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On the Riesz energy of measures

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Abstract

Representations for the Riesz kernel $|x-y|^{-s}$ $(s>0)$ are presented, which lead to new interpretations of the energy of measures. It is shown that the surface measure on the unit sphere in $\mathbb{R}^d$ solves a minimal energy problem independent of s (but intimately related to Riesz s-energy) and that n points on the unit circle with minimal discrete Riesz energy are nth roots of unity, unique up to rotation. Moreover, the energy of signed measures is estimated in terms of their discrepancy.

Keywords: Riesz kernel; Energy; Equidistribution; Fekete points; Discrepancy

1. Introduction

One motivation for the research presented in this paper is the problem of distributing n points equally on the unit sphere in $\mathbb{R}^3$, which has applications in various fields of mathematics, such as spherical approximation, numerical integration, quasi-Monte-Carlo methods, and discrete wavelet analysis, to mention only a few (see, for instance, [3,5,11,18,20]). It turned out that—among other—a "bionic" principle can give a reasonable solution from the point of view of constructive approximation: Taking the locations of electrons, which are restricted to the sphere (the conductor) and find themselves in a state of (global) minimum Coulomb energy, then these points are asymptotically well-distributed, even in the quantitative sense of discrepancy. This means that compared to the surface measure

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each part of the surface essentially gets its "most fair" share of points [7]. Moreover, it has been numerically shown that the distribution of such electrons follows certain geometric principles. The corresponding Dirichlet cells appear to partition the sphere into hexagons and pentagons. For instance, the Dirichlet cells of 32 electrons in equilibrium constitute the pattern of the standard soccer ball, and their dual structure is the one of the recently discovered C_{60} molecule (Buckminster fullerene) [27].

Yet, the principles working here have not been fully understood. There is still necessary a deeper analysis of the relations between the different concepts of energy, geometry, and equidistribution. The starting point for this paper are integral representations for the Riesz kernel $|x-y|^{-s}$ in $\mathbb{R}^d$ $(s>0)$. One interesting point of the corresponding formulas is that they factor into integrands independent of s, which are integrated against the weight dr/r^{1+s}. With this approach, the Riesz energy of a measure (or a signed measure) can be directly related to a square integral over the charges that this measure associates with dilated, translated and rotated copies of any fixed set. In particular, the energy of a signed measure—under certain restrictions—can be estimated in terms of the discrepancy of the two measures, based on homothetic images of the aforementioned given set.

For the case of the sphere it is shown that the normalized surface measure solves a minimal energy problem related to this new interpretation of Riesz energy. Moreover, it is shown that n points on the unit circle minimizing discrete energy with respect to a kernel, which is a decreasing convex function of arclength are given by the nth roots of unity and—in case of strict convexity—are unique up to rotation. In particular, this applies to the Riesz kernel with exponent $s>0$.

2. Notation and conventions

Let $d\geqslant 2$. Throughout this paper, $B(x,r)$ stands for the open ball in $\mathbb{R}^d$ of radius $r>0$, centered at x, and λ^d for the Lebesgue measure on $\mathbb{R}^d$. We denote the volume of the unit ball $B(0,1)$ by v_d and the surface of the unit sphere $S^{d-1} := \{x\in\mathbb{R}^d\colon |x|=1\}$ by ω_d. Here and in what follows, $|\cdot|$ stands for the Euclidean norm. Denote by σ the surface measure on S^{d-1}, normalized so that $\sigma(\mathbb{R}^d)=1$. Moreover, $diam(A)$ and $dist(z,A)$ are the diameter of a set $A\subset\mathbb{R}^d$ and the Euclidean distance from the point $z\in\mathbb{R}^d$ to A, respectively. $\#A$ is the number of elements of A. Let $SO(d)$ denote the group of rotations on $\mathbb{R}^d$ and H the Haar (unit) measure on $SO(d)$. Finally, $K\subset\mathbb{R}^d$ will be any (fixed) bounded measurable set with $\lambda^d(K)>0$.

3. The Riesz kernel

In this section, we present two integral representations of the classical Riesz kernel, which are fundamental for the subsequent considerations regarding Riesz energy.

Proposition 1. *Let $s>0$. Then for $x, y \in \mathbb{R}^d$, $x \neq y$,*

$$\frac{1}{|x-y|^s} = C(K,s,d) \int_0^\infty \int_{SO(d)} \lambda^d((x+rU(K)) \cap (y+rU(K)))\, dH(U) \frac{dr}{r^{d+1+s}},$$

where, setting $\mathbf{1} := (1,0,\dots,0) \in \mathbb{R}^d$, the constant $C(K,s,d)$ is given by

$$C(K,s,d)^{-1} = \int_0^\infty \int_{SO(d)} \lambda^d(tU(K) \cap (\mathbf{1}+tU(K)))\, dH(U) \frac{dt}{t^{d+1+s}}.$$

