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DISCRETE ENERGY ASYMPTOTICS ON A RIEMANNIAN CIRCLE

Johann S. Brauchart∗, Douglas P. Hardin†, and Edward B. Saff†

ABSTRACT. We derive the complete asymptotic expansion in terms of powers of N for the geodesic f-energy of N equally spaced points on a rectifiable simple closed curve Γ in $\mathbb{R}^p$, $p \geq 2$, as $N \to \infty$. For f decreasing and convex, such a point configuration minimizes the f-energy $\sum_{j \neq k} f(d(\mathbf{x}_j, \mathbf{x}_k))$, where d is the geodesic distance (with respect to Γ) between points on Γ. Completely monotonic functions, analytic kernel functions, Laurent series, and weighted kernel functions f are studied. Of particular interest are the geodesic Riesz potential $1/d^s$ ($s \neq 0$) and the geodesic logarithmic potential $\log(1/d)$. By analytic continuation we deduce the expansion for all complex values of s.

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1. Introduction

Throughout this article, Γ is a *Riemannian circle* (that is, a rectifiable simple closed curve in $\mathbb{R}^p$, $p \geq 2$) with length $|\Gamma|$ and associated (Lebesgue) arclength measure $\sigma = \sigma_\Gamma$. Choosing an orientation for Γ, we denote by $\ell(\mathbf{x}, \mathbf{y})$ the length of the arc of Γ from $\mathbf{x}$ to $\mathbf{y}$, where $\mathbf{x}$ precedes $\mathbf{y}$ on Γ. Thus $\ell(\mathbf{x}, \mathbf{y}) + \ell(\mathbf{y}, \mathbf{x}) = |\Gamma|$ for all $\mathbf{x}, \mathbf{y} \in \Gamma$. The *geodesic distance* $\mathrm{d}(\mathbf{x}, \mathbf{y})$ between $\mathbf{x}$ and $\mathbf{y}$ on Γ is given by

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the length of the shorter arc connecting $\mathbf{x}$ and $\mathbf{y}$; that is,

$$\mathrm{d}(\mathbf{x},\mathbf{y}) := \mathrm{d}_\Gamma(\mathbf{x},\mathbf{y}) := \min\{\ell(\mathbf{x},\mathbf{y}),\ell(\mathbf{y},\mathbf{x})\} = \frac{|\Gamma|}{2} - \left|\ell(\mathbf{x},\mathbf{y}) - \frac{|\Gamma|}{2}\right|. \tag{1}$$

The geodesic distance between two points on Γ can be at most $|\Gamma|/2$.

We remark that it would be sufficient to study the Euclidean circle with its arclength metric; however, for the purpose of emphasizing that our results hold as well for geodesic distances on a closed curve, we state them for the Riemannian circle.

Given a lower semicontinuous function $f : [0, |\Gamma|/2] \to \mathbb{R} \cup \{+\infty\}$, the discrete f-energy problem is concerned with properties of N point systems $\mathbf{z}^*_{1,N}, \dots, \mathbf{z}^*_{N,N}$ on Γ ($N \geq 2$) that minimize the f-energy functional

$$G_f(\mathbf{x}_1, \dots, \mathbf{x}_N) := \sum_{j \neq k} f(\mathrm{d}(\mathbf{x}_j, \mathbf{x}_k)) := \sum_{j=1}^{N} \sum_{\substack{k=1 \\ j \neq k}}^{N} f(\mathrm{d}(\mathbf{x}_j, \mathbf{x}_k)), \tag{2}$$

over all N point configurations ω_N of not necessarily distinct points $\mathbf{x}_1, \dots, \mathbf{x}_N$ on Γ. The following result asserts that equally spaced points (with respect to arclength) on Γ are minimal f-energy point configurations for a large class of functions f.

Proposition 1. *Let $f : [0, |\Gamma|/2] \to \mathbb{R} \cup \{+\infty\}$ be a lower semicontinuous function.*

(A) *If f is convex and decreasing, then the geodesic f-energy of N points on Γ attains a global minimum at N equally spaced points on Γ. If f is strictly convex, then these are the only configurations that attain a global minimum.*

(B) *If f is concave and decreasing, then the geodesic f-energy of N points on Γ attains a global minimum at antipodal systems ω_N with $\lceil N/2 \rceil$ points at $\mathbf{p}$ and $\lfloor N/2 \rfloor$ points at $\mathbf{q}$, where $\mathbf{p}$ and $\mathbf{q}$ are any pair of points on Γ with geodesic distance $|\Gamma|/2$. If f is strictly concave, then these are the only configurations that attain a global minimum.*

Part (A) of Proposition 1 follows from a standard "winding number argument" that can be traced back to the work of Fejes Tóth [15]. The result in the general form stated here appears explicitly in the work of M. Götz [17, Proposition 9] who uses a similar notion of "orbits." For completeness, we present in Section 4 a brief proof of Part (A).

Remark. Alexander and Stolarsky [2] studied the discrete and continuous energy problem for continuous kernel functions f on compact sets. In particular, they established the optimality of vertices of a regular N-gon circumscribed by a circle

$\mathcal{C}_a$ of radius a for various non-Euclidean metrics $\rho(\mathbf{x},\mathbf{y})$ (including the geodesic metric) with respect to an energy functional $E_{\sigma,\lambda}(\mathbf{x}_1,\dots,\mathbf{x}_N):=\sigma([\rho(\mathbf{x}_j,\mathbf{x}_k)]^\lambda)$, $0<\lambda\leq 1$, on $\mathcal{C}_a$ where σ is an elementary symmetric function on $\binom{n}{2}$ real variables. This result does not extend to the complete class of functions in Proposition 1 and vice versa. However, both cover the generalized sum of geodesic distances problem.

In the case of Riesz potentials we set

$$f_s(x):=-x^{-s},\quad s<0,\qquad f_0(x):=\log(1/x),\qquad f_s(x):=x^{-s},\quad s>0.$$

Then Proposition 1(A) asserts that equally spaced points are unique (up to translation along the simple closed curve Γ) optimal *geodesic f_s-energy* points for $s>-1$. (For $s>0$ this fact is also proved in the dissertation of S. Borodachov [6, Lemma V.3.1], see also [7].) Proposition 1(B) shows that for $s<-1$ and $N\geq 3$, antipodal configurations are optimal f_s-energy points, but equally spaced points are **not**. (We remark that if *Euclidean* distance is used instead of geodesic distance, then the N-th roots of unity on the unit circle cease to be optimal f_s-energy points when $s<-2$, cf. [5] and [10].)

For $s=-1$ in the geodesic case, equally spaced points are optimal but so are antipodal and other configurations. Fejes Tóth [16] showed that a configuration on the unit circle is optimal with respect to the *sum of geodesic distances** ($s=-1$) if and only if the system is centrally symmetric for an even number of points and, for an odd number of points, it is the union of a centrally symmetric set and a set $\{\mathbf{x}_1,\dots,\mathbf{x}_{2k+1}\}$ such that each half circle determined by $\mathbf{x}_j$ ($j=1,\dots,2k+1$) contains k of the points in its interior. (This result is reproved in [20].) These criteria easily carry over to Riemannian circles. In particular, any system of N equally spaced points on Γ and any antipodal system on Γ satisfy these criteria.

Remark. Equally spaced points on the unit circle are also *universally optimal* in the sense of Cohn and Kumar [11]; that is, they minimize the energy functional $\sum_{j\neq k} f(|\mathbf{x}_j-\mathbf{x}_k|^2)$ for any *completely monotonic* potential function f; that is, for a function f satisfying $(-1)^k f^{(k)}(x)>0$ for all integers $k\geq 0$ and all $x\in[0,2]$.

To determine the leading term in the energy asymptotics it is useful to consider the continuous energy problem. Let $\mathfrak{M}(\Gamma)$ denote the class of Borel probability measures supported on Γ. The *geodesic f-energy* of $\mu\in\mathfrak{M}(\Gamma)$ and the

*The analogue problem for the *sum of (Euclidean) distances* on the unit circle was also studied by Fejes Tóth [15] who proved that only (rotated copies) of the N-th roots of unity are optimal.

minimum geodesic f-energy of Γ are defined, respectively, as

$$\mathcal{I}_f^g[\mu] := \int\int f(\mathrm{d}(\mathbf{x},\mathbf{y}))\, d\mu(\mathbf{x})\, d\mu(\mathbf{y}), \qquad V_f^g(\Gamma) := \inf\left\{\mathcal{I}_f^g[\mu] : \mu \in \mathfrak{M}(\Gamma)\right\}.$$

The *continuous f-energy problem* concerns the existence, uniqueness, and characterization of a measure μ_Γ satisfying $V_f^g(\Gamma) = \mathcal{I}_f^g[\mu_\Gamma]$. If such a measure exists, it is called an *equilibrium measure on* Γ.

Proposition 2. *Let f be a Lebesgue integrable lower semicontinuous function on $[0, |\Gamma|/2]$ and convex and decreasing on $(0, |\Gamma|/2]$. Then the normalized arclength measure σ_Γ is an equilibrium measure on Γ and*

$$\lim_{N\to\infty} G_f(\omega_N^{(f)})/N^2 = V_f^g(\Gamma). \tag{3}$$

If, in addition, f is strictly decreasing, then σ_Γ is unique.

The proofs of the propositions in this introduction are given in Section 4.

