilon \to 0$, we get (43). □

4 The unit cube $U^d := [0,1]^d$.

In this section we prove that $g_{s,d}(U^d)$ exists when $s \geq d$. We first prove the result when $s > d$ by using the self-similarity of U^d to obtain estimates relating $\mathcal{G}_{s,d}(U^d, N)$ at different values of N. For $s = d$ the method is not immediately applicable. Instead we use results and techniques developed in [8] and [6] for the sphere S^d which actually yield $g_{d,d}(U^d)$ explicitly. The proof of the next theorem in the case $s = d$ is given separately in Section 4.1.

Theorem 4.1 *For $s \geq d$, the limit $g_{s,d}(U^d) := \lim_{N\to\infty} \mathcal{G}_{s,d}(U^d, N)$ exists and is finite and positive. Moreover, in the case $s = d$,*

$$g_{d,d}(U^d) = \mathcal{H}_d(\mathcal{B}^d) = \frac{2\pi^{d/2}}{d\,\Gamma(\frac{d}{2})}. \tag{44}$$

Proof. Case: $s > d$.
We first establish a lemma relating $\mathcal{G}_{s,d}(U^d, N)$ at different values of N.

Lemma 4.2 *Suppose $s > d$, $\gamma \in (0,1)$ and m is a positive integer. Then there is some constant $C > 0$ (independent of m, N or γ) such that*

$$\mathcal{G}_{s,d}(U^d, m^d N) \leq \gamma^{-s} \mathcal{G}_{s,d}(U^d, N) + C(1-\gamma)^{-s} N^{1-s/d}. \tag{45}$$

Proof. If m is a positive integer, let $I_m = \{0, \ldots, m-1\}^d \subset \mathbb{Z}^d$ and, for $\mathbf{i} \in I_m$, set $U_{m,\mathbf{i}} := (U^d + \mathbf{i})/m$. Note that $\mathcal{G}_{s,d}(U_{m,\mathbf{i}}, N) = m^s \mathcal{G}_{s,d}(U^d, N)$.

For $\mathbf{i} \in I_m$, let $\omega_N^{\mathbf{i}}$ be a set of N points in $(\gamma U^d + \mathbf{i})/m$ with minimum energy. Let $\omega_{m^d N} = \bigcup_{\mathbf{i} \in I_m} \omega_N^{\mathbf{i}}$. If $x \in \omega_N^{\mathbf{i}}$ and $y \in \omega_N^{\mathbf{j}}$, then $|x - y| \geq \delta := (1-\gamma)/m$

if $\|\mathbf{i}-\mathbf{j}\|_\infty = 1$ and $|x-y| \geq \|\mathbf{i}-\mathbf{j}\|_\infty/(2m)$ for $\|\mathbf{i}-\mathbf{j}\|_\infty > 1$. Then

$$\begin{aligned}
\mathcal{E}_s(U^d, m^d N) &\leq E_s(\omega_{m^d N}) \leq \sum_{\mathbf{i}\in I_m} E_s(\omega_N^{\mathbf{i}}) + \sum_{\substack{\mathbf{i}\neq\mathbf{j}\in I_m \\ x\in\omega_N^{\mathbf{i}},\, y\in\omega_N^{\mathbf{j}}}} \frac{1}{|x-y|^s} \\
&\leq \sum_{\mathbf{i}\in I_m} \left(\mathcal{E}_s(\frac{\gamma}{m}U^d, N) + \delta^{-s} 3^d N^2 + 2^s \sum_{\substack{\mathbf{j}\in I_m \\ \|\mathbf{i}-\mathbf{j}\|_\infty > 1}} m^s \|\mathbf{i}-\mathbf{j}\|_\infty^{-s} N^2 \right) \\
&= \sum_{\mathbf{i}\in I_m} \left(m^s \gamma^{-s} \mathcal{E}_s(U^d, N) + m^s \frac{3^d N^2}{(1-\gamma)^s} + 2^s \sum_{\substack{\mathbf{j}\in I_m \\ \|\mathbf{i}-\mathbf{j}\|_\infty > 1}} m^s \|\mathbf{i}-\mathbf{j}\|_\infty^{-s} N^2 \right) \\
&\leq m^{d+s} \left(\gamma^{-s} \mathcal{E}_s(U^d, N) + \frac{3^d N^2}{(1-\gamma)^s} + 2^s K N^2 \right)
\end{aligned}$$

where $K := \sum_{\mathbf{k}\in\mathbb{Z}^d\setminus\{\mathbf{0}\}} \|\mathbf{k}\|_\infty^{-s}$ is finite, and so

$$\mathcal{G}_{s,d}(U^d, m^d N) \leq \gamma^{-s} \mathcal{G}_{s,d}(U^d, N) + (1-\gamma)^{-s} (3^d + 2^s K) \frac{m^{s+d} N^2}{\tau_{s,d}(m^d N)}. \tag{46}$$

Since $m^{s+d} N^2 / \tau_{s,d}(m^d N) = N^{1-s/d}$, the inequality (45) follows from (46) with $C = 3^d + 2^s K$, which completes the proof of Lemma 4.2. □

Now suppose $\epsilon > 0$ and $0 < \gamma < 1$. Let C be the constant in (45) and let N^* be such that $\mathcal{G}_{s,d}(U^d, N^*) < \underline{g}_{s,d}(U^d) + \gamma^s \epsilon/2$ and $C(N^*)^{1-s/d} < (1-\gamma)^s \epsilon/2$. By Lemma 4.2 we then have

$$g_m := \mathcal{G}_{s,d}(U^d, m^d N^*) < \gamma^{-s}(\underline{g}_{s,d}(U^d) + \gamma^s \epsilon/2) + C(1-\gamma)^{-s}(N^*)^{1-s/d}$$

for any $m \in \mathbb{N}$, and hence

$$\limsup_{m\to\infty} g_m \leq \gamma^{-s} \underline{g}_{s,d}(U^d) + \epsilon.$$

For $N > N^*$, let m_N be the greatest integer such that $m_N^d N^* < N$. Then

$$\mathcal{G}_{s,d}(U^d, N) = \frac{\mathcal{E}_s(U^d, N)}{N^{1+s/d}} \leq \frac{\mathcal{E}_s(U^d, (m_N+1)^d N^*)}{(m_N^d N^*)^{1+s/d}} = (1 + 1/m_N)^{s+d} g_{m_N+1}$$

holds for all $N > N^*$, and thus

$$\limsup_{N\to\infty} \mathcal{G}_{s,d}(U^d, N) \leq \limsup_{N\to\infty} (1 + 1/m_N)^{s+d} g_{m_N+1} \leq \gamma^{-s} \underline{g}_{s,d}(U^d) + \epsilon.$$

Since this holds for all $0 < \gamma < 1$ and $\epsilon > 0$ we have that $\overline{g}_{s,d}(U^d) \leq \underline{g}_{s,d}(U^d)$ and, hence, $g_{s,d}(U^d)$ exists. By Lemma 3.1, $g_{s,d}(U^d)$ is finite and positive in the case $s > d$, which completes the proof in this case. □

4.1 Proof of Theorem 4.1 in the case $s = d$.

By Theorem 1.2 we know that $g_{d,d}(S^d)$ exists and is given as in (7). For $N \in \mathbb{N}$, let ω_N^* denote a set of N points in S^d minimizing the d-energy. Also from this theorem we have

$$\lim_{N\to\infty} \frac{|\omega_N^* \cap A|}{N} = \frac{\mathcal{H}_d(A)}{\mathcal{H}_d(S^d)} \tag{47}$$

whenever $A \subset S^d$ is such that the boundary ∂A (relative to the sphere) has $\mathcal{H}_d(\partial A) = 0$. Such a set A is called an **almost clopen** subset of S^d.