Proof. Since distance and Lebesgue measure are invariant under translation, we may assume that $x=0$. Moreover, w.l.o.g. $y = (|y|, 0, \dots, 0)$ by rotational invariance of the respective quantities. Now, for $r>0$ and $U \in SO(d)$,

$$\lambda^d(rU(K) \cap (y+rU(K))) = |y|^d \lambda^d\left(\frac{r}{|y|}U(K) \cap \left(\frac{y}{|y|} + \frac{r}{|y|}U(K)\right)\right),$$

so that making the change of variable $t = r/|y|$,

$$\begin{aligned}
&\int_0^\infty \int_{SO(d)} \lambda^d((x+rU(K)) \cap (y+rU(K)))\, dH(U) \frac{dr}{r^{d+1+s}} \\
&= \int_0^\infty \int_{SO(d)} |y|^d \lambda(tU(K) \cap (\mathbf{1}+tU(K)))\, dH(U) \frac{|y|\, dt}{(t|y|)^{d+1+s}} \\
&= C(K,s,d)^{-1} \frac{1}{|y|^s} = C(K,s,d)^{-1} \frac{1}{|x-y|^s}. \qquad \square
\end{aligned}$$

Example. Taking $K = B(0,1)$ in Proposition 1 it follows that

$$\frac{1}{|x-y|^s} = C(B(0,1),s,d) \int_0^\infty \lambda^d(B(x,r) \cap B(y,r)) \frac{dr}{r^{d+1+s}}. \tag{1}$$

Now,

$$\lambda^d(B(0,r) \cap B(\mathbf{1},r)) = \begin{cases} 2v_{d-1} r^d \int_{1/(2r)}^1 (\sqrt{1-t^2})^{d-1}\, dt, & \text{if } r>1/2, \\ 0, & \text{if } 1/2 \geqslant r > 0. \end{cases}$$

Consequently,

$$\begin{aligned}
C(B(0,1),s,d)^{-1} &= 2v_{d-1} \int_{1/2}^\infty \int_{1/(2r)}^1 (1-t^2)^{(d-1)/2}\, dt \frac{dr}{r^{1+s}} \\
&= \frac{2^{s+1}}{s} v_{d-1} \int_0^1 (1-t^2)^{(d-1)/2} t^s\, dt.
\end{aligned}$$

In particular, for $s=1$, $C(B(0,1),1,d) = \frac{d+1}{4v_{d-1}}$. If, in addition, $d=3$, then $C(B(0,1),1,3) = 1/\pi$ and (1) reduces to a formula for the Coulomb kernel which appears in [6]. $\square$

There is also a trivial integral representation of the Riesz kernel, which we state here for later reference.

Proposition 2. *Let* $s > 0$. *Then for* $x, y \in \mathbb{R}^d$, $x \neq y$,

$$\frac{1}{|x-y|^s} = s \int_{|x-y|}^{\infty} \frac{dr}{r^{1+s}}.$$

4. The Riesz energy of measures

Let $s > 0$ and let μ be a (positive Borel-) measure on $\mathbb{R}^d$. Its Riesz s-energy is given by

$$E_s(\mu) := \int \int \frac{1}{|x-y|^s} \, d\mu(x) \, d\mu(y).$$

By Proposition 1, changing the order of integration, the Riesz energy can be written in the form

$$E_s(\mu) = C(K, s, d) \int_0^{\infty} \int_{SO(d)} \int_{\mathbb{R}^d} [\mu(z + rU(K))]^2 \, d\lambda^d(z) \, dH(U) \frac{dr}{r^{d+1+s}}.$$

In particular, taking $K := B(0,1)$ this formula simplifies to

$$E_s(\mu) = C(B(0,1), s, d) \int_0^{\infty} \left(\int_{\mathbb{R}^d} [\mu(B(z,r))]^2 \, d\lambda^d(z) \right) \frac{dr}{r^{d+1+s}}. \tag{2}$$

From Proposition 2, making again a change in the order of integration, there follows that

$$E_s(\mu) = s \int_0^{\infty} \left(\int \mu(B(x,r)) \, d\mu(x) \right) \frac{dr}{r^{1+s}}. \tag{3}$$

Roughly speaking, relations (2) and (3) express that Riesz energy is determined by the charges that the measure associates with balls, where balls with smaller radius contribute more.

5. The energy of signed measures

Suppose ν is another (Borel-) measure on $\mathbb{R}^d$ such that the mixed energy

$$E_s[\mu, \nu] := \int \int \frac{1}{|x-y|^s} \, d\mu(x) \, d\nu(y)$$

is finite. Then the energy

$$\begin{aligned} E_s(\mu - \nu) &:= \int\int \frac{1}{|x-y|^s}\, d(\mu-\nu)(x)\, d(\mu-\nu)(y) \\ &= E_s(\mu) - 2E_s[\mu,\nu] + E_s(\nu) \end{aligned}$$

of the signed measure $\mu - \nu$ is well-defined, as we will henceforth always assume. By Proposition 1,

$$\begin{aligned} E_s(\mu-\nu) = C(K,s,d) \int_0^\infty \int_{SO(d)} \int_{\mathbb{R}^d} &[(\mu-\nu)(z + rU(K))]^2\, d\lambda^d(z)\, dH(U) \\ &\times \frac{dr}{r^{d+1+s}}. \end{aligned} \tag{4}$$

Later on, we will give an interpretation of (4) in terms of discrepancy. This formula should also be compared to Stolarsky's "invariance principle" [21,22] for measures on the unit sphere: Suppose there are given n (distinct) points $x_1, \ldots, x_n$ on S^{d-1} and denote by μ_n the atomic unit measure associating equal mass $1/n$ with each x_i. Let g be an integrable, (say) non-negative function and, with $p_0 := (1,0,\ldots,0) \in S^{d-1}$, look at the kernel

$$\rho(x,y) := \int_{SO(d)} \left| \int_{\langle U(x), p_0 \rangle}^{\langle U(y), p_0 \rangle} g(r)\, dr \right| dH(U) \quad (x, y \in S^{d-1}).$$