Note that (3) provides the first term in the asymptotic expansion of $G_f(\omega_N^{(f)})$ for large N; that is, $G_f(\omega_N^{(f)}) \sim V_f^g(\Gamma)\, N^2$ as $N \to \infty$. The goal of the present paper is to extend this asymptotic expansion to an arbitrary number of terms. The case when $\lim_{N\to\infty} G_f(\omega_N^{(f)})/N^2 \to \infty$ as $N \to \infty$ is also studied. For a certain class of functions f, satisfying $x^{s_0}\, f(z) \to a_0$ as $x \to 0^+$ for some $s_0 > 1$ and finite a_0, it turns out that the leading term is of the form $a_0 2\, \zeta(s_0) |\Gamma|^{-s_0} N^{1+s_0}$, where $\zeta(s)$ is the classical Riemann zeta function. However, such a leading term might even not exist. Indeed, if the function f has an essential singularity at 0 and is otherwise analytic in a sufficiently large annulus centered at zero, then the asymptotics of the geodesic f-energy of equally spaced points on Γ contains an infinite series part with rising positive powers of N determined by the principal part of the Laurent expansion of f at 0. Consequently, there is no "highest power of N", see Examples 11 and 12 below.

An outline of our paper is as follows. In Section 2, the geodesic f-energy of equally spaced points on Γ is investigated. In particular, completely monotonic functions, analytic kernel functions, Laurent series, and weighted kernel functions f are considered. Illustrative examples complement this study. In Section 3, the geodesic logarithmic energy and the geodesic Riesz s-energy of equally spaced points on Γ are studied. The results are compared with their counterparts when $\mathrm{d}(\cdot,\cdot)$ is replaced by the Euclidean metric. The proofs of the results are given in Section 4.

2. The geodesic f-energy of equally spaced points on Γ

Definition 3. Given a kernel function $f : [0, |\Gamma|/2] \to \mathbb{C} \cup \{+\infty\}$, the *discrete geodesic f-energy* of N equally spaced points $\mathbf{z}_{1,N}, \dots, \mathbf{z}_{N,N}$ on Γ is denoted by

$$\mathcal{M}(\Gamma, f; N) := \sum_{j \neq k} f(\mathrm{d}(\mathbf{z}_{j,N}, \mathbf{z}_{k,N})) = N \sum_{j=1}^{N-1} f(\mathrm{d}(\mathbf{z}_{j,N}, \mathbf{z}_{N,N})).$$

Set $N = 2M + \kappa$ ($\kappa = 0, 1$). Using the fact that the points are equally spaced, it can be easily shown that

$$\mathcal{M}(\Gamma, f; N) = 2N \sum_{n=1}^{\lfloor N/2 \rfloor} f(n\, |\Gamma| / N) - (1 - \kappa)\, f(|\Gamma| / 2) N. \tag{4}$$

An essential observation is that the geodesic f-energy has (when expressed in terms of powers of N) different asymptotics for even N and odd N. We remark that for real-valued functions f a configuration of equally spaced points is optimal with respect to the geodesic f-energy defined in (2), whenever f satisfies the hypotheses of Proposition 1(A).

An application of the generalized Euler-MacLaurin summation formula (see Proposition 20 below) yields an exact formula for $\mathcal{M}(\Gamma, f; N)$ in terms of powers of N. The asymptotic analysis of this expression motivates the following definition.

Definition 4. A function $f : [0, |\Gamma|/2] \to \mathbb{C} \cup \{+\infty\}$ is called *admissible* if the following holds:

(i) f has a continuous derivative of order $2p + 1$ on the interval $(0, |\Gamma|/2]$;

(ii) there exists a function $S_q(x)$ of the form $S_q(x) = \sum_{n=0}^{q} a_n\, x^{-s_n}$, where a_n and s_n ($n = 0, \dots, q$) are complex with $\operatorname{Re} s_0 > \operatorname{Re} s_1 > \cdots > \operatorname{Re} s_q$ [†] and $\operatorname{Re} s_q + 2p > 0$ or $s_q = -2p$ such that for some $\delta > 0$

  (a) $1 - \operatorname{Re} s_q + \delta > 0$,

  (b) $\displaystyle\int_0^x \{f(y) - S_q(y)\}\, dy = \mathcal{O}(x^{1+\delta-s_q})$ as $x \to 0^+$,

  (c) $\{f(x) - S_q(x)\}^{(\nu)} = \mathcal{O}(x^{\delta - s_q - \nu})$ as $x \to 0^+$ for all $\nu = 0, 1, \dots, 2p{+}1$.

For $p \geq 1$ an integer the following sum arises in the main theorems describing the asymptotics of $\mathcal{M}(\Gamma, f; N)$: Let $N = 2M + \kappa$, $\kappa = 0, 1$. Then

$$\mathcal{B}_p(\Gamma, f; N) := \frac{2}{|\Gamma|} N^2 \sum_{n=1}^{p} \frac{B_{2n}(\kappa/2)}{(2n)!} \left(|\Gamma| / N\right)^{2n} f^{(2n-1)}(|\Gamma| / 2), \tag{5}$$

[†] The powers in $S_q(x)$ are principal values.

where $B_m(x)$ denotes the Bernoulli polynomial of degree m defined by

$$\frac{z}{e^z - 1} e^{xz} = \sum_{m=0}^{\infty} \frac{B_m(x)}{m!} z^m, \qquad B_m(x) = \sum_{k=0}^{m} \binom{m}{k} B_{m-k} x^k,$$

where $B_0 = 1$, $B_1 = -1/2, \dots,$ are the so-called *Bernoulli numbers*. Recall that $B_{2k+1} = 0$, $(-1)^{k-1} B_{2k} > 0$ for $k = 1, 2, 3, \dots,$ and $B_n(1/2) = (2^{1-n} - 1) B_n$ for $n \geq 0$ ([1]).

Theorem 5 (general case)**.** *Let f be admissible in the sense of Definition 4 and suppose none of $s_0, s_1, \dots, s_q$ equals 1. Then, for $N = 2M + \kappa$ with $\kappa = 0$ or $\kappa = 1$,*

$$\mathcal{M}(\Gamma, f; N) = V_f(\Gamma)\, N^2 + \sum_{n=0}^{q} a_n \frac{2\,\zeta(s_n)}{|\Gamma|^{s_n}} N^{1+s_n} + \mathcal{B}_p(\Gamma, f; N) + \mathfrak{R}_p(\Gamma, f; N), \tag{6}$$

where

$$V_f(\Gamma) = \frac{2}{|\Gamma|} \sum_{n=0}^{q} a_n \frac{(|\Gamma|/2)^{1-s_n}}{1 - s_n} + \frac{2}{|\Gamma|} \int_0^{|\Gamma|/2} (f - S_q)(x)\, dx. \tag{7}$$

The remainder term satisfies $\mathfrak{R}_p(\Gamma, f; N) = \mathcal{O}(N^{1-2p}) + \mathcal{O}(N^{1-\delta+s_q})$ as $N \to \infty$ if $2p \neq \delta - \operatorname{Re} s_q$, whereas $\mathfrak{R}_p(\Gamma, f; N) = \mathcal{O}(N^{1-2p} \log N)$ if $2p = \delta - \operatorname{Re} s_q$.

The next result involves the *Euler-Mascheroni constant* defined by

$$\gamma := \lim_{n \to \infty} \left(1 + \frac{1}{2} + \frac{1}{3} + \frac{1}{4} + \dots + \frac{1}{n} - \log n \right).$$

Theorem 6 (exceptional case)**.** *Let f be admissible in the sense of Definition 4 and $s_{q'} = 1$ for some $1 \leq q' \leq q$.*[‡] *Then, for $N = 2M + \kappa$ with $\kappa = 0$ or $\kappa = 1$,*

$$\begin{aligned} \mathcal{M}(\Gamma, f; N) = {} & \frac{2}{|\Gamma|} a_{q'}\, N^2 \log N + V_f(\Gamma)\, N^2 + \sum_{\substack{n=0,\\ n \neq q'}}^{q} a_n \frac{2\,\zeta(s_n)}{|\Gamma|^{s_n}} N^{1+s_n} \\ & + \mathcal{B}_p(\Gamma, f; N) + \mathfrak{R}_p(\Gamma, f; N), \end{aligned}$$

where

$$V_f(\Gamma) = \frac{2}{|\Gamma|} \left\{ \sum_{\substack{n=0,\\ n \neq q'}}^{q} a_n \frac{(|\Gamma|/2)^{1-s_n}}{1 - s_n} + \int_0^{|\Gamma|/2} (f - S_q)(x)\, dx - a_{q'} (\log 2 - \gamma) \right\}. \tag{8}$$

The remainder term satisfies $\mathfrak{R}_p(\Gamma, f; N) = \mathcal{O}(N^{1-2p}) + \mathcal{O}(N^{1-\delta+s_q})$ as $N \to \infty$ if $2p \neq \delta - \operatorname{Re} s_q$, whereas $\mathfrak{R}_p(\Gamma, f; N) = \mathcal{O}(N^{1-2p} \log N)$ if $2p = \delta - \operatorname{Re} s_q$.

[‡] By Definition 4 there is only one such $s_{q'}$.

Remark. Both Theorems 5 and 6 show that only the coefficients of the nonpositive even powers of N depend on the parity of N. These dependencies appear in the sum $\mathcal{B}_p(\Gamma, f; N)$.

Remark. If $f(z) \equiv S_q(z) = \sum_{n=0}^{q} a_n z^{-s_n}$ for some q and $\operatorname{Re} s_0 > \cdots > \operatorname{Re} s_q$, then all expressions in Theorems 5 and 6 containing $f - S_q$ vanish. In general, the remainder term $\mathfrak{R}_p(\Gamma, f; N)$ is of order $\mathcal{O}(N^{1-2p})$, where the integer p satisfies $\operatorname{Re} s_q + 2p > 0$. In particular, this holds for the Riesz kernels (cf. Theorems 17 and 19 below).