Lemma 4.3 *For $N \in \mathbb{N}$, let ω_N^* denote a set of N points in S^d minimizing the d-energy. If A is an almost clopen subset of S^d, then*

$$\lim_{N\to\infty} \frac{E_d(\omega_N^* \cap A)}{\tau_{d,d}(N)} = g_{d,d}(S^d)\frac{\mathcal{H}_d(A)}{\mathcal{H}_d(S^d)}. \tag{48}$$

Proof. We first show that for any almost clopen subset K of S^d we have

$$\limsup_{N\to\infty} \frac{E_d(\omega_N^* \cap K)}{\tau_{d,d}(N)} \le g_{d,d}(S^d)\frac{\mathcal{H}_d(K)}{\mathcal{H}_d(S^d)}. \tag{49}$$

For this purpose we follow the argument given in [8]. Let $\{x_{i,N}^*\}_{i=1}^N$ denote the points of ω_N^* and for each i, set

$$U_{i,N}(x) := \sum_{j\neq i} |x - x_{j,N}^*|^{-d}, \qquad x \in S^d.$$

It is shown in inequality (6.6) of [8] that for every $r > 0$ sufficiently small we have

$$U_{i,N}(x_{i,N}^*) \le \frac{g_{d,d}(S^d) N \log N}{(1 - r^d g_{d,d}(S^d))} + \mathcal{O}_r(N) \qquad (N \to \infty). \tag{50}$$

Let $\Lambda(K,N) := \{i | x_{i,N}^* \in K\}$ and $N^K := |\Lambda(K,N)|$. Then from (50) we get

$$\begin{aligned} \frac{E_d(\omega_N^* \cap K)}{\tau_{d,d}(N)} &\le \frac{1}{\tau_{d,d}(N)} \sum_{i\in\Lambda(K,N)} U_{i,N}(x_{i,N}^*) \\ &\le \frac{N^K}{N} \frac{g_{d,d}(S^d)}{(1 - r^d g_{d,d}(S^d))} + \mathcal{O}_r\left(\frac{1}{\log N}\right). \end{aligned}$$

Letting $N \to \infty$ and then $r \to 0$ in this last inequality, we deduce from (47) that inequality (49) holds.

Now suppose that $A \subset S^d$ is almost clopen (with respect to $\mathcal{H}_d$), and let $B := S^d \setminus A$. For any set K, we put $K^N := \omega_N^* \cap K$. Then, clearly,

$$\frac{E_d(\omega_N^*)}{\tau_{d,d}(N)} = \frac{E_d(A^N)}{\tau_{d,d}(N)} + \frac{E_d(B^N)}{\tau_{d,d}(N)} + \frac{2}{\tau_{d,d}(N)} \sum_{\substack{x \in A^N \\ y \in B^N}} \frac{1}{|x-y|^d}. \tag{51}$$

We claim that, as $N \to \infty$, the last term in (51) tends to zero. To see this, let $\epsilon > 0$ be given and cover ∂A by an open (relative to S^d) set Ω_ϵ such that $\mathcal{H}_d(\Omega_\epsilon) < \epsilon$ and $\mathcal{H}_d(\partial\Omega_\epsilon) = 0$ (*e.g.*, let Ω_ϵ be a finite union of open balls). Then, since $\operatorname{dist}(A, B \setminus \Omega_\epsilon) > 0$ and $\operatorname{dist}(B, A \setminus \Omega_\epsilon) > 0$, it follows that, with $\tilde{A}_\epsilon := A \cap \Omega_\epsilon$, $\tilde{B}_\epsilon := B \cap \Omega_\epsilon$,

$$\begin{aligned} \limsup_{N\to\infty} \frac{2}{\tau_{d,d}(N)} \sum_{\substack{x \in A^N \\ y \in B^N}} \frac{1}{|x-y|^d} &= \limsup_{N\to\infty} \frac{2}{\tau_{d,d}(N)} \sum_{\substack{x \in \tilde{A}^N \\ y \in \tilde{B}^N}} \frac{1}{|x-y|^d} \\ &\leq \limsup_{N\to\infty} \frac{1}{\tau_{d,d}(N)} E_d(\bar{\Omega}_\epsilon^N). \end{aligned} \tag{52}$$

Since $\bar{\Omega}_\epsilon$ is almost clopen, we get from (49) and (52) that

$$\limsup_{N\to\infty} \frac{2}{\tau_{d,d}(N)} \sum_{\substack{x \in A^N \\ y \in B^N}} \frac{1}{|x-y|^d} \leq g_{d,d}(S^d) \frac{\mathcal{H}_d(\bar{\Omega}_\epsilon)}{\mathcal{H}_d(S^d)} \leq \frac{\epsilon g_{d,d}(S^d)}{\mathcal{H}_d(S^d)}.$$

As $\epsilon > 0$ is arbitrary, we have shown that the last term in (51) goes to zero as $N \to \infty$, as claimed. Consequently,

$$g_{d,d}(S^d) = \lim_{N\to\infty} \frac{E_d(\omega_N^*)}{\tau_{d,d}(N)} = \lim_{N\to\infty} \left(\frac{E_d(A^N)}{\tau_{d,d}(N)} + \frac{E_d(B^N)}{\tau_{d,d}(N)} \right). \tag{53}$$

Since A and B are almost clopen and $\mathcal{H}_d(A) + \mathcal{H}_d(B) = \mathcal{H}_d(S^d)$, it follows from (49) and (53) that

$$\lim_{N\to\infty} \frac{E_d(A^N)}{\tau_{d,d}(N)} = g_{d,d}(S^d) \frac{\mathcal{H}_d(A)}{\mathcal{H}_d(S^d)}$$

and

$$\lim_{N\to\infty} \frac{E_d(B^N)}{\tau_{d,d}(N)} = g_{d,d}(S^d) \frac{\mathcal{H}_d(B)}{\mathcal{H}_d(S^d)}.$$

□

Lemma 4.4 *Suppose A is a compact scalable subset of S^d. Then $g_{d,d}(A)$ exists and*

$$g_{d,d}(A) = \mathcal{H}_d(\mathcal{B}^d)/\mathcal{H}_d(A).$$

By saying A is a scalable subset of S^d, we mean that for every $\epsilon > 0$ there is a bi-Lipschitz mapping with constant $(1 + \epsilon)$ that maps the closure of A into its interior relative to S^d. Clearly the measure of the closure of such a set is equal to the measure of its interior, and so any scalable subset of S^d is almost clopen.