Here, $\langle \cdot, \cdot \rangle$ stands for the standard inner product in $\mathbb{R}^d$. Note that ρ is non-singular for $x = y$. Consider the spherical caps $C_r := \{p \in S^{d-1} \colon \langle p, p_0 \rangle \leqslant r\}$. Then Theorem 2 of [22] says that

$$\begin{aligned} &\int\int \rho(x,y)\, d\mu_n\, d\mu_n - \int\int \rho(x,y)\, d\sigma\, d\sigma \\ &\quad = 2\int_{-1}^{1} g(r) \int_{SO(d)} [(\mu_n - \sigma)(U(C_r))]^2\, dH(U)\, dr. \end{aligned}$$

We continue pointing out that (4) immediately leads to the following well-known conclusion on the positive definiteness of the energy functional [17].

Corollary 3. *The s-energy of a signed measure is positive, unless it is the zero-measure.*

We conclude this section with the following consequence of (3). Compared to (4) this formula lacks a non-negative integrand:

$$E_s(\mu-\nu) = s\int_0^\infty \left(\int (\mu-\nu)(B(x,r))\, d(\mu-\nu)(x) \right) \frac{dr}{r^{1+s}}. \tag{5}$$

6. Minimal energy on the sphere

This section is devoted to the minimal energy problem for measures on the unit sphere S^{d-1} in $\mathbb{R}^d$. It is well-known that for $0<s<d$, the normalized surface measure σ is the unique mass with minimal Riesz s-energy among all unit measures on S^{d-1}. But, as the following result shows, σ is the unique solution to a more general extremal problem, independent of s, which by (2) implies the minimal Riesz s-energy property.

Proposition 4. *Let $r>0$. For each unit measure μ on S^{d-1},*

$$\int_{\mathbb{R}^d} [\sigma(B(x,r))]^2 \, d\lambda^d(x) = \int_{\mathbb{R}^d} [\mu(B(x,r))]^2 \, d\lambda^d(x) - \int_{\mathbb{R}^d} [(\mu-\sigma)(B(x,r))]^2 \, d\lambda^d(x). \tag{6}$$

Corollary 5. *The normalized surface measure σ is the unique unit measure on S^{d-1} for which the L^2-norm of $x \mapsto \sigma(B(x,r))$ is minimal for each $r>0$.*

Remark. The "defect" $\int_{\mathbb{R}^d} [(\mu-\sigma)(B(x,r))]^2 \, d\lambda^d(x)$ on the right-hand side of (6) can be interpreted as an L^2-discrepancy of the signed measure $\mu - \sigma$.

Proof of Proposition 4. Let μ and ν be unit measures on S^{d-1}. Then

$$\int_{\mathbb{R}^d} \mu(B(x,r))\nu(B(x,r)) \, d\lambda^d(x) = \int_0^\infty \omega_d \rho^{d-1} \int_{S^d} \mu(B(\rho\zeta,r))\nu(B(\rho\zeta,r)) \, d\sigma(\zeta) \, d\rho. \tag{7}$$

Now, fix $\rho>0$ and write

$$\langle \mu, \nu \rangle := \int_{S^d} \mu(B(\rho\zeta,r))\nu(B(\rho\zeta,r)) \, d\sigma(\zeta).$$

Since $\zeta \mapsto \sigma(B(\rho\,\zeta,r))$ and $y \mapsto \sigma(B(\frac{y}{\rho},\frac{r}{\rho}))$ are constant on S^{d-1}, we have

$$\begin{aligned}
\langle \mu, \sigma \rangle &= \sigma(B(\rho\mathbf{1},r)) \int_{S^{d-1}} \mu(B(\rho\zeta,r)) \, d\sigma(\zeta) \\
&= \sigma(B(\rho\mathbf{1},r)) \int_{S^{d-1}} \sigma\left(B\left(\frac{y}{\rho},\frac{r}{\rho}\right)\right) d\mu(y) \\
&= \sigma(B(\rho\mathbf{1},r)) \int_{S^{d-1}} \sigma\left(B\left(\frac{y}{\rho},\frac{r}{\rho}\right)\right) d\sigma(y) \\
&= \langle \sigma, \sigma \rangle.
\end{aligned}$$

Hence,

$$\langle \sigma, \sigma \rangle = 2\langle \mu, \sigma \rangle - \langle \sigma, \sigma \rangle = \langle \mu, \mu \rangle - \langle \mu - \sigma, \mu - \sigma \rangle,$$

which by virtue of (7) implies the assertion of Proposition 4. □

For completeness, we formulate the aforementioned result on minimal s-energy on the sphere as a corollary to Proposition 4.

Corollary 6. *For $0<s<d$, the normalized surface measure on S^{d-1} is the unique unit measure on S^{d-1} with minimal Riesz s-energy. For $s\geqslant d$, there is no measure on S^{d-1} with finite Riesz s-energy.*

7. Discrete energy

One approach to the problem of distributing points uniformly on the sphere mentioned in the introduction is to approximate the surface measure by point masses which solve a discrete energy problem and thus mimic the minimal energy property of the surface measure.