Completely monotonic functions

A non-constant *completely monotonic* function $f : (0, \infty) \to \mathbb{R}$ has derivatives of all orders and satisfies $(-1)^k f^{(k)}(x) > 0$ (cf. [13]).[§] In particular, it is a continuous strictly decreasing convex function. Therefore, by Proposition 1, equally spaced points are optimal f-energy configurations on the Riemannian circle Γ.

By Bernstein's theorem [31, p. 161] a function is completely monotonic on $(0, \infty)$ if and only if it is the Laplace transformation $f(x) = \int_0^\infty e^{-xt} \, d\mu(t)$ of some nonnegative measure μ on $[0, \infty)$ such that the integral converges for all $x > 0$.

The following result applies in particular to completely monotonic functions.

Theorem 7. *Let f be the Laplace transform $f(x) = \int_0^\infty e^{-xt} \, d\mu(t)$ for some signed Borel measure μ on $[0, \infty)$ such that $\int_0^\infty t^m \, d|\mu|(t)$, $m = 0, 1, 2, \dots,$ are all finite. Then for all integers $p \geq 1$ and $N = 2M + \kappa$ with $\kappa = 0, 1$*

$$\mathcal{M}(\Gamma, f; N) = \left\{ \frac{2}{|\Gamma|} \int_0^\infty \frac{1 - e^{-t|\Gamma|/2}}{t} \, d\mu(t) \right\} N^2 + \sum_{n=0}^{2p} (-1)^n \frac{\mu_n}{n!} \frac{2\,\zeta(-n)}{|\Gamma|^{-n}} N^{1-n} + \mathcal{B}_p(\Gamma, f; N) + \mathcal{O}(N^{1-2p}),$$

where $\mu_m := \int_0^\infty t^m \, d\mu(t)$ denotes the m-th moment of μ.

Remark. The derivation of the (complete) asymptotic expansion for $\mathcal{M}(\Gamma, f; N)$ as $N \to \infty$ for Laplace transforms for which not all moments μ_m are finite, depends on more detailed knowledge of the behavior of $f(x)$ near the origin. For example, for integral transforms $G(x) = \int_0^\infty h(xt) g(t) \, dt$ there is a well-established theory of the asymptotic expansion of $G(x)$ at 0^+. See, [18], [19], [4] or [25] and [14]. These expansions give rise to results similar to our theorem above.

[§]A completely monotonic function on $(0, \infty)$ is necessarily analytic in the positive half-plane ([31]).

Remark. Recently, Koumandos and Pedersen [22] studied so-called *completely monotonic functions of integer order* $r \geq 0$; that is, functions f for which $x^r f(x)$ is completely monotonic. The completely monotonic functions of order 0 are the classical completely monotonic functions; those of order 1 are the so-called *strongly completely monotonic functions* satisfying that $(-1)^k x^{k+1} f^{(k)}(x)$ is non-negative and decreasing on $(0, \infty)$. In [22] it is shown that f is completely monotonic of order $\alpha > 0$ (α real) if and only if f is the Laplace transformation of a fractional integral of a positive Radon measure on $[0, \infty)$; that is,

$$f(x) = \int_0^\infty e^{-xt} \mathcal{J}_\alpha[\mu](t) \, dt, \qquad \mathcal{J}_\alpha[\mu](t) := \frac{1}{\Gamma(\alpha)} \int_0^t (t-s)^{\alpha-1} \, d\mu(s).$$

Results similar to Theorem 7 hold for these kinds of functions. However, the problem of giving an asymptotic expansion of $f(x)$ near the origin is more subtle.

Analytic kernel functions

If f is analytic in a disc with radius $|\Gamma|/2 + \varepsilon$ ($\varepsilon > 0$) centered at the origin, then f is admissible in the sense of Definition 4 and we have the following result.

Theorem 8. *Let $f(z) = \sum_{n=0}^\infty a_n z^n$ be analytic in $|z| < |\Gamma|/2 + \varepsilon$, $\varepsilon > 0$. Then for $N = 2M + \kappa$ with $\kappa = 0$ or $\kappa = 1$*

$$\mathcal{M}(\Gamma, f; N) = \left\{ \frac{2}{|\Gamma|} \int_0^{|\Gamma|/2} f(x) \, dx \right\} N^2 + \sum_{n=0}^{2p} a_n \frac{2\,\zeta(-n)}{|\Gamma|^{-n}} N^{1-n} + \mathcal{B}_p(\Gamma, f; N) + \mathcal{O}_{p,|\Gamma|,f}(N^{1-2p}).$$

Note that $\zeta(0) = -1/2$ and $\zeta(-2k) = 0$ for $k = 1, 2, 3, \dots$.

Example 9. If $f(x) = e^{-x}$, then for any positive integer p:

$$\mathcal{M}(\Gamma, f; N) = \frac{2}{|\Gamma|} \left(1 - e^{-|\Gamma|/2} \right) N^2 - N + \sum_{n=1}^{p} \frac{1}{(2n-1)!} \frac{2\,\zeta(1-2n)}{|\Gamma|^{1-2n}} N^{2-2n} - \sum_{n=1}^{p} \frac{B_{2n}(\kappa/2)}{(2n)!} \frac{2e^{-|\Gamma|/2}}{|\Gamma|^{1-2n}} N^{2-2n} + \mathcal{O}_{p,|\Gamma|,f}(N^{1-2p})$$

as $N = 2M + \kappa \to \infty$, where the notation of the last term indicates that the $\mathcal{O}$-constant depends on $p, |\Gamma|$ and f. Since $f(x)$ is a strictly decreasing convex function, by Proposition 1(A), equally spaced points are also optimal f-energy points. Thus, the relation above gives the complete asymptotics for the optimal N-point geodesic $e^{-(\cdot)}$-energy on Riemannian circles.

Laurent series kernels

If $f(z)$ is analytic in the annulus $0 < |z| < |\Gamma|/2 + \varepsilon$ ($\varepsilon > 0$) with a pole at $z = 0$, then f is admissible in the sense of Definition 4 and we obtain the following result.

Theorem 10. *Let f be analytic in the annulus $0 < |z| < |\Gamma|/2 + \varepsilon$ ($\varepsilon > 0$) having there the Laurent series expansion $f(z) = \sum_{n=-K}^{\infty} a_n z^n$, $K \geq 1$.*

(i) *If the residue $a_{-1} = 0$, then for $N = 2M + \kappa$ with $\kappa = 0, 1$*

$$\mathcal{M}(\Gamma, f; N) = V_f(\Gamma)\, N^2 + \sum_{\substack{n=-K,\\ n\neq -1}}^{2p} a_n \frac{2\,\zeta(-n)}{|\Gamma|^{-n}} N^{1-n} + \mathcal{B}_p(\Gamma, f; N) + \mathcal{O}_{p,|\Gamma|,f}(N^{1-2p}),$$

where the coefficient of N^2 is

$$V_f(\Gamma) = \frac{2}{|\Gamma|} \sum_{n=-K}^{\infty} a_n \frac{(|\Gamma|/2)^{1+n}}{1+n}.$$

(ii) *If the residue $a_{-1} \neq 0$, then for $N = 2M + \kappa$ with $\kappa = 0, 1$*

$$\mathcal{M}(\Gamma, f; N) = \frac{2}{|\Gamma|} a_{-1}\, N^2 \log N + V_f(\Gamma)\, N^2 + \sum_{\substack{n=-K,\\ n\neq -1}}^{2p} a_n \frac{2\,\zeta(-n)}{|\Gamma|^{-n}} N^{1-n} + \mathcal{B}_p(\Gamma, f; N) + \mathcal{O}_{p,|\Gamma|,f}(N^{1-2p}),$$

where the coefficient of N^2 is

$$V_f(\Gamma) = \frac{2}{|\Gamma|} \left\{ \sum_{\substack{n=-K,\\ n\neq -1}}^{\infty} a_n \frac{(|\Gamma|/2)^{1+n}}{1+n} - a_{-1}\,(\log 2 - \gamma) \right\}.$$

Next, we give two examples of kernels f each having an essential singularity at 0. Such kernels can also be treated in the given framework, since they satisfy an extended version of Definition 4; see Proof of Examples 11 and 12 in Section 4.

Example 11. Let $f(x) = e^{1/x} = \sum_{n=0}^{\infty} 1/(n!x^n)$, $x \in (0, +\infty)$, $f(0) = +\infty$. We define the entire function

$$F(z) := \sum_{n=2}^{\infty} \frac{\zeta(n)}{n!} z^n = -\gamma z - \frac{1}{2\pi i} \oint_{|w|=\rho<1} e^{z/w}\, \psi(1-w)\, dw, \qquad z \in \mathbb{C},$$

where $\psi(z)$ denotes the digamma function and we observe that, because of $0 < \zeta(n) - 1 < c2^{-n}$ for all integers $n \geq 2$ for some $c > 0$,

$$F(x) = e^x - 1 - x + \sum_{n=2}^{\infty} \frac{\zeta(n) - 1}{n!} x^n = e^x + \mathcal{O}(e^{x/2}) \qquad \text{as } x \to \infty.$$

Then

$$\begin{aligned}\mathcal{M}(\Gamma, f; N) &= 2N F(N/|\Gamma|) + \frac{2}{|\Gamma|} N^2 \log N + V_f(\Gamma)\, N^2 - N \\ &\quad + \sum_{n=1}^{p} \frac{2 B_{2n}(\kappa/2)}{(2n)!\, |\Gamma|^{1-2n}} N^{2-2n} f^{(2n-1)}(|\Gamma|/2) + \mathcal{O}_{p,|\Gamma|,f}(N^{1-2p}),\end{aligned}$$

where

$$\begin{aligned}V_f(\Gamma) &= 1 + \frac{2}{|\Gamma|} \sum_{n=2}^{\infty} \frac{1}{n!} \frac{(|\Gamma|/2)^{1-n}}{1-n} - \frac{2}{|\Gamma|} (\log 2 - \gamma) \\ &= e^{2/|\Gamma|} - \frac{2}{|\Gamma|} \left\{1 - 2\gamma + \log |\Gamma| + \mathrm{Ei}(2/|\Gamma|)\right\},\end{aligned}$$

where $\mathrm{Ei}(x) = -\int_{-x}^{\infty} e^{-t} t^{-1}\, dt$ is the exponential integral (taking the Cauchy principal value of the integral). In particular it follows that

$$\lim_{N\to\infty} \frac{\mathcal{M}(\Gamma, f; N)}{N\, e^{N/|\Gamma|}} = 2.$$

Since f is a strictly decreasing convex function on $(0, \infty)$, by Proposition 1(A), equally spaced points are also optimal. Thus, the above expansion gives the asymptotics of the optimal N-point $e^{1/(\cdot)}$-energy.