Proof. Suppose either $C = A$ or $C = B := S^d \setminus A$. Then (48) holds. We first prove that $\overline{g}_{d,d}(C) \leq \mathcal{H}_d(\mathcal{B}^d)/\mathcal{H}_d(C)$. For $\rho > 1$ and $N \in \mathbb{N}$, let $M[N] := \lfloor \rho \frac{\mathcal{H}_d(S^d)}{\mathcal{H}_d(C)} N \rfloor$ where $\lfloor x \rfloor$ denotes the integer part of x. Let $C^{M[N]} := \omega^*_{M[N]} \cap C$ and recall that (47) states that $|C^{M[N]}|/M[N] \to \mathcal{H}_d(C)/\mathcal{H}_d(S^d)$ as $N \to \infty$.

Then, for N large enough, we have

$$\rho^{-1} \frac{\mathcal{H}_d(C)}{\mathcal{H}_d(S^d)} \leq \frac{|C^{M[N]}|}{M[N]}$$

from which it follows that there is some N_ρ such that

$$N \leq |C^{M[N]}| \qquad (N > N_\rho), \tag{54}$$

and so $\mathcal{E}_d(C, N) \leq E_d(\omega^*_{M[N]} \cap C)$ for $N > N_\rho$. Thus we have

$$\begin{aligned} \overline{g}_{d,d}(C) &= \limsup_{N\to\infty} \frac{\mathcal{E}_d(C,N)}{\tau_{d,d}(N)} \\ &\leq \limsup_{N\to\infty} \frac{\tau_{d,d}(M[N])}{\tau_{d,d}(N)} \frac{E_d(\omega^*_{M[N]} \cap C)}{\tau_{d,d}(M[N])} \\ &\leq \rho^2 g_{d,d}(S^d) \frac{\mathcal{H}_d(S^d)}{\mathcal{H}_d(C)}, \end{aligned}$$

where (48) was used to obtain the last inequality. Since $\rho > 1$ is arbitrary, we have $\overline{g}_{d,d}(C) \leq \mathcal{H}_d(\mathcal{B}^d)/\mathcal{H}_d(C)$ for either $C = A$ or $C = B$.

Next we show $\underline{g}_{d,d}(A) \geq \mathcal{H}_d(\mathcal{B}^d)/\mathcal{H}_d(A)$. Let $(a_N)_{N\in\mathbb{N}}$ denote a sequence of natural numbers such that $\lim_{N\to\infty} \mathcal{G}_{d,d}(A, a_N) = \underline{g}_{d,d}(A)$. For $N \in \mathbb{N}$, let $b_N = \lceil (\mathcal{H}_d(B)/\mathcal{H}_d(A)) a_N \rceil$ where $\lceil x \rceil$ denotes the least integer greater than or equal to x and let $c_N = a_N + b_N$. Since A is scalable, there is a bi-Lipschitz mapping h with constant $(1+\epsilon)$ such that $h(A) \subset A^\circ$. Then $\delta := \operatorname{dist}(h(A), B) > 0$ and, as in the proof of Lemma 3.3, we have

$$\begin{aligned} \mathcal{E}_d(S^d, c_N) \leq \mathcal{E}_d(h(A) \cup B, c_N) &\leq \mathcal{E}_d(h(A), a_N) + \mathcal{E}_d(B, b_N) + 2\delta^{-s} a_N b_N \\ &\leq (1+\epsilon)^d \mathcal{E}_d(A, a_N) + \mathcal{E}_d(B, b_N) + 2\delta^{-d} c_N^2 \end{aligned}$$

and thus

$$\mathcal{G}_{d,d}(S^d, c_N) \leq (1+\epsilon)^d \mathcal{G}_{d,d}(A, a_N) \frac{\tau_{d,d}(a_N)}{\tau_{d,d}(c_N)} + \mathcal{G}_{d,d}(B, b_N) \frac{\tau_{d,d}(b_N)}{\tau_{d,d}(c_N)} + \frac{2\delta^{-d}}{\log(c_N)}.$$

Letting $N \to \infty$ and then $\epsilon \to 0$ gives

$$g_{d,d}(S^d) \leq \underline{g}_{d,d}(A) \left(\frac{\mathcal{H}_d(A)}{\mathcal{H}_d(S^d)} \right)^2 + \overline{g}_{d,d}(B) \left(\frac{\mathcal{H}_d(B)}{\mathcal{H}_d(S^d)} \right)^2 .$$

Using $\overline{g}_{d,d}(B) \leq \mathcal{H}_d(\mathcal{B}^d)/\mathcal{H}_d(B)$ and $\mathcal{H}_d(S^d) = \mathcal{H}_d(A) + \mathcal{H}_d(B)$ as well as Theorem 1.2, we get $\underline{g}_{d,d}(A) \geq \mathcal{H}_d(\mathcal{B}^d)/\mathcal{H}_d(A)$, which completes the proof of Lemma 4.4. □

Now we return to the $s = d$ case of the proof of Theorem 4.1. Recall that $\mathbb{P} : \mathbb{R}^d \to S^d$ denotes the stereographic projection defined by (30). Let $e_1 := (1, 0, \ldots, 0) \in \mathbb{R}^d$ and $\mathbf{1} := (1, 1, \ldots, 1) \in \mathbb{R}^d$. For $0 < \gamma < 1$, let

$$U_\gamma := \gamma U^d + e_1 - (\gamma/2)\mathbf{1} = [1 - \gamma/2, 1 + \gamma/2] \times [-\gamma/2, \gamma/2] \times \cdots \times [-\gamma/2, \gamma/2]$$

and let $A_\gamma := \mathbb{P}(U_\gamma)$. Note that A_γ is scalable, since the mappings $a \mapsto \mathbb{P}(r\mathbb{P}^{-1}(a) + (1 - r)e_1)$, for $0 < r < 1$, form a family of bi-Lipschitz mappings with constants approaching 1 as $r \to 1$ that map A_γ into its relative interior (cf. (31)). Thus $g_{d,d}(A_\gamma)$ exists and equals $\mathcal{H}_d(\mathcal{B}^d)/\mathcal{H}_d(A_\gamma)$. For $x \in U_\gamma$ and $0 < \gamma < 1/d$, we have $1 - \gamma \leq |x|^2 \leq (1 + \gamma/2)^2 + (d - 1)(\gamma/2)^2 \leq 1 + 2\gamma$. Using (31) it follows that for $\gamma < 1/d$, the function $h := \mathbb{P}^{-1}$ is bi-Lipschitz on A_γ with constant $(1 + \gamma)$ and such that $U_\gamma = h(A_\gamma)$. Then

$$\overline{g}_{d,d}(U^d) = \gamma^d \overline{g}_{d,d}(U_\gamma) = \gamma^d \overline{g}_{d,d}(h(A_\gamma)) \leq \gamma^d (1 + \gamma)^d g_{d,d}(A_\gamma) \qquad (55)$$

and, similarly,

$$\underline{g}_{d,d}(U^d) = \gamma^d \underline{g}_{d,d}(U_\gamma) \geq \gamma^d (1 + \gamma)^{-d} g_{d,d}(A_\gamma). \qquad (56)$$

Since $h = \mathbb{P}^{-1}$ is bi-Lipschitz on A_γ with constant $(1 + \gamma)$, it follows that $\lim_{\gamma \to 0^+} \gamma^{-d} \mathcal{H}_d(A_\gamma) = \mathcal{H}_d(U^d) = 1$ and so

$$\gamma^d g_{d,d}(A_\gamma) = \gamma^d \mathcal{H}_d(\mathcal{B}^d)/\mathcal{H}_d(A_\gamma) \to \mathcal{H}_d(\mathcal{B}^d)$$

as $\gamma \to 0$. Taking $\gamma \to 0$ in (55) and (56) we then have

$$\mathcal{H}_d(\mathcal{B}^d) \leq \underline{g}_{d,d}(U^d) \leq \overline{g}_{d,d}(U^d) \leq \mathcal{H}_d(\mathcal{B}^d)$$

which completes the proof of Theorem 4.1.

