

RIESZ ENERGY ON THE TORUS: REGULARITY OF MINIMIZERS

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ABSTRACT. We study sets of N points on the d -dimensional torus \mathbb{T}^d minimizing interaction functionals of the type

$$\sum_{\substack{i,j=1 \\ i \neq j}}^N f(x_i - x_j).$$

The main result states that for a class of functions f that behave like Riesz energies $f(x) \sim \|x\|^{-s}$ for $0 < s < d$, the minimizing configuration of points has optimal regularity w.r.t. a Fourier-analytic regularity measure that arises in the study of irregularities of distribution. A particular consequence is that they are optimal quadrature points in the space of trigonometric polynomials up to a certain degree. The proof extends to other settings and also covers less singular functions such as $f(x) = \exp(-N^{\frac{2}{d}}\|x\|^2)$.

1. INTRODUCTION AND MAIN RESULT

1.1. Introduction. This paper studies the regularity of minimizers of variational problems. More precisely, for a function $f : \mathbb{T}^d \rightarrow \mathbb{R}$ we will be interested in configuration of N points $\{x_1, x_2, \dots, x_N\} \subset \mathbb{T}^d$ that minimize the energy functional

$$\sum_{i \neq j} f(x_i - x_j).$$

These questions have a long and rich history: the choice $f(x_i - x_j) = \|x_i - x_j\|^{-1}$ on \mathbb{S}^2 is often interpreted as the minimal energy configuration of N electrons on a sphere and dates back to the physicist J. J. Thomson [23] in 1904. Minimizers are ‘roughly’ evenly spaced and what remains to be understood are fine structural details of the minimizing configuration. These questions are very relevant in mathematical physics (cf. Abrikosov lattices [1]). Since the field is extremely active, it has become increasingly difficult to summarize existing results, we refer to the survey of Blanc & Lewin [6] for an introduction into the crystallization conjecture, to a recent survey of Brauchart & Grabner [7] for an introduction to general problems of these type and to recent lecture notes of Serfaty [19].

1.2. Measuring Regularity. When studying the regularity of minimizers, the predominant measures are usually phrased in local terms: for example, is it true that $\min_{i \neq j} \|x_i - x_j\| \gtrsim N^{-1/d}$? Since the minimizers are assumed to be extremely regular and perhaps even close to lattices, it is reasonable to believe that this is indeed the case; the first results in this direction are due to Dahlberg [10] and this

2010 *Mathematics Subject Classification.* 31C20, 52C35, 74G65, 82B05.

The research of J.L. was supported in part by the National Science Foundation under award DMS-1454939.

has inspired many subsequent results. The purpose of our paper is to point out that by working with nonlocal measures of regularity, it is relatively simple to show that minimizing point sets are as regular as possible in this framework. Given a set of N points on the torus $\{x_1, \dots, x_N\} \subset \mathbb{T}^d$, we can quantify regularity by the size of the Fourier coefficients of the sum of Dirac measures placed in these points (since we work on the torus, the Fourier grid is given by \mathbb{Z}^d , which we assume without explicit mentioning in the sequel). The quantity we will study is given by

$$\sum_{\substack{\|k\| \leq X \\ k \neq 0}} \left| \widehat{\sum_{i=1}^N \delta_{x_i}}(k) \right|^2 = \sum_{\substack{\|k\| \leq X \\ k \neq 0}} \left| \sum_{n=1}^N e^{2\pi i \langle k, x_n \rangle} \right|^2,$$

where $X > 0$ is a free parameter. It is not new and played a prominent role in the L^2 -theory of irregularities of distribution, we refer to the seminal work of Beck [2, 3, 4] and Montgomery [16, 17, 18]. There is a fundamental inequality of Montgomery [17, 18] (see also the refinement [20]) that states that this quantity cannot be too small. More precisely, there exists a $c_d > 0$ such that for all point sets $\{x_1, \dots, x_N\} \subset \mathbb{T}^d$

$$\sum_{\substack{\|k\| \leq c_d N^{1/d} \\ k \neq 0}} \left| \sum_{n=1}^N e^{2\pi i \langle k, x_n \rangle} \right|^2 \geq N^2.$$

This inequality is sharp up to constants for sets of points satisfying a separation condition $\|x_i - x_j\| \gtrsim N^{-1/d}$ (see [20]). While, conversely, its validity does not imply $\sim N^{-1/d}$ separation, it does imply global regularity results at scales slightly coarser than that of nearest neighbors.