We begin by stating the minimal discrete energy problem in a general form.

Definition. Let E be an infinite subset of $\mathbb{R}^d$, $\Phi : E \times E \to \bar{\mathbb{R}}$ a kernel. Let $n \geqslant 2$. Points $x_1, \ldots, x_n \in E$ with the property that

$$\sum_{\substack{i,j=1 \\ i \neq j}} \Phi(x_i, x_j) = \inf_{y_1, \ldots, y_n \in E} \sum_{\substack{i,j=1 \\ i \neq j}} \Phi(y_i, y_j)$$

are called nth Φ-Fekete points on E.

The classical notion of Fekete points refers to the Newtonian kernel $\Phi(x,y) = |x-y|^{2-d}$ for $d \geqslant 3$ and the logarithmic kernel $\Phi(x,y) = -\log|x-y|$ for $d=2$. It is well-known that for compact E of positive capacity, the corresponding points are asymptotically distributed according to the equilibrium distribution of E. Moreover, for curves $E \subset \mathbb{R}^2$ or smooth surfaces $E \subset \mathbb{R}^d$ $(d \geqslant 3)$ the order of convergence can be quantified in terms of discrepancy (see [2,7] for details and [8] for an overview).

From Proposition 2, changing the order of integration, we have the following representation for the discrete Riesz energy of points.

Proposition 7. *Let $y_1, \ldots, y_n \in \mathbb{R}^d$. Then*

$$\sum_{\substack{i,j=1 \\ i \neq j}}^{n} \frac{1}{|y_i - y_j|^s} = s \int_0^\infty \left(\sum_{j=1}^{n} \#\{1 \leqslant i \leqslant n\colon\ y_i \in B(y_j, r),\ i \neq j\} \right) \frac{dr}{r^{1+s}}.$$

Taking $E = S^{d-1}$ $(d \geq 3)$ it can be proved via standard equilibrium techniques that Φ-Fekete points on the sphere for the Riesz kernel $\Phi(x,y) = |x-y|^{-s}$ are asymptotically distributed according to the surface measure, provided $s < d-1$. For $s \geq d-1$ these techniques fail, essentially due to the fact that there is no measure on S^{d-1} with finite Riesz s-energy. Using precise asymptotics for the minimal discrete energy [16] it is possible to prove equidistribution in the case $s = d-1$ [4,10]. However, yet there is no proof for the case $s > d-1$, even though mathematicians believe and physicists know that the corresponding extremal points need to be asymptotically equidistributed.

In a series of papers, Wagner has established upper and lower bounds for energies and potentials in various configurations [24–26]. By means of (2) and (3) one can find lower bounds for the discrete Riesz energy of points in terms of solutions to certain extremal problems. We illustrate this in what follows.

For $r > 0$ consider the extremal problem:

$$\text{Minimize} \quad \Phi_r(x_1, \ldots, x_n) = \sum_{j=1}^{n} \#\{1 \leq i \leq n\colon\ x_i \in B(x_j, r),\ \ i \neq j\}$$

$$\text{subject to} \quad x_1, \ldots, x_n \in S^{d-1}.$$

One may read this extremal task as follows: Suppose there are n inimical dictators on a planet that push the red button if the other is in the range of their missiles. Minimize the number of conflicts, given that all missiles have the same maximal range r (cf. [23] for a similar interpretation of the best packing problem). From Proposition 7, we immediately have

Corollary 8.

$$\inf_{y_1, \ldots, y_n \in S^{d-1}} \sum_{\substack{i,j=1 \\ i \neq j}}^{n} \frac{1}{|y_i - y_j|^s} \geq s \int_0^\infty \left(\inf_{x_1, \ldots, x_n \in S^{d-1}} \Phi_r(x_1, \ldots, x_n) \right) \frac{dr}{r^{1+s}}.$$

We conclude this section with an observation concerning Φ-Fekete points on the unit circle $E = S^1$. To this end, denote by $d(x,y)$ the distance between $x \in S^1$ and $y \in S^1$, measured in terms of arclength.

Proposition 9. *Suppose Φ is a function of arclength on S^1, i.e.,*

$$\Phi(x,y) = \phi(d(x,y)) \quad (x, y \in S^1).$$

If ϕ is decreasing and convex in $[0, \pi]$, then the nth *roots of unity are Φ-Fekete points on S^1. If, in addition, ϕ is strictly convex in $[0, 2\pi/n]$, then nth Φ-Fekete points on S^1 are unique up to rotation.*

Proof. Denote by $G = \{\zeta_1 = e^{2\pi i 0}, \ldots, \zeta_n = e^{2\pi i \frac{n-1}{n}}\}$, the group of nth roots of unity. Fix $1 \leqslant k \leqslant n-1$ and consider the transitive group action

$$\psi_k : G \to G, \quad g \mapsto e^{i2\pi \frac{k}{n}} g.$$

Then G is the union of mutually disjoint orbits $U_1^{(k)}, \ldots, U_{n_k}^{(k)}$, which are invariant under ψ_k: $\psi_k(U_i^{(k)}) = U_i^{(k)}$, $i = 1, \ldots, n_k$. Note that each $U_i^{(k)}$ consists of n/n_k elements.