Example 12. Let $\mathrm{J}_k(\lambda) = (-1)^k\, \mathrm{J}_{-k}(\lambda) := \frac{1}{2\pi} \int_0^{2\pi} \cos(k\theta - \lambda \sin\theta)\, d\theta$ denote the *Bessel function of the first kind of order* k whose generating function relation is given by (cf. [28, Exercise 5.5(10)])

$$f(x) = \exp\left[\frac{\lambda}{2}\left(x - \frac{1}{x}\right)\right] = \sum_{n=-\infty}^{\infty} \mathrm{J}_n(\lambda) x^n \qquad \text{for } |x| > 0.$$

For integers $m \geq 2$ we define the entire functions

$$F_m(z) := \sum_{n=m}^{\infty} \mathrm{J}_{-n}(\lambda)\, \zeta(n) z^n = \sum_{k=1}^{\infty} G_m(z/k), \quad G_m(z) := \sum_{n=m}^{\infty} \mathrm{J}_{-n}(\lambda) z^n, \quad z \in \mathbb{C}.$$

If λ is a zero of the Bessel function J_{-1}, then for positive integers p and $m \geq 2$ there holds

$$\begin{aligned}\mathcal{M}(\Gamma, f; N) = 2NF_m(N/|\Gamma|) &+ 2\sum_{n=2}^{m-1} \mathrm{J}_{-n}(\lambda)\,\zeta(n)\,|\Gamma|^{-n} N^{1+n} \\ &+ V_f(\Gamma)\,N^2 + |\Gamma|\,B_2(\frac{\kappa}{2}) f'(|\Gamma|/2) \\ &+ \sum_{n=2}^{p} \left\{ \frac{2B_{2n}}{2n} \frac{f^{2n-1}(|\Gamma|/2)}{(2n-1)!} + 2\,\mathrm{J}_{2n-1}(\lambda)\,\zeta(1-2n) \right\} |\Gamma|^{2n-1} N^{2-2n} \\ &+ \mathcal{O}(N^{1-2p})\end{aligned}$$

where

$$V_f(\Gamma) = \frac{2}{|\Gamma|} \sum_{\substack{n=-\infty,\\ n\neq\pm1}}^{\infty} \mathrm{J}_n(\lambda) \frac{(|\Gamma|/2)^{1+n}}{1+n}.$$

If, in addition, $\lambda < 0$, then $f(x)$ is a strictly decreasing convex function and, therefore, $\mathcal{M}(\Gamma, f; N)$ is also the minimal N-point f-energy on Γ and it follows from the observation

$$G_m(x/k) = \exp\left[-\frac{\lambda}{2}\left(\frac{x}{k} - \frac{k}{x}\right)\right] - \sum_{n=-\infty}^{m-1} J_n(\lambda)(-x/k)^n, \qquad k = 1, 2, 3, \dots,$$

that

$$\lim_{N\to\infty} \frac{\mathcal{M}(\Gamma, f; N)}{Nf(-N/|\Gamma|)} = 2.$$

If λ is not a zero of J_{-1}, then the above asymptotics must be modified to include a logarithmic term.

The *weighted* kernel function $f_s^w(x) = x^{-s} w(x)$

Given a weight function $w(x)$, the kernel $f_s^w(x) = x^{-s} w(x)$ gives rise to the so-called *geodesic weighted Riesz s-energy* of an N-point configuration $(\mathbf{x}_1, \dots, \mathbf{x}_N)$

$$G_s^w(\mathbf{x}_1, \dots, \mathbf{x}_N) := \sum_{j\neq k} \frac{w(\mathrm{d}(\mathbf{x}_j, \mathbf{x}_k))}{[\mathrm{d}(\mathbf{x}_j, \mathbf{x}_k)]^s}.$$

For the Euclidean metric the related weighted energy functionals are studied in [8].

If $w(x)$ is such that $f_s^w(x)$ is admissible in the sense of Definition 4, then Theorems 5 and 6 provide asymptotic expansions for the weighted geodesic Riesz s-energy of equally spaced points on a Riemannian circle Γ, which are also optimal configurations if $f_s^w(x)$ is strictly decreasing and convex (cf. Proposition 1(A)).

Theorem 13. *Let $w(z) = \sum_{n=0}^{\infty} a_n z^n$ be analytic in $|z| < |\Gamma|/2 + \varepsilon$, $\varepsilon > 0$. Set $f_s^w(z) := z^{-s} w(z)$. Then for integers $p, q > 0$ and $s \in \mathbb{C}$, s not an integer, such that $q - 2p < \operatorname{Re} s < 2 + q$ we have*

$$\mathcal{M}(\Gamma, f_s^w; N) = V_{f_s^w}(\Gamma)\, N^2 + \sum_{n=0}^{q} a_n \frac{2\,\zeta(s-n)}{|\Gamma|^{s-n}} N^{1+s-n} + \mathcal{B}_p(\Gamma, f_s^w; N) + \mathfrak{R}_p(\Gamma, f_s^w; N),$$

where $\mathcal{B}_p(\Gamma, f_s^w; N)$ is defined in (5). The coefficient of N^2 is the meromorphic continuation to $\mathbb{C}$ of the geodesic f_s^w-energy of Γ given by $(2/|\Gamma|) \int_0^{|\Gamma|/2} f_s^w(x)\, dx$ for $0 < s < 1$; that is,

$$V_{f_s^w}(\Gamma) = \frac{2}{|\Gamma|} \sum_{n=0}^{\infty} a_n \frac{(|\Gamma|/2)^{1+n-s}}{1+n-s}, \qquad s \neq 1, 2, 3, \dots.$$

The remainder $\mathfrak{R}_p(\Gamma, f_s^w; N)$ is of order $\mathcal{O}(N^{1-2p}) + \mathcal{O}(N^{s-2p})$ as $N \to \infty$.

Remark. For s is a positive integer the series $\sum_{n=0}^{\infty} a_n z^{n-s}$ is the Laurent expansion of $f(z)$ in $0 < |z| < |\Gamma|/2 + \varepsilon$ and Theorem 10 applies. For s is a non-positive integer the series $\sum_{n=0}^{\infty} a_n z^{n-s}$ is the power series expansion of $f(z)$ in $0 < |z| < |\Gamma|/2 + \varepsilon$ and Theorem 8 applies.

Example 14. Let $w(z) = \sin(z\pi/|\Gamma|)$. Then for $\operatorname{Re} s > 0$ not an integer

$$f_s^w(z) = z^{-s} w(z) = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)!} (\pi/|\Gamma|)^{2n+1} z^{2n+1-s}$$

and, by Theorem 13, the geodesic weighted Riesz s-energy of N equally spaced points has the asymptotic expansion ($0 < \operatorname{Re} s < 1 + 2p$)

$$\mathcal{M}(\Gamma, f_s^w; N) = V_{f_s^w}(\Gamma)\, N^2 + (\pi/|\Gamma|)^s \sum_{k=1}^{p} \frac{(-1)^{k-1}}{(2k-1)!} \frac{2\,\zeta(1+s-2k)}{\pi^{1+s-2k}} N^{2+s-2k} + \mathcal{B}_p(\Gamma, f_s^w; N) + \mathfrak{R}_p(\Gamma, f_s^w; N),$$

where $\mathcal{B}_p(\Gamma, f_s^w; N)$ is given in (5). The remainder $\mathfrak{R}_p(\Gamma, f_s^w; N)$ is of order $\mathcal{O}(N^{1-2p}) + \mathcal{O}(N^{s-2p})$ as $N \to \infty$ and

$$V_{f_s^w}(\Gamma) = \frac{2}{\pi} (|\Gamma|/\pi)^{-s} \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{(2k-1)!} \frac{(\pi/2)^{2k-s}}{2k-s}.$$

For $0 < s < 1$ we have

$$V_{f_s^w}(\Gamma) = \frac{2}{|\Gamma|} \int_0^{|\Gamma|/2} f_s^w(x)\, dx = \frac{\pi}{2} \frac{(|\Gamma|/2)^{-s}}{2-s}\, {}_1\mathrm{F}_2\!\left(\begin{matrix} 1-s/2 \\ 2-s/2, 3/2 \end{matrix}; -(\pi/4)^2 \right)$$

expressed in terms of a generalized ${}_1\mathrm{F}_2(;)$-hypergeometric function, which is analytic at s not an even integer. Hence, $V_{f_s^w}(\Gamma)$ is the meromorphic continuation to the complex plane of the integral $\frac{2}{|\Gamma|}\int_0^{|\Gamma|/2} f_s^w(x)\,dx$. We observe that for $s = 1/2$ we have $V_{f_s^w}(\Gamma) = 2\sqrt{2/|\Gamma|}\,\mathrm{S}(1)$, where $\mathrm{S}(u)$ is the Fresnel integral $\mathrm{S}(u) := \int_0^u \sin(x^2\pi/2)\,dx$.