1.3. Main Results. Our main result states the minimizing energy configuration for functions behaving like Riesz energies have to be as regular as possible w.r.t. the above regularity measure. One interesting implication is that they are good quadrature points for low-degree trigonometric polynomials (see below). Another remarkable aspect is that the argument does not require the set of points to be a global minimizers as long as their energy is close to that of the global minimizer.

Theorem 1. *Let $f : \mathbb{T}^d \rightarrow \mathbb{R}$ be given and assume there exists positive c_1, c_2 such that for all $x \in \mathbb{T}^d$, $k \in \mathbb{Z}^d$*

$$\frac{c_1}{\|x\|^s} \leq f(x) \leq \frac{c_2}{\|x\|^s} \quad \text{and} \quad \frac{c_1}{1 + \|k\|^{d-s}} \leq \widehat{f}(k) \leq \frac{c_2}{1 + \|k\|^{d-s}}.$$

Suppose furthermore that $\{x_1, \dots, x_N\} \subset \mathbb{T}^d$ satisfies

$$\sum_{i \neq j} f(x_i - x_j) \leq N^2 \int_{\mathbb{T}^d} f(x) dx + c_3 N^{1 + \frac{s}{d}}.$$

Then, for every $c_4 > 0$, we have

$$\sum_{\substack{\|k\| \leq c_4 N^{1/d} \\ k \neq 0}} \left| \sum_{n=1}^N e^{2\pi i \langle k, x_n \rangle} \right|^2 \lesssim_{c_1, c_2, c_3, c_4} N^2.$$

In particular, minimizing configurations as well as near-optimal configurations will be very evenly distributed on the torus. We will, after the proof of Theorem 1,

construct a family of functions that exhibit behavior of this type (in particular they behave like the Riesz kernel in the origin but are adapted to the Torus). The idea behind the proof is so general that the method is not restricted to these interaction energies; the following result is another application of this approach.

Theorem 2 (see [20]). *Every set of points $\{x_1, \dots, x_N\} \subset \mathbb{T}^d$ satisfying*

$$\sum_{i,j=1}^N \exp\left(-N^{\frac{2}{d}}\|x_i - x_j\|^2\right) \leq c_1 N$$

satisfies

$$\sum_{\substack{\|k\| \leq c_2 N^{1/d} \\ k \neq 0}} \left| \sum_{n=1}^N e^{2\pi i \langle k, x_n \rangle} \right|^2 \lesssim_{c_1, c_2} N^2.$$

This result, first proved in [20], was what originally motivated our interest in this problem. If the point set is well-distributed (i.e. $\|x_i - x_j\| \gtrsim N^{-1/d}$ whenever $i \neq j$), then the assumption is easily seen to hold and the conclusion follows; the interesting part is that any set of points minimizing this Gaussian interaction functional will necessarily behave like a set of well-separated points w.r.t. this Fourier-analytic regularity measure.

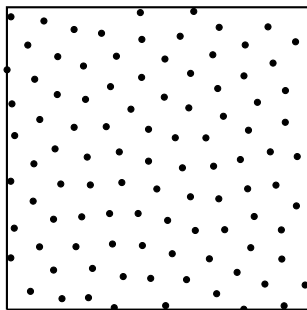


FIGURE 1. A local minimizer of the energy functional $f(x - y) = \exp(-N^{\frac{2}{d}}\|x - y\|^2)$ on \mathbb{T}^2 (picture taken from [22]).

1.4. Consequence for Regularity. The purpose of this section is to discuss implications of such a regularity statement: usually, such statements are given in terms of purely spatial properties (i.e. point separation, points being spread out, the empirical measure converging weakly to the uniform measure etc). Here, the regularity property is phrased on the Fourier side; we discuss implications for the spatial properties as well as their properties when used in numerical integration.

1. Integration error. While there is a vast literature on using minimizing configurations of interacting energy as sample points for quadrature, our argument provides a direct result for L^2 -functions with compact support in frequency space.

Corollary 1. *We have the identity*

$$\sup_{\text{supp}(\hat{f}) \subset B(0, X)} \left\| \int_{\mathbb{T}^d} f(x) dx - \frac{1}{N} \sum_{n=1}^N f(x_n) \right\|_{L^2} = \frac{\|f\|_{L^2}}{N} \left(\sum_{\substack{\|k\| \leq X \\ k \neq 0}} \left| \sum_{n=1}^N e^{2\pi i \langle k, x_n \rangle} \right|^2 \right)^{\frac{1}{2}}.$$

As a consequence, minimal configuration of an interacting energy functional like in Theorem 1 will have optimal error rates for the numerical integration of functions

$$\left\{ f \in L^2(\mathbb{T}^d) : \text{supp}(\hat{f}) \subset B(0, cN^{1/d}) \right\}.$$