Let $x_1, \ldots, x_n$ be any points on S^1, w.l.o.g. ordered in such a way that x_{i+1} is a neighbor of x_i. For sake of notation, define the auxiliary function F on G by

$$F(\zeta_i) = x_i \quad (i = 1, \ldots, n).$$

Rearranging the summation and taking into account the convexity of ϕ,

$$\begin{aligned} \frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^{n} \Phi(x_i, x_j) &= \sum_{k=1}^{[n/2]} \sum_{l=1}^{n_k} \sum_{\zeta \in U_l^{(k)}} \Phi(F(\zeta), F(\psi_k(\zeta))) \\ &= \sum_{k=1}^{[n/2]} \sum_{l=1}^{n_k} \frac{n}{n_k} \sum_{\zeta \in U_l^{(k)}} \frac{n_k}{n} \phi(d(F(\zeta), F(\psi_k(\zeta)))) \\ &\geqslant \sum_{k=1}^{[n/2]} \sum_{l=1}^{n_k} \frac{n}{n_k} \phi\left(\frac{n_k}{n} \sum_{\zeta \in U_l^{(k)}} d(F(\zeta), F(\psi_k(\zeta))) \right), \end{aligned} \tag{8}$$

where $[t]$ stands for the largest integer less than or equal to t. Now,

$$\sum_{\zeta \in U_l^{(k)}} d(F(\zeta), F(\psi_k(\zeta))) \leqslant \sum_{\zeta \in U_l^{(k)}} d(\zeta, \psi_k(\zeta)). \tag{9}$$

Moreover,

$$\frac{n_k}{n} \sum_{\zeta \in U_l^{(k)}} d(\zeta, \psi_k(\zeta)) = d(\xi, \psi_k(\xi)) \quad (\xi \in U_l^{(k)}). \tag{10}$$

Using (9), the monotonicity of ϕ, and (10) we can continue (8) to

$$\frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^{n} \Phi(x_i, x_j) \geqslant \sum_{k=1}^{[n/2]} \sum_{l=1}^{n_k} \sum_{\xi \in U_l^{(k)}} \phi(d(\xi, \psi_k(\xi))) = \frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^{n} \Phi(\zeta_i, \zeta_j).$$

If ϕ is strictly convex in $[0, 2\pi/n]$, then the inequality in (8) is strict, unless all arclength distances $d(F(\zeta_i), F(\psi_1(\zeta_i)))$ are the same. The latter can only occur in the case of rotated nth roots of unity. □

Corollary 10. *Let $r > 0$. The* n*th roots of unity are Φ-Fekete points for the kernel*

$$\Phi(x, y) = \lambda(B(x, r) \cap B(y, r)) \quad (x, y \in S). \tag{11}$$

For $r \geqslant \sin(\pi/n)$, the Fekete points for this kernel are unique (up to rotation).

Note that the kernel from Corollary 10 appears as the integrand in (1). The assertion of the following two immediate consequences of Proposition 9 were previously established in [1, Cor.2.1].

Corollary 11. *Let* $s>0$. *The* n*th roots of unity are the* (*up to a rotation unique*) Φ-*Fekete points for the Riesz kernel*

$$\Phi(x,y)=\frac{1}{|x-y|^s}\quad (x,y\in S).$$

Corollary 12. *The* n*th roots of unity are the* (*up to a rotation unique*) Φ-*Fekete points for the logarithmic kernel*

$$\Phi(x,y)=\log\frac{1}{|x-y|}\quad (x,y\in S).$$

8. Estimates for energy in terms of discrepancy

It has been established that—under certain restrictions—small Newtonian ($d\geqslant 3,\ s=d-2$) or logarithmic ($d=2$) energy of a signed measure $\mu-\nu$ guarantees that the two masses μ and ν are not too far from each other from the point of view of some uniform distance $\sup|\mu(B)-\nu(B)|$ based on a collection of relevant test sets $B\in\mathscr{B}$, i.e., from the point of view of discrepancy [2,12,14,15]. This insight can be used to give quantitative results on zero distributions arising in polynomial approximation [2].

The purpose of this section is to establish a converse relation, namely, in what sense small discrepancy implies small Riesz energy.

In general, different choices of classes of test sets result in notions of discrepancy which may have quite different behavior [19]. Here, motivated by (4), which actually states that the energy is some (non-uniform) square-integral discrepancy, we take as the collection of test sets the homethetic, i.e., rotated, dilated, and translated, images of one fixed set $K\subset\mathbb{R}^d$, which is bounded and of positive Lebesgue measure.

Definition. Let μ and ν be measures on $\mathbb{R}^d$. We call the quantity

$$D_K[\mu,\nu]:=\sup\{|(\mu-\nu)(z+rU(K))|:\ z\in\mathbb{R}^d,\ r>0,\ U\in SO(d)\}$$

the (homothetic) discrepancy between μ and ν, based on K.

Remark. This concept of discrepancy can also serve to estimate the error in multivariate integration in terms of continuity or smoothness properties of the integrand [9].

If $K=B(0,1)$, this notion coincides with ball discrepancy [5], and we write $D_{\text{ball}}[\mu,\nu]:=D_{B(0,1)}[\mu,\nu]$.