5 Almost clopen sets in $\mathbb{R}^d$

A Lebesgue measurable set $A \subset \mathbb{R}^d$ is said to be **almost clopen (with respect to d-dimensional Lebesgue measure)** if $\mathcal{H}_d(\partial A) = 0$ where ∂A denotes the boundary of A.

Theorem 5.1 *Suppose A is a bounded almost clopen set in $\mathbb{R}^d$. Then $g_{s,d}(A)$ exists for $s \geq d$ and*

$$g_{s,d}(A) = g_{s,d}(U^d)\mathcal{H}_d(A)^{-s/d}. \tag{57}$$

Remark. In particular, $g_{s,d}(A) = \infty$ if $\mathcal{H}_d(A) = 0$.

Proof. First, if $A = \gamma U^d$ then $g_{s,d}(A) = \gamma^{-s} g_{s,d}(U^d) = \mathcal{H}_d(A)^{-s/d} g_{s,d}(U^d)$ showing that A satisfies (57). Applying Corollary 3.4 inductively, it then follows that (57) holds if A is the union of a finite collection of cubes with disjoint interiors.

Next, for $n \in \mathbb{N}$, let $\mathcal{Q}_n$ denote the cubes q in $\mathbb{R}^d$ with vertices in the lattice $\mathbb{Z}^d/n$, let $\underline{A}_n$ denote the union of the cubes in $\mathcal{Q}_n$ that are also contained in A and let $\overline{A}_n$ denote the union of the cubes $\mathcal{Q}_n$ that meet the closure of A.

Suppose $\epsilon > 0$, then there is an open set V containing ∂A with $\mathcal{H}_d(V) < \epsilon$. If $q \in \mathcal{Q}_n$ is a subset of $\overline{A}_n \cap \underline{A}_n^c$, the complement of $\underline{A}_n$ in $\overline{A}_n$, then q meets ∂A. Since ∂A is compact and V^c is closed, the distance dist $(\partial A, V^c) > 0$.

Let n^* be large enough so that diam $q <$ dist $(\partial A, V^c)$ for $q \in \mathcal{Q}_{n^*}$. If $q \in \mathcal{Q}_{n^*}$ meets ∂A then $q \subset V$ and so we have $\overline{A}_n \cap \underline{A}_n^c \subset V$ for $n > n^*$. Hence,

$$\mathcal{H}_d(\underline{A}_n) \leq \mathcal{H}_d(\overline{A}_n) \leq \mathcal{H}_d(\underline{A}_n) + \epsilon \qquad (n > n^*)$$

showing that

$$\lim_{n\to\infty} \mathcal{H}_d(\underline{A}_n) = \lim_{n\to\infty} \mathcal{H}_d(\overline{A}_n) = \mathcal{H}_d(A).$$

Since $g_{s,d}(\overline{A}_n) \leq \underline{g}_{s,d}(A) \leq \overline{g}_{s,d}(A) \leq g_{s,d}(\underline{A}_n)$ and (57) holds for $\overline{A}_n$ and $\underline{A}_n$ it follows that (57) holds for A. □

We say that a sequence $\omega_N \subset A$, $N \in \mathcal{N}$, of sets of points in A is **asymptotically s-energy minimizing on** A for $s \geq d$ if

$$\lim_{N\to\infty} \frac{E_s(\omega_N)}{\tau_{s,d}(N)} = \underline{g}_{s,d}(A) \qquad (N \in \mathcal{N}).$$

Corollary 5.2 *Suppose A is a bounded, almost clopen set in $\mathbb{R}^d$, $\mathcal{H}_d(A) > 0$, B is an almost clopen subset of A and that $\omega_N \subset A$, $N \in \mathcal{N}$, is asymptotically s-energy minimizing on A. Then we have*

$$\lim_{\substack{N\to\infty \\ N\in\mathcal{N}}} \frac{|\omega_N \cap B|}{N} = \mathcal{H}_d(B)/\mathcal{H}_d(A). \qquad (N \in \mathcal{N}) \tag{58}$$

Proof. Note that $B' := A\backslash B$ is almost clopen (since $\partial B' \subset \partial A \cup \partial B$). Applying Theorem 5.1 to A, B and B' gives

$$\begin{aligned} g_{s,d}(A) &= g_{s,d}(U^d)\mathcal{H}_d(A)^{-s/d} \\ &= g_{s,d}(U^d)(\mathcal{H}_d(B) + \mathcal{H}_d(B'))^{-s/d} = \left(g_{s,d}(B)^{-d/s} + g_{s,d}(B')^{-d/s}\right)^{-s/d}. \end{aligned}$$

Then Lemma 3.2 implies (58). □

6 Separation

Proof of Theorem 2.3. For convenience we denote $x^*_{i,N}$ by x_i. For $i = 1, \ldots, N$, let

$$U_i(x) := \sum_{j \neq i} \frac{1}{|x - x_j|^s}. \tag{59}$$

Then $U_i(x_i) \leq U_i(x)$ for all $x \in A$. Let $0 < \delta < 1$ and set

$$r_0 := (\delta \mathcal{H}_d(A)/(N\mathcal{H}_d(B(0,1))))^{1/d}$$

and

$$D_j := B(x_j, r_0), \quad \mathcal{D}_i := A \setminus \bigcup_{j \neq i} D_j.$$

Then

$$\mathcal{H}_d(\mathcal{D}_i) \geq \mathcal{H}_d(A) - N r_0^d \mathcal{H}_d(B(0,1)) = \mathcal{H}_d(A)(1 - \delta) > 0 \tag{60}$$

and we have

$$\begin{aligned} U_i(x_i) &\leq \frac{1}{\mathcal{H}_d(\mathcal{D}_i)} \int_{\mathcal{D}_i} U_i(x)\, d\mathcal{H}_d(x) \\ &= \frac{1}{\mathcal{H}_d(\mathcal{D}_i)} \sum_{j \neq i} \int_{\mathcal{D}_i} \frac{1}{|x - x_j|^s}\, d\mathcal{H}_d(x) \\ &\leq \frac{1}{\mathcal{H}_d(\mathcal{D}_i)} \sum_{j \neq i} \int_{A \backslash D_j} \frac{1}{|x - x_j|^s}\, d\mathcal{H}_d(x). \end{aligned} \tag{61}$$