As an application of the theorems of this section, we recover results recently given in [10] regarding the complete asymptotic expansion of the Euclidean Riesz s-energy $\mathcal{L}_s(N)$ of the N-th roots of unity on the unit circle $\mathbb{S}^1$ in the complex plane $\mathbb{C}$. Indeed, if $|z-w|$ denotes the Euclidean distance between two points ζ and z in $\mathbb{C}$, then from the identities $|z-\zeta|^2 = 2(1-\cos\psi) = 4[\sin(\psi/2)]^2$, where ψ denotes the angle "between" ζ and z on $\mathbb{S}^1$, we obtain the following relation between Euclidean and geodesic Riesz s-kernel:

$$|z-\zeta|^{-s} = |2\,(1-\cos\psi)|^{s/2} = \left|2\sin\frac{\psi}{2}\right|^s = \left|2\sin\frac{\mathrm{d}(\zeta,z)}{2}\right|^s, \qquad \zeta, z \in \mathbb{S}^1.$$

Thus, for $\zeta, z \in \mathbb{S}^1$ there holds

$$|z-\zeta|^{-s} = f_s^w(\mathrm{d}(\zeta,z)), \;\; w(x) := \left(\operatorname{sinc}\frac{x}{2}\right)^{-s}, \;\; f_s^w(x) = x^{-s}\operatorname{sinc}^{-s}(x/2), \quad (9)$$

where the "sinc" function, defined as $\operatorname{sinc} z = (\sin z)/z$ is an entire function that is non-zero for $|z| < \pi$ and hence, has a logarithm $g(z) = \log\operatorname{sinc} z$ that is analytic for $|z| < \pi$ (we choose the branch such that $\log\operatorname{sinc} 0 = 0$). The function $\operatorname{sinc}^{-s}(z/2) := \exp[-s\log\operatorname{sinc}(z/2)]$ is even and analytic on the unit disc $|z| < 2\pi$ and thus has a power series representation of the form

$$\operatorname{sinc}^{-s}(z/2) = \sum_{n=0}^{\infty} \alpha_n(s) z^{2n}, \quad |z| < 2\pi, \; s \in \mathbb{C}.$$

It can be easily seen that for $s > -1$ and $s \neq 0$ the function $(\operatorname{sgn} s) f_s^w(x)$ ¶ is a convex and decreasing function. Hence, application of Proposition 1(A) reproves the well-known fact that the N-th roots of unity and their rotated copies are the only optimal f_s^w-energy configurations for s in the range $(-1,0)\cup(0,\infty)$. (We remind the reader that, in contrast to the geodesic case, in the Euclidean case the N-th roots of unity are optimal for $s \geq -2$, $s \neq 0$, and they are unique up to rotation for $s > -2$, see discussion in [10].) The complete asymptotic expansion of $\mathcal{L}_s(N) = \mathcal{M}(\mathbb{S}^1, f_s^w; N)$ can be obtained from Theorem 13 if s is not an integer, from Theorem 10 if s is a positive integer, and from Theorem 8 if s is a negative integer. (We leave the details to the reader.) For $s \in \mathbb{C}$ with

¶The function $\operatorname{sgn} s$ denotes the sign of s. It is defined to be -1 if $s < 0$, 0 if $s = 0$, and 1 if $s > 0$.

$s \neq 0, 1, 3, 5, \dots$ and $q - 2p < \operatorname{Re} s < 2 + q$, the Euclidean Riesz s-energy for the N-th roots of unity is given by (cf. [10, Theorem 1.1])

$$\begin{aligned} \mathcal{L}_s(N) = V_s\, N^2 + \frac{2\,\zeta(s)}{(2\pi)^s} N^{1+s} + \sum_{n=1}^{q} \alpha_n(s) \frac{2\,\zeta(s-2n)}{(2\pi)^{s-2n}} N^{1+s-2n} \\ + \mathcal{O}(N^{1-2p}) + \mathcal{O}(N^{s-2p}) \end{aligned} \tag{10}$$

as $N \to \infty$, where (cf. [10])

$$V_s = \frac{2^{-s}\,\Gamma((1-s)/2)}{\sqrt{\pi}\,\Gamma(1-s/2)}, \qquad \alpha_n(s) = \frac{(-1)^n B_{2n}^{(s)}(s/2)}{(2n)!}, \quad n = 0, 1, 2, \dots. \tag{11}$$

Here, $B_n^{(\alpha)}(x)$ is the generalized Bernoulli polynomial, where $B_n(x) = B_n^{(1)}(x)$. Notice the absence of the term $\mathcal{B}_p(\Gamma, f_s^w; N)$, which follows from the fact that odd derivatives of $f_s^w(x)$ evaluated at π assume the value 0. (This can be seen, for example, from Faà di Bruno's differentiation formula.)

The entirety of positive odd integers s constitutes the class of exceptional cases regarding the Euclidean Riesz s-energy of the N-th roots of unity. For such s Theorem 10(ii) provides the asymptotic expansion of $\mathcal{L}_s(N) = \mathcal{M}(\mathbb{S}^1, f_s^w; N)$, which features an $N^2 \log N$ term as leading term. That is, for $s = 2L + 1$, $L = 0, 1, 2, \dots$, we have from Theorem 10(ii) that (cf. [10, Thm. 1.2])

$$\begin{aligned} \mathcal{L}_s(N) = \frac{\alpha_L(s)}{\pi} N^2 \log N + V_{f_s^w}(\mathbb{S}^1) N^2 \\ + \sum_{\substack{m=0, \\ m \neq L}}^{p+L} \alpha_m(s) \frac{2\,\zeta(s-2m)}{(2\pi)^{s-2m}} N^{1+s-2m} + \mathcal{O}(N^{1-2p}), \end{aligned} \tag{12}$$

where the coefficients $\alpha_m(s)$ are given in (11) and

$$V_{f_s^w}(\mathbb{S}^1) = \frac{1}{\pi} \left\{ \sum_{\substack{m=0, \\ m \neq L}}^{\infty} \alpha_m(s) \frac{\pi^{2m+1-s}}{2m+1-s} - \alpha_L(s) \left(\log 2 - \gamma \right) \right\}.$$

We remark that in [10, Thm. 1.2] we also give a computationally more accessible representation of $V_{f_s^w}(\mathbb{S}^1)$. The appearance of the $N^2 \log N$ terms can be understood on observing that the constant V_s in (10) has its simple poles at positive odd integers s and when using a limit process as $s \to K$ (K a positive odd integer) in (10), the simple pole at $s = K$ need to be compensated by the simple pole of the Riemann zeta function in the coefficient of an appropriate lower-order term. This interplay produces eventually the $N^2 \log N$ term.

3. Geodesic Riesz s-energy of equally spaced points

Here, we state theorems concerning the geodesic Riesz s-energy of equally spaced points on Γ that follow of the results from the preceding section together with asymptotic properties of generalized harmonic numbers. The proofs are given in Section 4.

Definition 15. The *discrete geodesic Riesz s-energy* of N equally spaced points $\mathbf{z}_{1,N}, \dots, \mathbf{z}_{N,N}$ on Γ is given by

$$\mathcal{M}_s(\Gamma; N) := \sum_{j \neq k} [\mathrm{d}(\mathbf{z}_{j,N}, \mathbf{z}_{k,N})]^{-s} = N \sum_{j=1}^{N-1} [\mathrm{d}(\mathbf{z}_{j,N}, \mathbf{z}_{N,N})]^{-s}, \qquad s \in \mathbb{C}.$$

The *discrete logarithmic geodesic energy* of N equally spaced points $\mathbf{z}_{1,N}, \dots, \mathbf{z}_{N,N}$ on Γ enters in a natural way by taking the limit

$$\mathcal{M}_{\log}(\Gamma; N) := \lim_{s \to 0} \frac{\mathcal{M}_s(\Gamma; N) - N(N-1)}{s} = \sum_{j \neq k} \log \frac{1}{\mathrm{d}(\mathbf{z}_{j,N}, \mathbf{z}_{k,N})}. \tag{13}$$

We are interested in the asymptotics of $\mathcal{M}_s(\Gamma; N)$ for large N for all values of s in the complex plane and we shall compare them with the related asymptotics for the Euclidean case given in our recent paper [10]. In the following we use the notation

$$\mathcal{I}_s^g[\mu] := \iint \frac{d\mu(\mathbf{x})\, d\mu(\mathbf{y})}{[\mathrm{d}(\mathbf{x}, \mathbf{y})]^s}, \qquad V_s^g(\Gamma) := \inf\{\mathcal{I}_s^g[\mu] : \mu \in \mathfrak{M}(\Gamma)\},$$

$$\mathcal{I}_{\log}^g[\mu] := \iint \log \frac{1}{\mathrm{d}(\mathbf{x}, \mathbf{y})}\, d\mu(\mathbf{x})\, d\mu(\mathbf{y}), \qquad V_{\log}^g(\Gamma) := \inf\{\mathcal{I}_{\log}^g[\mu] : \mu \in \mathfrak{M}(\Gamma)\}.$$

3.1. The geodesic logarithmic energy

Theorem 16. *Let q be a positive integer. For $N = 2M + \kappa$, $\kappa = 0, 1$*

$$\begin{aligned} \mathcal{M}_{\log}(\Gamma; N) = V_{\log}^g(\Gamma)\, N^2 - N \log N + N \log \frac{|\Gamma|}{2\pi} \\ - \sum_{n=1}^{q} \frac{B_{2n}(\kappa/2)}{(2n-1)\, 2n} 2^{2n} N^{2-2n} + \mathcal{O}_{q,\kappa}(N^{-2q}) \end{aligned}$$

as $N \to \infty$. Here, $V_{\log}^g(\Gamma) = 1 - \log(|\Gamma|/2)$.