Suppose μ and ν are unit measures on $\mathbb{R}^d$ with support contained in a compact set, say, M. It is clear that in order to estimate Riesz energy in terms of discrepancy one needs to impose restrictions on the masses' densities. We will do this by assuming that there exist $\beta > s$ and $c \geqslant 1$ such that

$$\sup_{x \in \mathbb{R}^d} (\mu + \nu)(B(x,r)) \leqslant c r^\beta \quad (r > 0). \tag{12}$$

Such an assumption guarantees finite s-energy as can be seen from the following remark, which is also of independent interest.

Lemma. *Let $s > 0$. Suppose ρ_1, ρ_2 are finite measures, and set*

$$\varphi(r) := \sup_{x \in \mathbb{R}^d} \rho_1(B(x,r)) \quad (r > 0).$$

If $\int_0^1 \frac{\varphi(r)}{r^{1+s}} dr < \infty$, then ρ_1 and ρ_2 have finite mixed s-energy $E_s[\rho_1, \rho_2]$.

Proof. From Proposition 2,

$$\begin{aligned} E_s[\rho_1, \rho_2] &= s \int_0^\infty \int \rho_1(B(x,r))\, d\rho_2(x) \frac{dr}{r^{1+s}} \\ &\leqslant s\rho_2(\mathbb{R}^d) \left(\int_0^1 \frac{\varphi(r)\, dr}{r^{1+s}} + \rho_1(\mathbb{R}^d) \int_1^\infty \frac{dr}{r^{1+s}} \right) < \infty. \qquad \square \end{aligned}$$

We start by estimating Riesz energy in terms of ball discrepancy.

Proposition 13. *Suppose μ and ν are unit measures on $\mathbb{R}^d$ satisfying* (12). *Then*

$$E_s(\mu - \nu) \leqslant \frac{2\beta}{\beta - s} c^{s/\beta} D_{\text{ball}}[\mu, \nu]^{1 - s/\beta}.$$

We remark that the dependence of this estimate on the dimension d is implicitly given by assumption (12). In particular, for $s \geqslant d$ no such β exists.

Proof. Let $\delta > 0$. By (5) and (12),

$$\begin{aligned} E_s(\mu - \nu) &\leqslant s \int_0^\infty \left| \int (\mu - \nu)(B(x,r))\, d(\mu - \nu)(x) \right| \frac{dr}{r^{1+s}} \\ &\leqslant 2\, s \int_0^\delta c r^\beta \frac{dr}{r^{1+s}} + 2s \int_\delta^\infty D_{\text{ball}}[\mu, \nu] \frac{dr}{r^{1+s}} \\ &= 2c \frac{s}{\beta - s} \delta^{\beta - s} + 2\delta^{-s} D_{\text{ball}}[\mu, \nu]. \end{aligned}$$

Inserting $\delta := (D_{\text{ball}}[\mu, \nu]/c)^{1/\beta}$ gives the desired estimate. $\square$

Remark. With the same method, it is possible to derive estimates for the logarithmic energy of a signed measure in terms of discrepancy. If μ and v are unit measures with (12) and compact support, then the logarithmic energy

$$E_{\log}(\mu - v) := \int\int \frac{1}{|x-y|}\, d(\mu - v)(x)\, d(\mu - v)(y)$$

can also be written in the form

$$E_{\log}(\mu - v) = \int_0^\infty \left(\int (\mu - v)(B(x,r))\, d(\mu - v)(x) \right) \frac{dr}{r}.$$

If, say, the support of the measures satisfies $M \subset B(0, 1/2)$, for $0 < \delta \leqslant 1$,

$$E_{\log}(\mu - v) \leqslant 2c\frac{\delta^\beta}{\beta} + 2D_{\text{ball}}[\mu, v] \log\frac{1}{\delta}.$$

Setting $\delta := (D_{\text{ball}}[\mu, v]/c)^{1/\beta}$ gives

$$E_{\log}(\mu - v) \leqslant 2\frac{D_{\text{ball}}[\mu, v]}{\beta}\left(1 + \log\frac{c}{D_{\text{ball}}[\mu, v]}\right).$$

We illustrate the sharpness of Proposition 13 with the following

Example. Let $n \in \mathbb{N}$, say $n > 2$ odd. Consider the nth roots of unity ζ_j on S^1 (see the proof of Proposition 9), and set $I_j = \{z \in S^1 \colon d(z, \zeta_j) \leqslant \frac{2\pi}{4n}\}$. Look at the unit measures

$$\mu_n := 2\sum_{j=1}^n \sigma_{|I_j}, \quad v = \sigma.$$

Then $\mu_n - v = \mu_n^* - v_n^*$, where the positive measures

$$\mu_n^* = \sum_{j=1}^n \sigma_{|I_j}, \quad v_n^* = \sigma - \sum_{j=1}^n \sigma_{|I_j}$$

have complementary support. Moreover, v_n^* is the image of μ_n^* under a rotation by an angle $\frac{2\pi}{2n}$. In particular,

$$E_s(\mu_n^*) = E_s(v_n^*) \quad (0 < s < 1). \tag{13}$$

We will now show that for some constant $\gamma_1 > 0$ independent of n,

$$E_s[\mu_n^* - v_n^*, \mu_n^*] \geqslant \gamma_1 \left(\frac{1}{n}\right)^{1-s}. \tag{14}$$

Then, by virtue of (13),

$$\begin{aligned} E_s(\mu_n - \sigma) = E_s(\mu_n^* - v_n^*) &= 2E_s(\mu_n^*) - 2E_s[\mu_n^*, v_n^*] \\ &\geqslant 2\gamma_1\left(\frac{1}{n}\right)^{1-s} = 2\gamma_1 (D_{\text{ball}}[\mu_n, \sigma])^{1-s}. \end{aligned}$$

Since $\mu + \nu = \mu_n + \sigma$ satisfies (12) with $\beta = 1$, this establishes the sharpness of Proposition 13 with respect to the exponent to which the discrepancy is raised.