Proof. The argument follows quickly from an expansion in Fourier series: the frequency $k = 0$ cancels with the integral

$$\begin{aligned} \frac{1}{N} \sum_{i=1}^N f(x_i) - \int_{\mathbb{T}^d} f(x) dx &= \frac{1}{N} \sum_{n=1}^N \sum_{\|k\| \leq X} \hat{f}(k) e^{2\pi i \langle k, x_n \rangle} - \int_{\mathbb{T}^d} f(x) dx \\ &= \sum_{\substack{\|k\| \leq X \\ k \neq 0}} \hat{f}(k) \frac{1}{N} \sum_{n=1}^N e^{2\pi i \langle k, x_n \rangle} \end{aligned}$$

A simple application of the Cauchy-Schwarz inequality yields

$$\begin{aligned} \sum_{\substack{\|k\| \leq X \\ k \neq 0}} \hat{f}(k) \frac{1}{N} \sum_{n=1}^N e^{2\pi i \langle k, x_n \rangle} &\leq \left(\sum_{\substack{\|k\| \leq X \\ k \neq 0}} |\hat{f}(k)|^2 \right)^{\frac{1}{2}} \left(\sum_{\substack{\|k\| \leq X \\ k \neq 0}} \left| \frac{1}{N} \sum_{n=1}^N e^{2\pi i \langle k, x_n \rangle} \right|^2 \right)^{\frac{1}{2}} \\ &= \frac{\|f\|_{L^2}}{N} \left(\sum_{\substack{\|k\| \leq X \\ k \neq 0}} \left| \sum_{n=1}^N e^{2\pi i \langle k, x_n \rangle} \right|^2 \right)^{\frac{1}{2}}. \end{aligned}$$

Equality for the supremum then follows from L^2 -duality (i.e. picking $\hat{f}(k)$ so as to obtain equality in the Cauchy-Schwarz inequality). The fact that this is optimal up to constants follows from [20]. \square

2. Spatial regularity. Almost orthogonality to low-frequency trigonometric polynomials has obvious implications for spatial properties. We refer especially to classical discrepancy theory where usually the other route is highlighted: notions of irregularity of distribution are bounded from above by Fourier-analytic quantities; we refer especially to Erdős-Turan-Koksma inequality and the books [11, 12, 15, 18] for an overview. Here we shall merely focus on the notion of L^2 -discrepancy and highlight the connection to our result; for simplicity, we restrict our attention to the two-dimensional case $d = 2$. Let $S \subset \mathbb{T}^2$ be a measurable set and define the discrepancy of a point set $\{x_1, \dots, x_N\} \subset \mathbb{T}^2$ with respect to S as

$$D(S) = \# \{1 \leq i \leq N : x_i \in S\} - N|S|.$$

For any fixed S this quantity may be quite small (say ≤ 1) even if the points are distributed in a rather irregular fashion. It therefore makes sense to consider the quantity over an entire family of sets and one fairly canonical approach is to simply consider all possible translations of S and define

$$d_S(x) := D(S + x) = D(\{s + x : s \in S\}).$$

A simple computation shows that we can express the averaged square error in terms of Fourier coefficients as

$$\int_{\mathbb{T}^2} d_S(x)^2 dx = \sum_{k \neq 0} |\widehat{\chi_S}(k)|^2 \left| \sum_{n=1}^N e^{2\pi i \langle k, x_n \rangle} \right|^2,$$

where χ_S is the characteristic function of the set S .

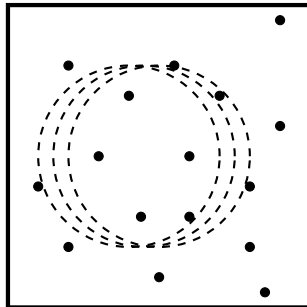


FIGURE 2. L^2 -discrepancy: moving a shape over the points and integrating the square of the difference between the number of points inside the shape and the expected number.

This quantity depends on both the behavior of the Fourier transform of the characteristic function of S as well as the behavior of the exponential sum; our result guarantees that the sum over the second term up to frequencies $\|k\| \lesssim N^{1/d}$ will be small, which is the best possible behavior one could ask of that expression.