Let $R >$ diam A. It is easy to verify that for $0 < r < 1$ and $y \in A$

$$\begin{aligned} \int_{A \backslash B(y,r)} \frac{1}{|x - y|^s}\, d\mathcal{H}_d(x) &\leq \int_{B(0,R) \backslash B(0,r)} \frac{1}{|u|^s}\, d\mathcal{H}_d(u) \\ &\leq \begin{cases} c_s / r^{s-d} & \text{for } s > d, \\ c_d \log(R/r) & \text{for } s = d, \end{cases} \end{aligned} \tag{62}$$

where the positive constants c_s, c_d are independent of y and r. Using the estimates (60) and (62) we get for $s > d$,

$$U_i(x_i) \leq \frac{(N-1)c_s \left(\delta \mathcal{H}_d(A)/N\mathcal{H}_d(B(0,1))\right)^{1-s/d}}{(1-\delta)\mathcal{H}_d(A)} \leq k_s N^{s/d} \tag{63}$$

and for $s = d$,

$$U_i(x_i) \le k_d N \log N, \tag{64}$$

where the constants k_s, k_d are independent of N and i. Finally, since for each $i = 1, \dots, N$, we have $|x_i - x_j|^{-s} \le U_i(x_i)$ for $i \ne j$, inequality (16) follows from (63) and (64). □

Lemma 6.1 *For the closed unit ball $\mathcal{B}^d := \bar{B}(0,1) \subset \mathbb{R}^d$, there is a d-energy asymptotically optimal sequence $(\omega_N)_{N\in\mathbb{N}}$ of N-point configurations $\omega_N = \{x_{1,N}, \dots, x_{N,N}\}$ for $\mathcal{B}^d$ such that for $N \ge 2$*

$$\min_{i\ne j} |x_{i,N} - x_{j,N}| \ge (2 + \sqrt{d})^{-1} N^{-1/d}.$$

Proof. By Theorems 4.1 and 5.1, we have that $g_{d,d}(\mathcal{B}^d) = 1$. For a positive integer m let $\Omega^m := (\frac{1}{m}\mathbb{Z})^d \cap \mathcal{B}^d$ and for $\mathbf{j} \in (\frac{1}{m}\mathbb{Z})^d$ let $U_{m,\mathbf{j}} := \frac{1}{m}[-1/2, 1/2]^d + \mathbf{j}$ denote the d dimensional cube of side length $1/m$ (with sides parallel to the coordinate axes) and center $\mathbf{j}$. Since

$$B(0, (1 - \sqrt{d}/m)) \subset \bigcup_{\mathbf{j}\in\Omega^m} U_{m,\mathbf{j}} \subset B(0, (1 + \sqrt{d}/m)),$$

we have

$$(m - \sqrt{d})^d \mathcal{H}_d(\mathcal{B}^d) \le |\Omega^m| \le (m + \sqrt{d})^d \mathcal{H}_d(\mathcal{B}^d). \tag{65}$$

Fix $k > \sqrt{d}$. If $x \in U_{m,\mathbf{j}}$ and $|\mathbf{j}| \ge k/m$, then $|\mathbf{j}| \ge |x| - \sqrt{d}/(2m) > 0$ and so

$$\begin{aligned}
\sum_{\substack{\mathbf{j}\in(\frac{1}{m}\mathbb{Z})^d \\ 0<|\mathbf{j}|\le 2}} \frac{1}{|\mathbf{j}|^d} &\le \sum_{\substack{\mathbf{j}\in(\frac{1}{m}\mathbb{Z})^d \\ 0<|\mathbf{j}|<k/m}} \frac{1}{|\mathbf{j}|^d} + m^d \sum_{\substack{\mathbf{j}\in(\frac{1}{m}\mathbb{Z})^d \\ k/m\le|\mathbf{j}|\le 2}} \frac{1}{|\mathbf{j}|^d}\frac{1}{m^d} \\
&\le \sum_{\substack{\mathbf{j}\in(\frac{1}{m}\mathbb{Z})^d \\ 0<|\mathbf{j}|<k/m}} \frac{1}{|\mathbf{j}|^d} + m^d \int_{k/m<|x|<2} \frac{1}{(|x| - \sqrt{d}/(2m))^d}\, d\mathcal{H}_d(x) \\
&\le 2^d k^d m^d + m^d \int_{(k-\sqrt{d}/2)/m}^{2} \frac{(r + \sqrt{d}/(2m))^{d-1}}{r^d} \mathcal{H}_{d-1}(S^{d-1}) dr \\
&\le 2^d k^d m^d + m^d (1 + \sqrt{d}/k)^{d-1} \mathcal{H}_{d-1}(S^{d-1}) \int_{(k-\sqrt{d}/2)/m}^{2} \frac{1}{r} dr \\
&= 2^d k^d m^d + m^d \mathcal{H}_{d-1}(S^{d-1})(1 + \sqrt{d}/k)^{d-1} \log\left(\frac{2m}{k - \sqrt{d}/2}\right).
\end{aligned}$$

Hence using (65) and the preceding estimate we obtain

$$\begin{aligned}
&E_d(\Omega^m) = \sum_{i\in\Omega^m} \sum_{\substack{\mathbf{j}\in\Omega^m \\ \mathbf{j}\ne i}} \frac{1}{|\mathbf{j} - \mathbf{i}|^d} \le |\Omega^m| \sum_{\substack{\mathbf{j}\in(\frac{1}{m}\mathbb{Z})^d \\ 0<|\mathbf{j}|\le 2}} \frac{1}{|\mathbf{j}|^d} \\
&\le m^d (m + \sqrt{d})^d \mathcal{H}_d(\mathcal{B}^d) \left(2^d k^d + \mathcal{H}_{d-1}(S^{d-1})(1 + \sqrt{d}/k)^{d-1} \log\left(\frac{2m}{k - \sqrt{d}/2}\right)\right).
\end{aligned}$$

Suppose $N \geq 2$. Now choose $m = \lceil (N/\mathcal{H}_d(\mathcal{B}^d))^{1/d} + \sqrt{d} \rceil$. Then using (65) we get

$$(m - \sqrt{d} - 1)^d \mathcal{H}_d(\mathcal{B}^d) \leq N \leq (m - \sqrt{d})^d \mathcal{H}_d(\mathcal{B}^d) \leq |\Omega^m|. \tag{66}$$

Hence we may let ω_N consist of N distinct points from Ω^m. Then

$$\frac{E_d(\omega_N)}{N^2 \log N} \leq \frac{E_d(\Omega^m)}{N^2 \log N}$$
$$\leq \left(\frac{m^d (m + \sqrt{d})^d}{(m - \sqrt{d} - 1)^{2d}} \right) \frac{2^d k^d + \mathcal{H}_{d-1}(S^{d-1})(1 + \sqrt{d}/k)^{d-1} \log \left(\frac{2m}{k - \sqrt{d}/2} \right)}{\mathcal{H}_d(\mathcal{B}^d) \log((m - \sqrt{d} - 1)^d \mathcal{H}_d(\mathcal{B}^d))}.$$