In order to establish (14), let $x \in I_j$ and introduce $\delta = \delta(x) \in [0, \frac{2\pi}{4n}]$ via $d(x, \zeta_j) = \frac{2\pi}{4n} - \delta$. Moreover, write $B(x,r) \cap S = \{z \in S^1 : d(x,z) < \alpha\}$, more precisely, $\alpha = \alpha(r) = 2\arcsin(r/2)$. Now,

$$g_n(r,x) := (\mu_n - \nu_n^*)(B(x,r)) = \begin{cases} 0, & \text{if } r = \alpha = 0, \\ 2\delta/(2\pi), & \text{if } \alpha = \delta, \\ 2\delta/(2\pi), & \text{if } \alpha = \frac{2\pi}{2n} - \delta, \\ -2\delta/(2\pi), & \text{if } \alpha = \frac{2\pi}{2n} + \delta, \\ -2\delta/(2\pi), & \text{if } \alpha = \frac{4\pi}{2n} - \delta, \\ 2\delta/(2\pi), & \text{if } \alpha = \frac{4\pi}{2n} + \delta, \\ \vdots, & \vdots \end{cases} \tag{15}$$

and this function is linear (in α) in between these knots (cf. Fig. 1).

Now,

$$E_s(\mu_n^* - \nu_n^*) = s \int \int_0^\infty g_n(r,x) \frac{dr}{r^{1+s}} d\mu_n^*(x). \tag{16}$$

By (15),

$$\int_0^\infty g_n(r,x) \frac{dr}{r^{1+s}} = \sum_{i=1}^\infty \left\{ \int_{\alpha = i\frac{\pi}{n}}^{\alpha=(i+1)\frac{\pi}{n}} |g_n(r,x)| \frac{dr}{r^{1+s}} - \int_{\alpha=(i+1)\frac{\pi}{n}}^{\alpha=(i+2)\frac{\pi}{n}} |g_n(r,x)| \frac{dr}{r^{1+s}} \right\}, \tag{17}$$

where we note that the sum on the right-hand side is only formally "infinite". It follows from (17) and (15) that

$$\int_0^\infty g_n(r,x) \frac{dr}{r^{1+s}} \geqslant 0,$$

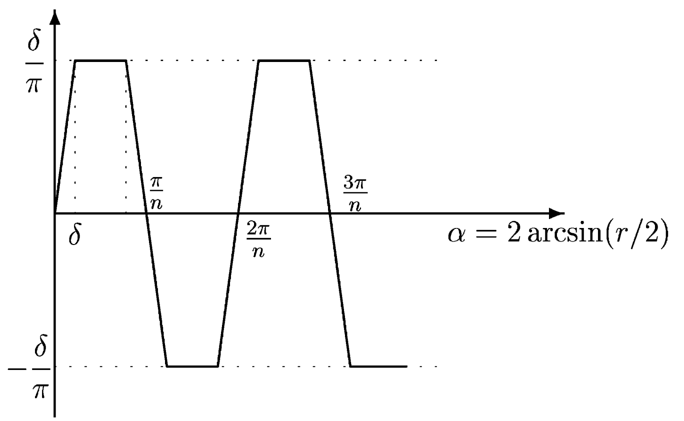

Fig. 1. $g_n(r,x)$.

and, for (say) $\frac{\pi}{4n} \leqslant \delta \leqslant \frac{\pi}{3n}$,

$$\int_0^\infty g_n(r,x)\frac{dr}{r^{1+s}} \geqslant \int_0^{\alpha=\frac{2\pi}{n}} g_n(r,x)\left(\frac{1}{r^{1+s}} - \frac{1}{\alpha^{1+s}}\right) dr + 0 + \cdots$$

$$\geqslant \gamma_2 \int_{\alpha=\delta}^{\alpha=\frac{\pi}{2n}n} 2\delta \frac{dr}{r^{1+s}} \geqslant \gamma_3 \delta^{1-s} \geqslant \gamma_4 \left(\frac{1}{n}\right)^{1-s}$$

with $\gamma_2, \gamma_3, \gamma_4 > 0$ independent of n. Integrating this inequality against $d\mu_n^*(x)$ it follows that (see (16)),

$$E_s(\mu_n^* - v_n^*, \mu_n^*) \geqslant \gamma_1 \frac{1}{n} \sum_{j=1}^{n} \left(\frac{1}{n}\right)^{1-s},$$

which we were supposed to show. □

Remark. It is established in Hüsing [13] that the logarithmic energy of a signed measure is—roughly stated—bounded from below by the square of the discrepancy, and that such estimates are sharp from various points of view. The previous considerations point out that such a lower bound is not attained in canonic examples. This gives some explanation why it is not possible to obtain sharp quantitative estimates for the zero distribution of certain extremal polynomials, e.g., Fekete-polynomials, via energy-techniques. More refined methods have to be used [2].