Remark. The parity of N affects the coefficients of the powers N^{2-2m}, $m \geq 1$. The N^2-term vanishes for curves Γ with $|\Gamma| = 2e$ and the N-term vanishes when $|\Gamma| = 2\pi$. By contrast, the Euclidean logarithmic energy of N equally spaced points on the unit circle is given by (cf. [10])

$$\mathcal{L}_{\log}(N) = -N \log N.$$

3.2. The geodesic Riesz s-energy

The next result provides the complete asymptotic formula for all $s \neq 1$. This exceptional case, in which a logarithmic term arises, is described in Theorem 19.

Theorem 17 (general case)**.** *Let q be a positive integer. Then for all $s \in \mathbb{C}$ with $s \neq 1$ and $\operatorname{Re} s + 2q \geq 0$ there holds*

$$\begin{aligned} \mathcal{M}_s(\Gamma; N) = V_s^g(\Gamma)\, N^2 + \frac{2\,\zeta(s)}{|\Gamma|^s} N^{1+s} \\ - \frac{1}{(|\Gamma|/2)^s} \sum_{n=1}^{q} \frac{B_{2n}(\kappa/2)}{(2n)!} (s)_{2n-1} 2^{2n} N^{2-2n} + \mathcal{O}_{s,q,\kappa}(N^{-2q}) \end{aligned} \tag{14}$$

as $N \to \infty$, where $V_s^g(\Gamma) = (|\Gamma|/2)^{-s}/(1-s)$ and $N = 2M + \kappa$, $\kappa = 0, 1$.

In (14) the symbol $(s)_n$ denotes the Pochhammer symbol defined as $(s)_0 = 1$ and $(s)_{n+1} = (n+s)(s)_n$ for integers $n \geq 0$.

Remark. It is interesting to compare (14) with (10). It should be noted that in both the geodesic and the Euclidean case, the respective asymptotics have an N^2-term whose coefficient is the respective energy integral of the limit distribution (which is the normalized arc-length measure) or its appropriate analytic continuation, and an N^{1+s}-term with the coefficient $2\,\zeta(s)/|\Gamma|^s$. Regarding the latter, it has been shown in [27] that for $s > 1$ the dominant term of the asymptotics for the (Euclidean) Riesz s-energy of optimal energy N-point systems for any one-dimensional rectifiable curves in $\mathbb{R}^p$ is given by $2\,\zeta(s)/|\Gamma|^s N^{1+s}$. Regarding the remaining terms of the asymptotics of $\mathcal{M}_s(\Gamma; N)$ and $\mathcal{L}_s(N)$ one sees that the exponents of the powers of N do not depend on s in the geodesic case but do depend on s in the Euclidean case.

Remark. In the general case $s \neq 1$, the asymptotic series expansion (14) is not convergent, except for $s = 0, -1, -2, \dots$ when the infinite series reduces to a finite sum. The former follows, for example, from the ratio test and properties of the Bernoulli numbers and the latter from properties of the Pochhammer symbol $(a)_n$.

For a negative integer s we have the following result.

Proposition 18. *Let p be a positive integer. Then*

$$\begin{aligned} \mathcal{M}_{-p}(\Gamma; N) = \frac{(|\Gamma|/2)^p}{p+1} N^2 + \frac{(|\Gamma|/2)^p}{p+1} \sum_{n=1}^{\lfloor p/2 \rfloor} \binom{p+1}{2n} B_{2n}(\kappa/2)\, 2^{2n} N^{2-2n} \\ + \frac{2\,|\Gamma|^p}{p+1} \left(B_{p+1}(\kappa/2) - B_{p+1} \right) N^{1-p} \end{aligned}$$

for $N = 2M + \kappa$, $\kappa = 0, 1$. The right-most term above vanishes for even p.

Remark. The corresponding *Euclidean* Riesz $(-m)$-energy of N-th roots of unity [10, Eq. (1.19)] reduces to[‖]

$$\mathcal{L}_{-m}(N) = V_{-m} N^2 \quad \text{if } m = 2, 4, 6, \dots \text{ and } N \text{ is sufficiently large.}$$

Remark. The quantity $\mathcal{M}_{-1}(\mathbb{S}; N)$ gives the maximum sum of *geodesic* distances on the unit circle. Corollary 18 yields

$$\mathcal{M}_{-1}(\mathbb{S}; N) = \frac{\pi}{2}\left(N^2 - \kappa\right), \qquad N = 2M + \kappa,\ \kappa = 0, 1. \tag{15}$$

We remark that L. Fejes Tóth [16] conjectured (and proved for $N \leq 6$) that the maximum sum of geodesic distances on the *unit sphere* $\mathbb{S}^2$ *in* $\mathbb{R}^3$ is also given by the right-hand side in (15). This conjecture was proved by Sperling [30] for even N [**] and by Larcher [24] for odd N.[††] An essential observation is that the sum of geodesic distances does not change if a given pair of antipodal points $(\mathbf{x}, \mathbf{x}')$ is rotated simultaneously, since $\mathrm{d}(\mathbf{x}, \mathbf{y}) + \mathrm{d}(\mathbf{x}', \mathbf{y}) = \pi$ for every $\mathbf{y} \in \mathbb{S}^2$.

In the exceptional case $s = 1$ a logarithmic term appears.

Theorem 19. *Let $q \geq 1$ be an integer. For $N = 2M + \kappa$, $\kappa = 0, 1$,*

$$\begin{aligned}\mathcal{M}_1(\Gamma; N) = \frac{2}{|\Gamma|} N^2 \log N - \frac{\log 2 - \gamma}{|\Gamma|/2} N^2 - \frac{2}{|\Gamma|} \sum_{n=1}^{q} \frac{B_{2n}(\kappa/2)}{2n} 2^{2n} N^{2-2n} \\ - \theta_{q,N,\kappa} \frac{2}{|\Gamma|} \frac{B_{2q+2}(\kappa/2)}{2q+2} 2^{2q+2} N^{-2q},\end{aligned} \tag{16}$$

where $0 < \theta_{q,N,\kappa} \leq 1$ depends on q, N and κ.

Remark. A comparison of the asymptotics (16) and the corresponding result for the Euclidean Riesz 1-energy of N-th roots of unity (cf. (12) and [10, Thm. 1.2]),

$$\begin{aligned}\mathcal{L}_1(N) = \frac{1}{\pi} N^2 \log N + \frac{\gamma - \log(\pi/2)}{\pi} N^2 \\ + \sum_{n=1}^{q} \frac{(-1)^n B_{2n}(1/2)}{(2n)!} \frac{2\,\zeta(1-2n)}{(2\pi)^{1-2n}} N^{2-2n} + \mathcal{O}(N^{1-2q}),\end{aligned}$$

shows that for $|\Gamma| = 2\pi$ the dominant term is the same and the coefficients of all other powers of N differ. The latter is obvious for the N^2-term, and for the

[‖] We caution the reader that in [10] the condition 'N is sufficiently large' is missing from formula (1.19). Direct computation shows that (1.19) is true for $N > m$. Exact formulas for $\mathcal{L}_{2k}(N)$, k a non-zero integer, have been derived and appear in [9].

[**] Sperling mentions that his proof can be easily generalized to higher-dimensional spheres.

[††] Larcher also characterizes all optimal configurations.

N^{2-2n}-term, follows from the fact that the coefficient in (16) multiplied by π is rational whereas the coefficient in the asymptotics for $\mathcal{L}_1(N)$ multiplied by π is transcendental. Interestingly, except for $s = 1$, there are no other exceptional cases with an $N^2 \log N$ term in the asymptotics of $\mathcal{M}_s(\Gamma; N)$, whereas in the asymptotics of $\mathcal{L}_s(N)$ there appears an $N^2 \log N$ term whenever s is a positive integer, cf. [10, Thm. 1.2].

4. Proofs

P r o o f o f P r o p o s i t i o n 1. **Part (A).** The proof utilizes the "winding number" argument of L. Fejes Tóth. The key idea is to regroup the terms in the sum in (2) with respect to its m nearest neighbors ($m = 1, \dots, N$) and then use convexity and Jensen's inequality.