On taking $N \to \infty$ (and thus $m \to \infty$) we get

$$\limsup_{N \to \infty} \frac{E_d(\omega_N)}{N^2 \log N} \leq \frac{\mathcal{H}_{d-1}(S^{d-1})}{d\, \mathcal{H}_d(\mathcal{B}^d)} (1 + \sqrt{d}/k)^{d-1} = (1 + \sqrt{d}/k)^{d-1}$$

for any $k \geq \sqrt{d}$ (here we recall $\mathcal{H}_{d-1}(S^{d-1}) = d\, \mathcal{H}_d(\mathcal{B}^d)$). Letting $k \to \infty$ then shows that $(\omega_N)_{N \in \mathbb{N}}$ is d-energy asymptotically optimal for $\mathcal{B}^d$. Using $\mathcal{H}_d(\mathcal{B}^d) \geq 1$ and the definition of m, we have $m \leq N^{1/d}(2 + \sqrt{d})$ and thus

$$\min_{x \neq y \in \omega_N} |x - y| = 1/m \geq (2 + \sqrt{d})^{-1} N^{-1/d}$$

which completes the proof. □

7 Compact sets

Proof of Theorem 2.1. Let $\epsilon > 0$ and G be an almost clopen set (since A is compact, G could be chosen to be the union of a finite collection of open balls) such that $G \supset A$ and $\mathcal{H}_d(G \setminus A) < \epsilon$. Then, from Theorem 5.1,

$$\underline{g}_{s,d}(A) \geq g_{s,d}(G) = g_{s,d}(U^d) \mathcal{H}_d(G)^{-s/d} \geq g_{s,d}(U^d)(\mathcal{H}_d(A) + \epsilon)^{-s/d}. \tag{67}$$

If $\mathcal{H}_d(A) = 0$ then (67) shows $\underline{g}_{s,d}(A) = \overline{g}_{s,d}(A) = \infty$; if $\mathcal{H}_d(A) > 0$, then since (67) holds for arbitrary $\epsilon > 0$, we get

$$\underline{g}_{s,d}(A) \geq g_{s,d}(U^d) \mathcal{H}_d(A)^{-s/d}. \tag{68}$$

We next show $\overline{g}_{s,d}(A) \leq g_{s,d}(U^d) \mathcal{H}_d(A)^{-s/d}$. The case $\mathcal{H}_d(A) = 0$ was already considered above and so we assume $\mathcal{H}_d(A) > 0$. Let

$$A^* := \{x \in A \mid \limsup_{r \to 0^+} \frac{\mathcal{H}_d(\bar{B}(x,r) \cap A)}{\mathcal{H}_d(\bar{B}(x,r))} = 1\}.$$

The Lebesgue Density Theorem (e.g., see [13]) states that $\mathcal{H}_d(A \setminus A^*) = 0$. For $0 < \epsilon < 1$, let

$$C_\epsilon := \{\bar{B}(x,r) \mid x \in A^*,\ 0 < r < 1,\ \frac{\mathcal{H}_d(\bar{B}(x,r) \cap A)}{\mathcal{H}_d(\bar{B}(x,r))} > 1 - \epsilon\}. \tag{69}$$

By the Besicovitch Covering Theorem (cf. [13]), there is a countable collection of pairwise disjoint closed balls $\{B_i := \bar{B}(x_i, r_i)\} \subset C_\epsilon$ that covers almost all of A^* and hence almost all of A. Choose n large enough so that

$$\mathcal{H}_d\left(\bigcup_{i=1}^{n} A \cap B_i\right) = \sum_{i=1}^{n} \mathcal{H}_d(A \cap B_i) \geq (1-\epsilon)\mathcal{H}_d(A). \tag{70}$$

Let $i \in \{1, \ldots, n\}$ be fixed and let ω_N denote an asymptotically minimal sequence of configurations for B_i such that

$$\delta_N := \min_{x,y \in \omega_N,\, x \neq y} |x - y| \geq r_i (CN)^{-1/d}$$

for some positive constant C independent of i. (Recall Theorem 2.3 states that, in the case $s > d$, any minimal sequence for B_i must satisfy such a separation condition while Lemma 6.1 implies the existence of such a sequence in the case $s = d$.)

For $0 < \nu < 1/2$, let $r := \nu \delta_N$ and set

$$\omega_N^\nu := \{x \in \omega_N \mid \mathrm{dist}(x, A \cap B_i) \leq r\}.$$

Then

$$B(x,r) \cap B(y,r) = \emptyset \qquad \text{for } x, y \in \omega_N,\ x \neq y,$$

and

$$B(x,r) \cap A = \emptyset \qquad \text{for } x \in \omega_N \setminus \omega_N^\nu.$$

Since, for any fixed constant less than 1/2, say 1/4, at least this fraction of every $B(x,r)$, $x \in B_i$, is contained in B_i for N sufficiently large (and hence r sufficiently small), we have

$$\mathcal{H}_d(B_i \cap A^c) \geq \mathcal{H}_d\Big(\bigcup_{x \in \omega_N \setminus \omega_N^\nu} B_i \cap B(x,r)\Big) \geq (1/4)|\omega_N \setminus \omega_N^\nu|\, \mathcal{H}_d(B(0,1)) r^d,$$

which implies

$$|\omega_N \setminus \omega_N^\nu| \leq 4\mathcal{H}_d(B_i \cap A^c)\mathcal{H}_d(B(0,1))^{-1}(\nu\delta_N)^{-d} \leq 4C\frac{\epsilon}{\nu^d}N,$$

where we have used (cf. (69)) $\mathcal{H}_d(B_i \cap A^c) \leq \epsilon \mathcal{H}_d(B_i) = \epsilon r_i^d \mathcal{H}_d(B(0,1))$. Thus

$$|\omega_N^\nu| = N - |\omega_N \setminus \omega_N^\nu| \geq N(1 - 4C\epsilon\nu^{-d}). \tag{71}$$

If $x \in \omega_N^\nu$, then there exists $y \in A \cap B_i$ such that $|x-y| \leq r$. For each $x \in \omega_N^\nu$, let $\phi_{N,\nu}(x)$ be one such y, and let

$$\lambda_{N,\nu} := \{\phi_{N,\nu}(x) \mid x \in \omega_N^\nu\}.$$

Note that for $x, y \in \omega_N^\nu$ we have

$$\begin{aligned} |\phi_{N,\nu}(x) - \phi_{N,\nu}(y)| &\geq |x-y| - |\phi_{N,\nu}(x) - x| - |\phi_{N,\nu}(y) - y| \\ &\geq (1-2\nu)|x-y|, \end{aligned} \tag{72}$$

and so

$$E_s(\lambda_{N,\nu}) \leq (1-2\nu)^{-s} E_s(\omega_N). \tag{73}$$

Let $M := \lceil N/(1-4C\epsilon\nu^{-d}) \rceil$. Then

$$|\lambda_{M,\nu}| \geq (1-4C\epsilon\nu^{-d})M \geq N,$$

and so we have

$$\begin{aligned} \frac{\mathcal{E}_s(A \cap B_i, N)}{\tau_{s,d}(N)} &\leq \left(\frac{E_s(\lambda_{M,\nu})}{\tau_{s,d}(M)}\right)\left(\frac{\tau_{s,d}(M)}{\tau_{s,d}(N)}\right) \\ &\leq \frac{1}{(1-2\nu)^s}\left(\frac{\tau_{s,d}(M)}{\tau_{s,d}(N)}\right)\left(\frac{E_s(\omega_M)}{\tau_{s,d}(M)}\right). \end{aligned} \tag{74}$$

From the definition of M it follows (even in the case $s = d$) that

$$\lim_{N\to\infty} \tau_{s,d}(M)/\tau_{s,d}(N) = \left(\frac{1}{1-4C\epsilon\nu^{-d}}\right)^{1+s/d}$$

and hence

$$\overline{g}_{s,d}(A \cap B_i) \leq \frac{1}{(1-2\nu)^s}\left(\frac{1}{1-4C\epsilon\nu^{-d}}\right)^{1+s/d} g_{s,d}(B_i) \tag{75}$$

for any $(4C\epsilon)^{1/d} < \nu < 1/2$.