In this spirit, we introduce another natural regularity measure: instead of taking the discrepancy with respect to the characteristic function of a set, we may define discrepancy with respect to a localized measure; more precisely, given a set of points $\{x_1, \dots, x_N\} \subset \mathbb{T}^d$, a parameter $t > 0$ and a fixed point $x \in \mathbb{T}^d$, we can define the *heat discrepancy* via

$$d_{t,\Delta}(x) := \sum_{n=1}^N [e^{t\Delta}\delta_x](x_n) - N.$$

Here and henceforth, $e^{t\Delta}$ denotes the heat propagator defined via

$$e^{t\Delta}f = \sum_{k \in \mathbb{Z}^d} e^{-t\|k\|^2} \widehat{f}(k) e^{2\pi i \langle k, x \rangle}.$$

It corresponds to the solution of the heat equation at time $t/(4\pi^2)$ and can be simultaneously understood as a Fourier multiplier and mollification operator. Note that $e^{t\Delta}\delta_x$ in particular may be understood as, roughly, a Gaussian centered at x at carrying most of its mass at scale $\sim t^{1/2}$. Moreover, the function $e^{t\Delta}\delta_x$ is scaled so as to have total integral 1: subtracting N then yields a function that has integral 0 when integrated over \mathbb{T}^d and its deviation from 0 (*i.e.*, its L^2 -norm) serves as a natural measure of irregularity. We would expect this function to be roughly at order $\sim N$ in most points for $t \ll N^{-\frac{2}{d}}$ independently of the set of points and then to become more regular as t increases. We will show in the next Corollary that the

point sets for Riesz-type potentials as in Theorem 1 have good regularity properties with respect to the heat discrepancy.

Corollary 2. *We have, for any set of points and all $t \gtrsim N^{-\frac{2}{d}}$,*

$$\int_{\mathbb{T}^d} d_{t,\Delta}(x)^2 dx \gtrsim Nt^{-\frac{d}{2}}.$$

Any minimizing point set considered in Theorem 1 satisfies

$$\int_{\mathbb{T}^d} d_{N^{-\frac{2}{d}+\alpha},\Delta}(x)^2 dx \lesssim_d (\log N)^{\frac{d-s}{2}} N^2 N^{-\frac{\alpha}{2}(d-s)}.$$

This result clearly shows that on a local scale things have to be rather well-distributed; more precisely, we obtain matching upper and lower bounds (up to a logarithm) for $t \sim N^{-\frac{2}{d}}$ (i.e., $\alpha = 0$, corresponding to regularity on the finest scale $\sqrt{t} \sim N^{-\frac{1}{d}}$). However, for any $\alpha > 0$ (which means spatial scale slightly coarser than just nearest neighbors), we obtain an upper bound that is polynomially smaller than the trivial estimate $\sim N^2$. Moreover, for small values of s (corresponding to a long-range interaction energy), this is arbitrarily close to the universal lower bound satisfied by all point sets. This is similar in spirit to recent results [9, 19] on *rigidity* of minimizing point configurations (the number of points in boxes is more regularly distributed than random).

1.5. Open questions. These results motivate many questions.

- (1) While we give an explicit construction of a function satisfying the properties in §2.2, we do not know whether $f(x) = \|x\|^{-s}$ restricted on torus for $0 < s < d$ satisfies the assumptions of the Theorem 1 (the missing property that would need to be established being $\widehat{f}(k) \gtrsim (1 + \|k\|)^{d-s}$, we refer to Hare & Roginskaya [14] for results in this direction).
- (2) It would be interesting to understand the behavior of the Fourier-analytic quantity for other cutoff-values. Is it possible to prove bounds on

$$\sum_{\substack{\|k\| \leq X \\ k \neq 0}} \left| \sum_{n=1}^N e^{2\pi i \langle k, x_n \rangle} \right|^2 \quad \text{for arbitrary } X?$$

We do not know what happens for $X \lesssim N^{\frac{1}{d}}$. For $X \gtrsim N^{\frac{1}{d}}$ it is likely that

$$\sum_{\substack{\|k\| \leq X \\ k \neq 0}} \left| \sum_{n=1}^N e^{2\pi i \langle k, x_n \rangle} \right|^2 \sim NX^d$$

since this would be implied by the conjecture that the points are maximally separated $\|x_i - x_j\| \gtrsim N^{-1/d}$ (see [20] for a proof).

- (3) Our argument is heavily based on properties of Fourier series while the underlying problem should actually display fairly universal behavior on arbitrary compact manifolds. It could be interesting to further investigate this line of research by trying to see whether similar results hold true on the sphere \mathbb{S}^{d-1} , where spherical harmonics provide a fairly accessible function basis to work with. An encouraging Montgomery-type result on the sphere was established by Bilyk & Dai [5].