W.l.o.g. we assume that $\mathbf{w}_1, \dots, \mathbf{w}_N$ on Γ are ordered such that $\mathbf{w}_k$ precedes $\mathbf{w}_{k+1}$ (denoted $\mathbf{w}_k \prec \mathbf{w}_{k+1}$). We identify $\mathbf{w}_{j+N}$ with $\mathbf{w}_j$ for $j = 1, \dots, N-1$. By convexity

$$\begin{aligned}\sum_{j=1}^{N} \sum_{\substack{k=1\\k\neq j}}^{N} f(\mathrm{d}(\mathbf{w}_j, \mathbf{w}_k)) &= N \sum_{k=1}^{N-1} \left[\frac{1}{N} \sum_{j=1}^{N} f(\mathrm{d}(\mathbf{w}_j, \mathbf{w}_{j+k})) \right] \\ &\geq N \sum_{k=1}^{N-1} f\Big(\frac{1}{N} \sum_{j=1}^{N} \mathrm{d}(\mathbf{w}_j, \mathbf{w}_{j+k}) \Big).\end{aligned} \tag{17}$$

Let $\mathbf{z}_{1,N} \prec \cdots \prec \mathbf{z}_{N,N}$ be N equally spaced (with respect to the metric d) points on Γ. Set $\mathbf{z}_{0,N} = \mathbf{z}_{N,N}$. Assuming further that this metric d also satisfies

$$\frac{1}{N} \sum_{j=1}^{N} \mathrm{d}(\mathbf{x}_j, \mathbf{x}_{j+k}) \leq \mathrm{d}(\mathbf{z}_{0,N}, \mathbf{z}_{k,N}), \qquad k = 1, \dots, N-1, \tag{18}$$

for every ordered N-point configuration $\mathbf{x}_1 \prec \cdots \prec \mathbf{x}_N$ with $\mathbf{x}_j = \mathbf{x}_{j+N}$, it follows that

$$G_f(\mathbf{w}_1, \dots, \mathbf{w}_N) \geq N \sum_{k=1}^{N-1} f(\mathrm{d}(\mathbf{z}_{0,N}, \mathbf{z}_{k,N})) = G_f(\mathbf{z}_{1,N}, \dots, \mathbf{z}_{N,N}).$$

It remains to show that the geodesic distance satisfies (18). From

$$\mathrm{d}(\mathbf{x}_j, \mathbf{x}_k) = \min\left\{\ell(\mathbf{x}_j, \mathbf{x}_k), |\Gamma| - \ell(\mathbf{x}_j, \mathbf{x}_k)\right\} \qquad \text{if } 0 \leq k - j < N$$

and additivity of the distance function $\ell(\cdot,\cdot)$ it follows that

$$\sum_{j=1}^{N} \mathrm{d}(\mathbf{x}_j,\mathbf{x}_{j+k}) \leq \begin{cases} \displaystyle\sum_{j=1}^{N} \ell(\mathbf{x}_j,\mathbf{x}_{j+k}) = \sum_{j=1}^{N}\sum_{n=1}^{k} \ell(\mathbf{x}_{j+n-1},\mathbf{x}_{j+n}) = |\Gamma|\, k, \\ \displaystyle\sum_{j=1}^{N} \left(|\Gamma| - \ell(\mathbf{x}_j,\mathbf{x}_{j+k})\right) = |\Gamma|\,(N-k) \end{cases}$$

and therefore

$$\frac{1}{N}\sum_{j=1}^{N} \mathrm{d}(\mathbf{x}_j,\mathbf{x}_{j+k}) \leq \min\{|\Gamma|\, k/N, |\Gamma|\,(N-k)\,/N\} = \mathrm{d}(\mathbf{z}_{0,N},\mathbf{z}_{k,N}).$$

In the case of a strictly convex function f we have equality in (17) if and only if the points are equally spaced. This shows uniqueness (up to translation along the simple closed curve Γ) of equally spaced points.

Part (B). Given $N = 2M + \kappa$ ($\kappa = 0, 1$), let ω_N denote the antipodal set with $M + \kappa$ points placed at the North Pole and M points at the South Pole of Γ, where both Poles can be any two points on Γ with geodesic distance $|\Gamma|/2$. Thus, the geodesic distance between two points in ω_N is either 0 or $|\Gamma|/2$. Hence

$$G_f(\omega_N) = 2M\,(M+\kappa)\, f(|\Gamma|\,/2) = \frac{1}{2} f(|\Gamma|\,/2)\left(N^2 - \kappa\right). \tag{19}$$

Since adding a constant to G_f does not change the positions of optimal f-energy points, we may assume w.l.o.g. that $f(0) = 0$. In fact, we will prove the equivalent assertion that if f is a non-constant convex and increasing function with $f(0) = 0$, then the functional G_f has a maximum at ω_N, which is unique (up to translation along Γ) if f is strictly increasing. (Note that by these assumptions $f(x) \geq 0$.) Indeed, any N-point system X_N of points $\mathbf{x}_1, \dots, \mathbf{x}_N$ from Γ satisfies

$$\begin{aligned} G_f(X_N) &= f(|\Gamma|\,/2) \sum_{j\neq k} \frac{f(\mathrm{d}(\mathbf{x}_j,\mathbf{x}_k))}{f(|\Gamma|\,/2)} \leq f(|\Gamma|\,/2) \sum_{j\neq k} \frac{\mathrm{d}(\mathbf{x}_j,\mathbf{x}_k)}{|\Gamma|\,/2} \\ &= f(|\Gamma|\,/2) \frac{G_{\mathrm{id}}(X_N)}{|\Gamma|\,/2} \leq f(|\Gamma|\,/2) \frac{G_{\mathrm{id}}(\omega_N)}{|\Gamma|\,/2} = \frac{1}{2} f(|\Gamma|\,/2)\left(N^2 - \kappa\right), \end{aligned}$$

where we used that antipodal configurations are optimal for the "sum of distance function" (f is the identity function id) and relation (19) with $f \equiv \mathrm{id}$. Note that the first inequality is strict if there is at least one pair (j,k) such that $0 < \mathrm{d}(\mathbf{x}_j,\mathbf{x}_k) < |\Gamma|/2$. On the other hand, if $X_N = \omega_N$, then equality holds everywhere. $\square$

Proof of Proposition 2. For Lebesgue integrable functions f the minimum geodesic f-energy $V_f^g(\Gamma)$ is finite, since $\mathcal{I}_f^g[\sigma_\Gamma] = \int f(\mathrm{d}(\mathbf{x},\mathbf{y}))\, d\sigma_\Gamma(\mathbf{x}) =$

$(2/|\Gamma|)\int_0^{|\Gamma|/2} f(\ell)\,d\ell \neq \infty$ ($\mathbf{y} \in \Gamma$ arbitrary). Moreover, for lower semicontinuous functions f, a standard argument (see [23]) shows that the sequence $\{G_f(\omega_N^{(f)})/[N(N-1)]\}_{N\geq 2}$ is monotonically increasing. Since f is Lebesgue integrable, this sequence is bounded from above by $\mathcal{I}_f^g[\sigma_\Gamma]$; thus, the limit $\lim_{N\to\infty} G_f(\omega_N^{(f)})/N^2$ exists in this case. If f also satisfies the hypotheses of Proposition 1(A), then $\lim_{N\to\infty} G_f(\omega_N^{(f)})/N^2 = \mathcal{I}_f^g[\sigma_\Gamma]$. (By a standard argument, one constructs a family of continuous functions $F_\varepsilon(x)$ with $F_\varepsilon(x) = f(x)$ outside of ε-neighborhoods at points of discontinuity of f, $f(x) \geq F_\varepsilon(x)$ everywhere and $\lim_{\varepsilon\to 0} F_\varepsilon(x) = f(x)$ wherever f is continuous at x. Then the lower bound follows from weak-star convergence of $\nu[\omega_N^{(F_\varepsilon)}]$ as $N\to\infty$ and, subsequently, letting $\varepsilon \to 0$.) □

We next present some auxiliary results that are needed to prove the main Theorems 5 and 6. We begin with the following generalized Euler-MacLaurin summation formula.

Proposition 20. *Let $\omega = 0$ or $\omega = 1/2$. Let $M \geq 2$. Then for any function h with continuous derivative of order $2p+1$ on the interval $[1-\omega, M+\omega]$ we have*

$$\begin{aligned}\sum_{k=1}^{M} h(k) = \int_a^b h(x)\,dx &+ (1/2-\omega)\left\{h(a)+h(b)\right\}\\ &+ \sum_{k=1}^{p} \frac{B_{2k}(\omega)}{(2k)!}\left\{h^{(2k-1)}(b) - h^{(2k-1)}(a)\right\}\\ &+ \frac{1}{(2p+1)!}\int_a^b C_{2p+1}(x) h^{(2p+1)}(x)\,dx, \qquad a = 1-\omega, b = M+\omega,\end{aligned}$$

where $C_k(x)$ is the periodized Bernoulli polynomial $B_k(x - \lfloor x \rfloor)$.

P r o o f. For $\omega = 0$, the above formula is the classical Euler-MacLaurin summation formula (cf., for example, [3]). For $\omega = 1/2$, iterated application of integration by parts yields the desired result. □

Let f have a continuous derivative of order $2p+1$ on the interval $(0, |\Gamma|/2]$. Then applying Proposition 20 with $h(x) = f(x|\Gamma|/N)$ and $\omega = \kappa/2$, where $N = 2M + \kappa \geq 2$, $\kappa = 0, 1$, we obtain

$$\begin{aligned}\mathcal{M}(\Gamma, f; N) &= 2N \sum_{n=1}^{\lfloor N/2 \rfloor} f(n\,|\Gamma|\,/N) - (1-\kappa)\, f(|\Gamma|\,/2)N\\ &= 2N \int_{1-\omega}^{N/2} f(x|\Gamma|/N)\,dx + 2\left(\frac{1}{2}-\omega\right) N \left\{f((1-\omega)|\Gamma|/N) + f(|\Gamma|/2)\right\}\end{aligned}$$

$$+ 2N \sum_{k=1}^{p} \frac{B_{2k}(\omega)}{(2k)!} \left\{ f(x|\Gamma|/N) \right\}^{(2k-1)} \Big|_{1-\omega}^{N/2}$$
$$+ \frac{2N}{(2p+1)!} \int_{1-\omega}^{N/2} C_{2p+1}(x) \left\{ f(x|\Gamma|/N) \right\}^{(2p+1)} (x) \, dx$$
$$- 2 \left(\frac{1}{2} - \omega \right) f(|\Gamma|/2) N.$$