Now Theorem 5.1 implies $g_{s,d}(B_i) = g_{s,d}(U^d)\mathcal{H}_d(B_i)^{-s/d}$ and so using Lemma 3.3 and inequalities (75) and (70) we obtain

$$\begin{aligned} \overline{g}_{s,d}(A) &\leq \overline{g}_{s,d}\left(\bigcup_{i=1}^n A \cap B_i\right) \\ &\leq \left(\sum_{i=1}^n \overline{g}_{s,d}(A \cap B_i)^{-d/s}\right)^{-s/d} \\ &\leq \frac{1}{(1-2\nu)^s}\left(\frac{1}{1-4C\epsilon\nu^{-d}}\right)^{1+s/d} g_{s,d}(U^d)\left(\sum_{i=1}^n \mathcal{H}_d(B_i)\right)^{-s/d} \\ &\leq \frac{1}{(1-2\nu)^s}\left(\frac{1}{1-4C\epsilon\nu^{-d}}\right)^{1+s/d} g_{s,d}(U^d)(1-\epsilon)^{-s/d}\mathcal{H}_d(A)^{-s/d} \end{aligned} \tag{76}$$

for any $0 < \epsilon < 1$ and any $(4C\epsilon)^{1/d} < \nu < 1/2$. By first taking $\epsilon \to 0$ and then $\nu \to 0$ we have

$$\overline{g}_{s,d}(A) \leq g_{s,d}(U^d)\mathcal{H}_d(A)^{-s/d} \tag{77}$$

which combined with (68) completes the proof. □

Proof of Theorem 2.2. Let $B \subset A$ be a measurable set such that $\mathcal{H}_d(\partial_r B) = 0$, where $\partial_r B := \partial B \cap \overline{(A \setminus B)}$ is the relative boundary of B. Then $A = A_1 \cup A_2$, where $A_1 := B \cup \partial_r B$, and $A_2 := (A \setminus B) \cup \partial_r(A \setminus B)$ are compact sets and $\mathcal{H}_d(\partial_r(A\setminus B)) = 0$. Since $\mathcal{H}_d(A) = \mathcal{H}_d(A_1)+\mathcal{H}_d(A_2)$ we can apply Theorem 2.1 and Lemma 3.2 to deduce that

$$\frac{|\omega_N \cap A_1|}{N} \longrightarrow \frac{\mathcal{H}_d(B)}{\mathcal{H}_d(A)} \quad \text{as } N \to \infty. \tag{78}$$

On writing $A = \partial_r B \cup \overline{A \setminus \partial_r B}$ we similarly have

$$\frac{|\omega_N \cap \partial_r B|}{N} \longrightarrow 0 \quad \text{as } N \to \infty$$

which together with (78) gives (15) and thus (13). □

8 d-Rectifiable manifolds in $\mathbb{R}^{d'}$

In Section 2 we defined the notion of a d-rectifiable manifold. More generally, a set $A \subset \mathbb{R}^{d'}$ is said to be a **d-dimensional rectifiable set** if A is $\mathcal{H}_d$ measurable, $\mathcal{H}_d(A) < \infty$, and $\mathcal{H}_d$-almost all of A is contained in the countable union of Lipschitz images of bounded subsets of $\mathbb{R}^d$ (see [5], [11], and [13]). Clearly, any d-rectifiable manifold is a d-dimensional rectifiable set.

We shall need the following result of Federer concerning d-dimensional rectifiable sets:

Lemma 8.1 ([5, 3.2.18], [13, 3.11]) *Suppose $A \subset \mathbb{R}^{d'}$ is a d-dimensional rectifiable set and $\epsilon > 0$. Then there exists a countable collection $\{K_i \mid i = 1, 2, \ldots\}$ of compact subsets of $\mathbb{R}^d$ and bi-Lipschitz mappings $\psi_i : K_i \to \mathbb{R}^{d'}$, $i = 1, 2, \ldots$, with constant $(1 + \epsilon)$ such that $\psi_1(K_1), \psi_2(K_2), \psi_3(K_3)\ldots$ are pairwise disjoint subsets of A that cover $\mathcal{H}_d$-almost all of A.*

Proposition 8.2 *Suppose $A \subset \mathbb{R}^{d'}$ is a compact, d-dimensional rectifiable set and $s \geq d$. Then*

$$\overline{g}_{s,d}(A) \leq g_{s,d}(U^d)\mathcal{H}_d(A)^{-s/d}. \tag{79}$$

Proof. If $\mathcal{H}_d(A) = 0$, then the right hand side of (79) is understood to be ∞ and (79) holds trivially. Now suppose $0 < \epsilon < \mathcal{H}_d(A)$. Let $K_1, K_2, \ldots$ and

$\psi_1, \psi_2, \ldots$ be as in Lemma 8.1. Let $n \in \mathbb{N}$ be large enough so that

$$\sum_{i=1}^{n} \mathcal{H}_d(\psi_i(K_i)) \geq \mathcal{H}_d(A) - \epsilon. \tag{80}$$

Since $\psi_1(K_1), \ldots, \psi_n(K_n)$ are disjoint compact subsets of A, we may use Lemma 3.3, Theorem 2.1, (80), and the fact that ψ_i is bi-Lipschitz with constant $(1+\epsilon)$ to get

$$\begin{aligned} \overline{g}_{s,d}(A) &\leq \overline{g}_{s,d}\left(\bigcup_{i=1}^{n} \psi_i(K_i)\right) \\ &\leq \left(\sum_{i=1}^{n} \overline{g}_{s,d}(\psi_i(K_i))^{-d/s}\right)^{-s/d} \\ &\leq g_{s,d}(U^d)(1+\epsilon)^{2s}\left(\sum_{i=1}^{n} \mathcal{H}_d(\psi_i(K_i))\right)^{-s/d} \\ &\leq g_{s,d}(U^d)(1+\epsilon)^{2s}(\mathcal{H}_d(A) - \epsilon)^{-s/d}. \end{aligned} \tag{81}$$

Since ϵ is arbitrary, (81) shows $\overline{g}_{s,d}(A) \leq g_{s,d}(U^d)\mathcal{H}_d(A)^{-s/d}$. □

Proposition 8.3 *Suppose $s \geq d$ and that $A \subset \mathbb{R}^{d'}$ is as in Theorem 2.4 with the property that for each $\epsilon > 0$ there is some $\delta > 0$ such that $\underline{g}_{s,d}(B) \geq 1/\epsilon$ whenever B is a compact subset of A with $\mathcal{H}_d(B) < \delta$. Then $\underline{g}_{s,d}(A) \geq g_{s,d}(U^d)\mathcal{H}_d(A)^{-s/d}$.*

Proof. Suppose $\epsilon > 0$. Again let (K_i, ψ_i), $i = 1, 2, \ldots$, be as in Lemma 8.1. Let $\delta > 0$ be such that $\underline{g}_{s,d}(B) \geq (\epsilon)^{-s/d}$ whenever B is a compact subset of A with $\mathcal{H}_d(B) < \delta$. Let n be large enough so that

$$\sum_{i=1}^{n} \mathcal{H}_d(\psi_i(K_i)) \geq \mathcal{H}_d(A) - \delta. \tag{82}$$