2. PROOFS

Lemma 1. *Let $0 < s < d$ be fixed. Then, for all $x, y \in \mathbb{T}^d$ and all $t > 0$,*

$$\int_{\mathbb{T}^d} \int_{\mathbb{T}^d} \frac{[e^{t\Delta}\delta_x](a) [e^{t\Delta}\delta_y](b)}{\|a - b\|^s} da db \lesssim_{d,s} \frac{1}{\|x - y\|^s}.$$

Proof. We prove the result on Euclidean space \mathbb{R}^d , the result on the Torus then follows by transplantation for short times and is easily seen to be true for large times (for large times, the left-hand side converges to a universal constant). On \mathbb{R}^d , we can make explicit use of the fact that convolution with the Riesz potential $\|x\|^{-s}$ is a Fourier multiplier R . Fourier multipliers commute and thus

$$\begin{aligned} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \frac{[e^{t\Delta}\delta_x](a) [e^{t\Delta}\delta_y](b)}{\|a - b\|^s} da db &= \int_{\mathbb{R}^d} \left(\int_{\mathbb{R}^d} \frac{[e^{t\Delta}\delta_x](a)}{\|a - b\|^s} da \right) [e^{t\Delta}\delta_y](b) db \\ &= \langle Re^{t\Delta}\delta_x, e^{t\Delta}\delta_y \rangle \\ &= \langle Re^{2t\Delta}\delta_0, \delta_{y-x} \rangle \end{aligned}$$

This last expression is completely explicit, $e^{2t\Delta}\delta_0$ is a Gaussian centered in the origin to which the Riesz transform is applied; the result then follows from an explicit computation: we obtain

$$\langle Re^{2t\Delta}\delta_0, \delta_{y-x} \rangle = \frac{1}{(8\pi t)^{d/2}} \int_{\mathbb{R}^d} \frac{e^{-\frac{\|z\|^2}{8t}}}{\|z - (y - x)\|^s} dz.$$

We abbreviate the unit vector $w = (y - x)/\|y - x\|$ and argue that

$$\int_{\mathbb{R}^d} \frac{e^{-\frac{\|z\|^2}{8t}}}{\|z - (y - x)\|^s} dz = \frac{1}{\|y - x\|^s} \int_{\mathbb{R}^d} \frac{e^{-\frac{\|z\|^2}{8t}}}{\|\frac{z}{\|x-y\|} - w\|^s} dz$$

We can rewrite this integral as

$$\int_{\mathbb{R}^d} \frac{e^{-\frac{\|z\|^2}{8t}}}{\|\frac{z}{\|x-y\|} - w\|^s} dz = \int_{\mathbb{R}^d} \frac{e^{-\|\frac{z}{\|x-y\|}\|^2 \frac{\|x-y\|^2}{8t}}}{\|\frac{z}{\|x-y\|} - w\|^s} dz = \|x - y\|^{-d} \int_{\mathbb{R}^d} \frac{e^{-\|s\|^2 \frac{\|x-y\|^2}{8t}}}{\|s - w\|^s} ds.$$

Altogether, this implies, with the substitution $t^* = t\|x - y\|^2$ that

$$\langle Re^{2t\Delta}\delta_0, \delta_{y-x} \rangle = \frac{1}{\|x - y\|^s} \frac{1}{(8\pi t^*)^{d/2}} \int_{\mathbb{R}^d} \frac{e^{-\frac{\|s\|^2}{8t^*}}}{\|s - w\|^s} ds$$

We can use rotational invariance to assume that $w = (1, 0, 0, \dots, 0)$. This turns the remaining expression into a function of t^* which is finite for every $t^* \geq 0$, converges to 0 as $t^* \rightarrow \infty$ and is thus bounded. \square

2.1. Proof of Theorem 1.

Proof. We assume that the function f satisfies an estimate

$$\min_{x_1, \dots, x_N} \sum_{i \neq j} f(x_i - x_j) - N^2 \int_{\mathbb{T}^d} f(x) dx \lesssim N^{1+\frac{s}{d}}.$$

We will henceforth fix N and let $\{x_1, \dots, x_N\} \subset \mathbb{T}^d$ be a point set for which this inequality is satisfied. The first step of the argument consists in a mollification of the Dirac point masses: this leads to well-defined functions on which we can apply Fourier analysis. Since $\widehat{f}(k) \geq 0$, we have that for any $x, y \in \mathbb{T}$ and any measure μ

$$\langle e^{t\Delta} \mu, e^{t\Delta} (f * \mu) \rangle = \sum_{k \in \mathbb{Z}^d} e^{-2t\|k\|^2} |\widehat{\mu}(k)|^2 \widehat{f}(k)$$

is monotonically decaying in t . This suggests using the heat kernel as a mollifier. We observe that the self-interactions are at scale