If the concept of discrepancy is not based on balls, but on the homothetic images of some fixed set K, then the method to derive upper bounds for energy has to be modified:

In what follows, $c_1, c_2, \ldots$ denote positive constants, depending at most on K, d, c, and M. Let $1 \geqslant \delta > 0$. A precise value for δ will be specified later. By (4),

$$\begin{aligned} &C(K,s,d)^{-1}\, E_s(\mu - v) \\ &\quad = \left\{\int_0^\delta + \int_\delta^1 + \int_1^\infty\right\} \int_{SO(d)} \int_{\mathbb{R}^d} [(\mu - v)(z + rU(K))]^2 \, d\lambda^d(x)\, dH(U)\, \frac{dr}{r^{d+1+s}} \\ &\quad =: I_1(\delta) + I_2(\delta) + I_3. \end{aligned} \tag{18}$$

Now, since

$$\lambda^d((x + rU(K)) \cap (y + rU(K))) \begin{cases} = 0, & \text{if } |x-y| \geqslant 2\, diam(K) r, \\ \leqslant \lambda^d(K) r^d, & \text{otherwise,} \end{cases}$$

and taking into account (12), it follows that

$$\begin{aligned} I_1(\delta) &= \int_0^\delta \int_{SO(d)} \int \int \lambda^d((x+rU(K))\cap(y+rU(K))) \\ &\qquad \times d(\mu-\nu)\, d(\mu-\nu)\, dH(U)\, \frac{dr}{r^{d+1+s}} \\ &\leqslant \int_0^\delta \int \int_{|x-y|\leqslant c_2 r} c_1 r^d\, d(\mu+\nu)(y)\, d(\mu+\nu)(x)\, \frac{dr}{r^{d+1+s}} \\ &\leqslant \frac{c_3}{\beta-s}\,\delta^{\beta-s}. \end{aligned} \tag{19}$$

Moreover, since

$$[(\mu-\nu)(z+rU(K))]^2 \begin{cases} =0, & \text{if } |z|\geqslant diam(M)+diam(K)r, \\ \leqslant D_K[\mu,\nu]^2, & \text{otherwise}, \end{cases}$$

we have

$$\begin{aligned} I_2(\delta) &\leqslant \int_\delta^1 \int_{|z|\leqslant c_4} D_K[\mu,\nu]^2\, d\lambda^d(z)\, \frac{dr}{r^{d+1+s}} \\ &\leqslant \frac{c_5}{d+s}\,\delta^{-d-s}\, D_K[\mu,\nu]^2. \end{aligned} \tag{20}$$

In addition,

$$\begin{aligned} I_3 &\leqslant \int_1^\infty \int_{|z|\leqslant c_5 r} D_K[\mu,\nu]^2\, d\lambda^d(z)\, \frac{dr}{r^{d+1+s}} \\ &\leqslant \frac{c_6}{s}\, D_K[\mu,\nu]^2. \end{aligned} \tag{21}$$

Combining (18)–(21) it follows that

$$E_s(\mu-\nu)\leqslant c_7\left(\frac{\delta^{\beta-s}}{\beta-s}+\frac{\delta^{-d-s}}{d+s}D_K[\mu,\nu]^2+\frac{1}{s}D_K[\mu,\nu]^2\right).$$

Inserting $\delta := D_K[\mu,\nu]^{2/(\beta+d)}$ we arrive at

Proposition 14. *Suppose ν and μ are unit measures with support in a compact set M, satisfying* (12) *with $\beta>s$. Then there exists a constant $C_0 = C_0(K,M,c,\beta,s,d)$ such that*

$$E_s(\mu-\nu)\leqslant C_0 D_K[\mu,\nu]^{2\frac{\beta-s}{d+\beta}}.$$

Remark. Suppose that in the situation of Proposition 14 the support of the measures μ and ν is such that

$$\lambda^d(\{x\in\mathbb{R}^d \mid dist(x,M)\leqslant r\})\leqslant c_8 r^p \quad (0<r\leqslant 1)$$

as, for instance, in the case when μ and ν are concentrated on a sufficiently smooth, closed, bounded, $(d-p)$-dimensional hypersurface in $\mathbb{R}^d$. Then $(\mu-\nu)(z+rU(K))=0$ if $dist(z,M)\geqslant c_8 r^p$ and, therefore, the estimate for $I_2(\delta)$ can be improved to

$$I_2(\delta)\leqslant \int_\delta^1 \int_{dist(z,M)\leqslant c_8 r^p} D_K[\mu,\nu]^2\, d\lambda^d(z)\, \frac{dr}{r^{d+1+s}}$$
$$\leqslant \frac{c_9}{d+s-p}\,\delta^{-d-s+p} D_K[\mu,\nu]^2.$$

Thus, with $\delta := D_K[\mu,\nu]^{2/(\beta+d-p)}$,

$$E_s(\mu-\nu)\leqslant C_1 D_K[\mu,\nu]^{2\frac{\beta-s}{(d-p)+\beta}},$$

where $C_1 = C_1(K,M,c,\beta,s,d,p)$.

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