Since A is a Borel set and $\mathcal{H}_d(A) < \infty$, then $\mathcal{H}_d|_A$ is a Radon measure on $\mathbb{R}^{d'}$ (cf. [11, 1.11]). If $K \subset A$ is compact and $\epsilon > 0$, then there is some relatively open set $G \subset A$ such that $K \subset G$ and such that $\mathcal{H}_d(G) \leq \mathcal{H}_d(K) + \epsilon$. Furthermore, we may choose G to be $\mathcal{H}_d$-almost clopen relative to A. Indeed, if G is not almost clopen then we can construct an almost clopen set $\mathcal{G}$ with the same properties as G in the following way. Let $C(x,r) = \{y \in \mathbb{R}^{d'} \mid |y - x| = r\}$. Since $\mathcal{H}_d(A) < \infty$, the set $\{r > 0 \mid \mathcal{H}_d(C(x,r) \cap A) > 0\}$ is at most countable. Since $K \subset A$ is compact, there is a relatively open cover of K of the form $\{B(x_i, r_i) \cap A \mid i = 1, \ldots, m\}$ where $B(x_i, r_i) \cap A \subset G$ and $\mathcal{H}_d(C(x_i, r_i) \cap A) = 0$. Let $\mathcal{G} = \bigcup_{i=1}^{m} B(x_i, r_i) \cap A$, then $K \subset \mathcal{G} \subset G$, $\mathcal{G}$ is a relatively open subset of A, and $\mathcal{H}_d(\bar{\mathcal{G}}) = \mathcal{H}_d(\mathcal{G}) \leq \mathcal{H}_d(K) + \epsilon$.

Using arguments similar to those in the proof of Theorem 2.1, we can find for $i = 1, \ldots, n$ a relatively open subset G_i of A such that $\psi_i(K_i) \subset G_i$ and

$$\underline{g}_{s,d}(\bar{G}_i) \geq \left(\underline{g}_{s,d}(\psi_i(K_i))^{-d/s} + \epsilon/2^i\right)^{-s/d}. \tag{83}$$

Let $G_0 := A \setminus \bigcup_{i=1}^n \bar{G}_i$. Then $\bar{G}_0 \subset A \setminus \bigcup_{i=1}^n \psi_i(K_i)$ and thus, using (82), we obtain $\mathcal{H}_d(\bar{G}_0) \leq \delta_0$ and hence

$$\underline{g}_{s,d}(G_0) \geq \epsilon^{-s/d}. \tag{84}$$

Since ψ_i is bi-Lipschitz on K_i with constant $(1+\epsilon)$ we have, using Theorem 2.1,

$$\begin{aligned} \underline{g}_{s,d}(\psi_i(K_i)) &\geq (1+\epsilon)^{-s} g_{s,d}(K_i) \\ &= (1+\epsilon)^{-s} g_{s,d}(U^d)\mathcal{H}_d(K_i)^{-s/d} \\ &\geq (1+\epsilon)^{-2s} g_{s,d}(U^d)\mathcal{H}_d(\psi_i(K_i))^{-s/d}. \end{aligned} \tag{85}$$

Since $A \subset \bigcup_{i=0}^n \bar{G}_i$, we again use Lemma 3.2 together with (82)–(85) to obtain

$$\begin{aligned} \underline{g}_{s,d}(A) &\geq \left(\sum_{i=0}^n \underline{g}_{s,d}(\bar{G}_i)^{-d/s}\right)^{-s/d} \\ &\geq \left(\sum_{i=0}^n \epsilon/2^i + \sum_{i=1}^n \underline{g}_{s,d}(\psi_i(K_i))^{-d/s}\right)^{-s/d} \\ &\geq \left(2\epsilon + (1+\epsilon)^{2d} g_{s,d}(U^d)^{-d/s} \sum_{i=1}^n \mathcal{H}_d(\psi_i(K_i))\right)^{-s/d} \\ &\geq \left(2\epsilon + (1+\epsilon)^{2d} g_{s,d}(U^d)^{-d/s}\mathcal{H}_d(A)\right)^{-s/d}. \end{aligned} \tag{86}$$

Taking $\epsilon \to 0$ in (86) then completes the proof. □

Proof of Theorem 2.4. Suppose $A \subset \mathbb{R}^{d'}$ is a d-rectifiable manifold. Since any d-rectifiable manifold is a d-dimensional rectifiable set, Proposition 8.2 implies $\overline{g}_{s,d}(A) \leq g_{s,d}(U^d)\mathcal{H}_d(A)^{-s/d}$.

We next show that A also satisfies the hypotheses of Proposition 8.3 which will then imply that $g_{s,d}(A)$ exists and is given by

$$g_{s,d}(A) = g_{s,d}(U^d)\mathcal{H}_d(A)^{-s/d}. \tag{87}$$

Since A is a d-rectifiable manifold, we have $A = \bigcup_{k=1}^n \phi_k(K_k)$ where $K_k \subset \mathbb{R}^d$ is compact and ϕ_k is bi-Lipschitz on K_k with constant L_k for $k = 1, \ldots, n$. Let $L := \max\{L_k \mid k = 1, \ldots, n\}$.

Suppose B is a compact subset of A. For $k = 1, \ldots, n$, let $B_k := B \cap \phi_k(K_k)$. Then by Lemma 3.2 and Theorem 2.1

$$\begin{aligned} \underline{g}_{s,d}(B) &\geq \left(\sum_{k=1}^{n} \underline{g}_{s,d}(B_k)^{-d/s} \right)^{-s/d} \qquad (88) \\ &\geq L^{-s} \left(\sum_{k=1}^{n} \underline{g}_{s,d}(\phi_k^{-1}(B_k))^{-d/s} \right)^{-s/d} \\ &\geq L^{-s} g_{s,d}(U^d) \left(\sum_{k=1}^{n} \mathcal{H}_d(\phi_k^{-1}(B_k)) \right)^{-s/d} \\ &\geq n^{-s/d} L^{-2s} g_{s,d}(U^d) \mathcal{H}_d(B)^{-s/d} \end{aligned}$$

from which it follows that A satisfies the hypotheses of Proposition 8.3, thereby proving (87).

Once we have the formula (87), the proof of Theorem 2.2 may be repeated without change to show that (13) holds for asymptotically optimal s-energy N-point configurations in A.

Finally, to prove the separation estimates (16) for an optimal N-point s-energy configuration $\lambda_N^* = \{y_{1,N}^*, \ldots, y_{N,N}^*\}$ for A, when $A = \phi(K)$, $K \subset \mathbb{R}^d$, K compact and ϕ bi-Lipschitz on K, we can imitate the argument given in Section 6.1 for the proof of Theorem 2.3. For this purpose we replace the definition of $U_i(x)$ in (59) by

$$U_i(x) := \sum_{j \neq i} \frac{1}{|\phi(x) - \phi(x_{j,N})|^s},$$

where $x_{j,N} = \phi^{-1}(y_{j,N}^*)$. The details are left to the reader. □

Acknowledgements. We thank the referees, S. Borodachov, and J. Brauchart for their careful reading of the manuscript and their helpful comments.

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