$$\begin{aligned} \langle e^{t\Delta} \delta_x, e^{t\Delta} (f * \delta_x) \rangle &= \langle e^{t\Delta} \delta_0, e^{t\Delta} (f * \delta_0) \rangle \\ &= \sum_{k \in \mathbb{Z}^d} e^{-2t\|k\|^2} \widehat{f}(k) \lesssim_{c_2} \sum_{k \in \mathbb{Z}^d} \frac{e^{-2t\|k\|^2}}{1 + \|k\|^{d-s}} \\ &\lesssim 1 + \sum_{1 \leq \|k\| \leq t^{-1/2}} \frac{1}{\|k\|^{d-s}} + \sum_{\|k\| \geq t^{-1/2}} \frac{e^{-2t\|k\|^2}}{\|k\|^{d-s}} \\ &\lesssim 1 + \int_1^{t^{-1/2}} \frac{r^{d-1}}{r^{d-s}} dr + \int_{t^{-1/2}}^\infty \frac{e^{-tr^2} r^{d-1}}{r^{d-s}} dr \\ &\lesssim 1 + t^{-\frac{s}{2}} + \int_{t^{-1/2}}^\infty e^{-tr^2} r^{s-1} dr. \end{aligned}$$

This last integral can be bounded after substituting $x = tr^2$

$$\begin{aligned} \int_{t^{-1/2}}^\infty e^{-tr^2} r^{s-1} dr &= \int_1^\infty e^{-x} \left(\frac{x}{t}\right)^{\frac{s-1}{2}} \frac{dx}{2\sqrt{x}\sqrt{t}} \\ &= t^{-\frac{s}{2}} \int_1^\infty e^{-x} x^{\frac{s}{2}-1} dx \lesssim_s t^{-\frac{s}{2}}. \end{aligned}$$

Combining this with Lemma 1 implies that, for all $t > 0$,

$$\begin{aligned} \sum_{i,j=1}^N \left\langle e^{t\Delta} \sum_{i=1}^N \delta_{x_i} * f, e^{t\Delta} \sum_{i=1}^N \delta_{x_i} \right\rangle &= N \langle e^{t\Delta} \delta_0 * f, e^{t\Delta} \delta_0 \rangle \\ &\quad + \sum_{\substack{i,j=1 \\ i \neq j}}^N \left\langle e^{t\Delta} \sum_{i=1}^N \delta_{x_i} * f, e^{t\Delta} \sum_{i=1}^N \delta_{x_i} \right\rangle \\ &\lesssim N t^{-\frac{s}{2}} + \sum_{i \neq j} f(x_i - x_j). \end{aligned}$$

A simple application of the Fourier transform shows

$$\begin{aligned} \sum_{i,j=1}^N \left\langle e^{t\Delta} \sum_{i=1}^N \delta_{x_i} * f, e^{t\Delta} \sum_{i=1}^N \delta_{x_i} \right\rangle &= \sum_{k \in \mathbb{Z}^d} e^{-2t\|k\|^2} \left| \sum_{n=1}^N e^{2\pi i \langle k, x_n \rangle} \right|^2 \widehat{f}(k) \\ &= N^2 \int_{\mathbb{T}^d} f(x) dx + \sum_{\substack{k \in \mathbb{Z}^d \\ k \neq 0}} e^{-2t\|k\|^2} \left| \sum_{n=1}^N e^{2\pi i \langle k, x_n \rangle} \right|^2 \widehat{f}(k). \end{aligned}$$

As a consequence, we have the estimate

$$\sum_{\substack{k \in \mathbb{Z}^d \\ k \neq 0}} e^{-2t\|k\|^2} \left| \sum_{n=1}^N e^{2\pi i \langle k, x_n \rangle} \right|^2 \widehat{f}(k) \lesssim Nt^{-\frac{s}{2}} + N^{1+\frac{s}{d}}.$$

We set $t = N^{-\frac{2}{d}}$ and obtain $Nt^{-\frac{s}{2}} \sim N^{1+\frac{s}{d}}$. Moreover,

$$\begin{aligned} N^{1+\frac{s}{d}} &\gtrsim \sum_{\substack{k \in \mathbb{Z}^d \\ k \neq 0}} e^{-2N^{-\frac{2}{d}}\|k\|^2} \left| \sum_{n=1}^N e^{2\pi i \langle k, x_n \rangle} \right|^2 \widehat{f}(k) \\ &\geq \sum_{\substack{\|k\| \leq N^{1/d} \\ k \neq 0}} e^{-2N^{-\frac{2}{d}}\|k\|^2} \left| \sum_{n=1}^N e^{2\pi i \langle k, x_n \rangle} \right|^2 \widehat{f}(k) \\ &\gtrsim \frac{1}{N^{\frac{d-s}{d}}} \sum_{\substack{\|k\| \leq N^{1/d} \\ k \neq 0}} \left| \sum_{n=1}^N e^{2\pi i \langle k, x_n \rangle} \right|^2, \end{aligned}$$

which is the desired result. \square

2.2. Existence of functions with the desired properties. The purpose of this section is to quickly discuss that there are indeed functions satisfying the assumptions of the Theorem 1 and behaving like a Riesz kernel. We fix $0 < s < d$ and recall that the Bessel potential is defined as the function $G_s : \mathbb{R}^d \setminus \{0\} \rightarrow \mathbb{R}$

$$\mathcal{F}^{-1} \frac{\widehat{f}(\xi)}{(1 + 4\pi^2|\xi|^2)^{s/2}} = G_s * f.$$

Taking the Fourier transform G_s can be defined on $\mathbb{R}^d \setminus \{0\}$ via

$$G_s(x) = \frac{1}{(4\pi)^{s/2} \Gamma(s/2)} \int_0^\infty e^{-\frac{\pi|x|^2}{y} - \frac{y}{4\pi}} y^{-1-\frac{d-s}{2}} dy$$

and satisfies $G_s(x) \geq 0$ as well as the asymptotics

$$\begin{aligned} G_s(x) &= (c_{d,s} + o(1))|x|^{-(d-s)} && \text{as } |x| \rightarrow 0 \\ G_s(x) &= (c_{d,s}^* + o(1))|x|^{-\frac{d+1-s}{2}} e^{-|x|} && \text{as } |x| \rightarrow \infty. \end{aligned}$$

We can now consider the function $f_s : \mathbb{T}^d \setminus \{0\} \rightarrow \mathbb{R}$ via

$$f_s(x) = \sum_{k \in \mathbb{Z}^d} G_s(x+k).$$

The asymptotics show that the first property is satisfied, we observe that

$$\widehat{f}_s(k) = \widehat{G}_s(k) = \frac{1}{(1 + 4\pi^2\|k\|^2)^{s/2}} \sim \frac{1}{1 + \|k\|^s}.$$

It remains to show that

$$\min_{x_1, \dots, x_N} \sum_{i \neq j} f_s(x_i - x_j) \leq N^2 \int_{\mathbb{T}^d} f(x) dx + c_3 N^{1+\frac{d-s}{d}},$$

which follows from $|f_s(x)| \lesssim_{s,d} \|x\|^{s-d}$ and a recent result of Hardin, Saff, Simanek & Su [13] (this result actually determines the constant c_3 for an explicit potential with the same asymptotic behavior).

2.3. Proof of Theorem 2.

Proof. We simplify the argument from [20] for the convenience of the reader. The proof proceeds along the same lines as before. It is to see, by considering a lattice, that the energy of any minimal-energy configuration is bounded from above by

$$\sum_{i,j=1}^N \exp\left(-N^{\frac{2}{d}}\|x_i - x_j\|^2\right) \lesssim N \sum_{j=1}^{\infty} j^{d-1} \exp(-j^2) \lesssim N.$$

We start by remarking that we can use the short-time asymptotic of the heat kernel to write

$$\exp\left(-N^{\frac{2}{d}}\|x_i - x_j\|^2\right) = (1 + o(1))\pi^{d/2} \frac{1}{N} \left[e^{(N^{2/d}/4)\Delta} \delta_{x_i} \right](x_j).$$

This allows us to write

$$\begin{aligned} cN^2 &\gtrsim N \sum_{i,j=1}^N \exp\left(-N^{\frac{2}{d}}\|x_i - x_j\|^2\right) \gtrsim \sum_{i,j=1}^N \left[e^{(N^{2/d}/4)\Delta} \delta_{x_i} \right](x_j) \\ &\gtrsim \sum_{k \in \mathbb{Z}^d} e^{-\frac{4\|k\|^2}{N^{2/d}}} \left| \sum_{n=1}^N e^{2\pi i \langle k, x_n \rangle} \right|^2 \geq N^2 + \sum_{k \neq 0} e^{-\frac{4\|k\|^2}{N^{2/d}}} \left| \sum_{n=1}^N e^{2\pi i \langle k, x_n \rangle} \right|^2 \\ &\gtrsim \sum_{\substack{\|k\| \leq N^{1/d} \\ k \neq 0}} \left| \sum_{n=1}^N e^{2\pi i \langle k, x_n \rangle} \right|^2 \end{aligned}$$

which is the desired result. \square

2.4. Proof of Corollary 2.

Proof. We observe that

$$d_{t,\Delta}(x) = \sum_{n=1}^N \langle e^{t\Delta} \delta_x, \delta_{x_n} \rangle - N = \left\langle \delta_x, e^{t\Delta} \sum_{n=1}^N \delta_{x_n} \right\rangle - N$$

and thus, by taking the Fourier transform and Plancherel's theorem,

$$\int_{\mathbb{T}^d} d_{t,\Delta}(x)^2 dx = \sum_{\substack{k \in \mathbb{Z}^d \\ k \neq 0}} e^{-t\|k\|^2} \left| \sum_{n=1}^N e^{2\pi i \langle k, x_n \rangle} \right|^2.$$

For every set of points and every $t \gtrsim N^{-2/d}$, we have

$$\sum_{\substack{k \in \mathbb{Z}^d \\ k \neq 0}} e^{-t\|k\|^2} \left| \sum_{n=1}^N e^{2\pi i \langle k, x_n \rangle} \right|^2 \gtrsim \sum_{\substack{k \in \mathbb{Z}^d \\ \|k\| \leq t^{-1/2}}} \left| \sum_{n=1}^N e^{2\pi i \langle k, x_n \rangle} \right|^2 \gtrsim N t^{-\frac{d}{2}},$$

where the last step is Montgomery's Lemma. Conversely, for any set of points under consideration, we have

$$\begin{aligned} \int_{\mathbb{T}^d} d_{t,\Delta}(x)^2 dx &\lesssim \sum_{\substack{\|k\| \leq X \\ k \neq 0}} e^{-t\|k\|^2} \left| \sum_{n=1}^N e^{2\pi i \langle k, x_n \rangle} \right|^2 + \sum_{\|k\| \geq X} e^{-t\|k\|^2} \left| \sum_{n=1}^N e^{2\pi i \langle k, x_n \rangle} \right|^2 \\ &\lesssim X^{d-s} \sum_{\substack{\|k\| \leq X \\ k \neq 0}} e^{-t\|k\|^2} \left| \sum_{n=1}^N e^{2\pi i \langle k, x_n \rangle} \right|^2 \widehat{f}(k) + N^2 \sum_{\|k\| \geq X} e^{-t\|k\|^2}. \end{aligned}$$

The first sum is easy to bound from above by simply summing over all $k \in \mathbb{Z}^d, k \neq 0$, which yields

$$\sum_{i,j=1}^N \left\langle e^{(t/2)\Delta} \sum_{i=1}^N \delta_{x_i} * f, e^{(t/2)\Delta} \sum_{i=1}^N \delta_{x_i} \right\rangle - N^2 \int_{\mathbb{T}^d} f(x) dx \lesssim N t^{-\frac{s}{2}} + N^{1+\frac{s}{d}}.$$

We can estimate the second sum using the incomplete gamma function

$$\sum_{\|k\| \geq X} e^{-t\|k\|^2} \lesssim \int_X^\infty e^{-tr^2} r^{d-1} dr \lesssim_d t^{-\frac{d}{2}} \Gamma\left(\frac{d}{2}, X^2 t\right)$$

and a simple asymptotic estimate, valid for $X \gtrsim t^{-1/2}$, simplifies this to

$$t^{-\frac{d}{2}} + t^{-\frac{d}{2}} \Gamma\left(\frac{d}{2}, X^2 t\right) \lesssim X^{d-2} t^{-1} e^{-X^2 t}.$$

Altogether, this implies

$$\int_{\mathbb{T}^d} d_{t,\Delta}(x)^2 dx \lesssim_d X^{d-s} (N t^{-\frac{s}{2}} + N^{1+\frac{s}{d}}) + X^{d-2} t^{-1} N^2 e^{-X^2 t}.$$

We now substitute $X = t^{-1/2} Y$ (and require $Y \gtrsim 1$), which simplifies the expression

$$\begin{aligned} \int_{\mathbb{T}^d} d_{t,\Delta}(x)^2 dx &\lesssim_d Y^{d-s} \left(N t^{-\frac{d}{2}} + N^{1+\frac{s}{d}} t^{\frac{s-d}{2}} \right) + N t^{-\frac{d}{2}} \left[Y^{d-2} e^{-Y^2} N \right] \\ &\lesssim Y^{d-s} N t^{-\frac{d}{2}} \left(N^{1/d} t^{1/2} \right)^s + N t^{-\frac{d}{2}} \left[Y^{d-2} e^{-Y^2} N \right]. \end{aligned}$$

For $t = N^{-2/d+\alpha}$, the result follows from setting $Y \sim c\sqrt{\log N}$. \square

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