Regrouping the terms in the last relation and using the fact that $B_{2k+1} = B_{2k+1}(1/2) = 0$ for $k = 1, 2, 3, \dots$ and $B_1(\omega) = \omega - 1/2$, we derive the exact representation

$$\begin{aligned} \mathcal{M}(\Gamma, f; N) = N^2 \frac{2}{|\Gamma|} \int_{(1-\omega)|\Gamma|/N}^{|\Gamma|/2} f(y) \, dy - \mathcal{A}_p(\Gamma, f; N) \\ + \mathcal{B}_p(\Gamma, f; N) + \mathcal{R}_p(\Gamma, f; N) \end{aligned} \tag{20}$$

valid for every integer $N \geq 2$, where

$$\begin{aligned} \mathcal{A}_p(\Gamma, f; N) &:= -2B_1(\omega) f((1-\omega)|\Gamma|/N) \\ &\quad - 2N \sum_{k=1}^{p} \frac{B_{2k}(\omega)}{(2k)!} \left\{ f(x|\Gamma|/N) \right\}^{(2k-1)} \Big|_{1-\omega} \\ &= \frac{2}{|\Gamma|} N^2 \sum_{r=1}^{2p} \frac{B_r(\omega)}{r!} \left(|\Gamma|/N \right)^r f^{(r-1)}((1-\omega)|\Gamma|/N), \end{aligned} \tag{21a}$$

$$\mathcal{B}_p(\Gamma, f; N) := \frac{2}{|\Gamma|} N^2 \sum_{k=1}^{p} \frac{B_{2k}(\omega)}{(2k)!} \left(|\Gamma|/N \right)^{2k} f^{(2k-1)}(|\Gamma|/2), \tag{21b}$$

$$\mathcal{R}_p(\Gamma, f; N) := 2N \frac{\left(|\Gamma|/N \right)^{2p+1}}{(2p+1)!} \int_{1-\omega}^{N/2} C_{2p+1}(x) f^{(2p+1)}(x|\Gamma|/N) \, dx. \tag{21c}$$

If f is admissible in the sense of Definition 4, then by linearity

$$\mathcal{M}(\Gamma, f; N) = \mathcal{M}(\Gamma, S_q; N) + \mathcal{M}(\Gamma, f - S_q; N),$$

where the term $\mathcal{M}(\Gamma, S_q; N)$ contains the asymptotic expansion of $\mathcal{M}(\Gamma, f; N)$ and the term $\mathcal{M}(\Gamma, f - S_q; N)$ is part of the remainder term. The next lemma provides estimates for the contributions to the remainder term in the asymptotic expansion of $\mathcal{M}(\Gamma, f; N)$ as $N \to \infty$.

Lemma 21. *Let f be admissible in the sense of Definition 4. Then as $N \to \infty$:*

$$N^2 \frac{2}{|\Gamma|} \int_0^{(1-\omega)|\Gamma|/N} (f - S_q)(y) \, dy = \mathcal{O}(N^{1-\delta+s_q}),$$

$$\mathcal{A}_p(\Gamma, f - S_q; N) = \mathcal{O}(N^{1-\delta+s_q}),$$

$$\mathcal{R}_p(\Gamma, f - S_q; N) = \begin{cases} \mathcal{O}(N^{1-2p}) & \textit{if } 2p \neq \delta - \operatorname{Re} s_q, \\ \mathcal{O}(N^{1-2p}\log N) & \textit{if } 2p = \delta - \operatorname{Re} s_q. \end{cases}$$

The $\mathcal{O}$*-term depends on* $|\Gamma|$, p, s_q, *and* f.

Proof. The first relation follows directly from Definition 4(ii.a). The second estimate follows from Definition 4(ii.b) and (21a); that is, for some positive constant C

$$\begin{aligned} |\mathcal{A}_p(\Gamma, f - S_q; N)| &\leq \frac{2}{|\Gamma|} N^2 \sum_{r=1}^{2p} \frac{|B_r(\omega)|}{r!} \left(|\Gamma|/N\right)^r \left|(f - S_q)^{(r-1)}((1-\omega)|\Gamma|/N)\right| \\ &\leq C \frac{2}{|\Gamma|} N^2 \sum_{r=1}^{2p} \frac{|B_r(\omega)|}{r!} \left(|\Gamma|/N\right)^r (1-\omega)^{\delta - \operatorname{Re} s_q - r + 1} \\ &\qquad \times \left(|\Gamma|/N\right)^{r + \delta - \operatorname{Re} s_q - r + 1}. \end{aligned}$$

The last estimate follows from Definition 4(ii.b), (21c) and the fact that

$$|C_{2p+1}(x)| \leq (2p+1)\,|B_{2p}| \qquad \text{for all real } x \text{ and all } p = 1, 2, \dots; \tag{22}$$

that is, for some positive constant C

$$\begin{aligned} |\mathcal{R}_p(\Gamma, f - S_Q; N)| &\leq 2N \frac{\left(|\Gamma|/N\right)^{2p+1}}{(2p+1)!} \int_{1-\omega}^{N/2} |C_{2p+1}(x)| \left|(f - S_q)^{(2p+1)}(x\frac{|\Gamma|}{N})\right| dx \\ &\leq 2CN \frac{B_{2p}}{(2p)!} \left(|\Gamma|/N\right)^{\delta - \operatorname{Re} s_q} \int_{1-\omega}^{N/2} x^{\delta - 1 - 2p - \operatorname{Re} s_q}\, dx. \end{aligned}$$

□

Other functions arising in the asymptotics of $\mathcal{M}(\Gamma, f; N)$ are defined next.

Definition 22. Let $\omega = 0, 1/2$ and p be a positive integer. For $s \in \mathbb{C}$, $s \neq 1$,

$$\begin{aligned} \zeta_p(\omega, y; s) := &\frac{1}{s-1} \sum_{r=0}^{2p} \frac{B_r(\omega)}{r!} (-1)^r (s-1)_r \, (1-\omega)^{1-s-r} \\ &- \frac{(s)_{2p+1}}{(2p+1)!} \int_{1-\omega}^{y} C_{2p+1}(x) x^{-s-1-2p}\, dx, \end{aligned}$$

which we call *incomplete zeta function* and

$$\Psi_p(\omega, y) := -\log(1-\omega) + \sum_{r=1}^{2p} \frac{B_r(\omega)}{r} (-1)^r (1-\omega)^{-r} - \int_{1-\omega}^{y} \frac{C_{2p+1}(x)}{x^{2+2p}}\, dx.$$

Proposition 23. *Let $\omega = 0, 1/2$. Then*

$$
\begin{aligned}
\Psi_p(\omega, y) &= \lim_{s\to 1}(\zeta_p(\omega, y; s) - 1/(s-1)),\\
\zeta_p(\omega, y; -n) &= -\frac{B_{n+1}}{n+1} = \zeta(-n), \qquad n = 0, 1, \dots, 2p,\\
\zeta_p(\omega, y; s) - \zeta(s) &= \frac{(s)_{2p+1}}{(2p+1)!}\int_y^\infty C_{2p+1}(x) x^{-s-1-2p}\, dx, \qquad \operatorname{Re} s + 2p > 0,\\
\zeta(s) &= \lim_{y\to\infty} \zeta_p(\omega, y; s), \qquad \operatorname{Re} s + 2p > 0,\\
\Psi_p(\omega, y) - \gamma &= \int_y^\infty C_{2p+1}(x) x^{-2-2p}\, dx,\\
\gamma &= \lim_{y\to\infty} \Psi_p(\omega, y).
\end{aligned}
$$

P r o o f. The second relation follows from [26, Eq. 2.8(13)], $B_{2k+1}(\omega) = 0$ for $\omega = 0, 1/2$ and $k \geq 1$ and [1, Eq. 23.2.15]. The representations and therefore the limit relations for $\zeta(s)$ and γ follow from Proposition 20. □

P r o o f o f T h e o r e m 5. Let f be admissible in the sense of Definition 4. In the representation (20) we can write the integral as follows: Set $a := (1-\omega)|\Gamma|/N$, then

$$
\begin{aligned}
\frac{2}{|\Gamma|}\int_a^{|\Gamma|/2} f(y)\, dy &= \frac{2}{|\Gamma|}\int_a^{|\Gamma|/2} S_q(x)\, dx + \frac{2}{|\Gamma|}\int_a^{|\Gamma|/2} (f - S_q)(x)\, dx\\
&= \frac{2}{|\Gamma|}\sum_{n=0}^{q} a_n \int_a^{|\Gamma|/2} x^{-s_n}\, dx + \frac{2}{|\Gamma|}\int_0^{|\Gamma|/2} (f - S_q)(x)\, dx\\
&\quad - \frac{2}{|\Gamma|}\int_0^{a} (f - S_q)(x)\, dx\\
&= V_f(\Gamma) - \frac{2}{|\Gamma|}\sum_{n=0}^{q} a_n \frac{a^{1-s_n}}{1-s_n} - \frac{2}{|\Gamma|}\int_0^{a} (f - S_q)(x)\, dx.
\end{aligned}
$$

Defining

$$
\begin{aligned}
\widetilde{\mathfrak{R}}_p(f - S_q; N) := &-\frac{2}{|\Gamma|}N^2 \int_0^{(1-\omega)|\Gamma|/N} (f - S_q)(x)\, dx - \mathcal{A}_p(\Gamma, f - S_q; N)\\
&+ \mathcal{R}_p(\Gamma, f - S_q; N),
\end{aligned}
$$

formula (20) becomes (in condensed notation)

$$
\mathcal{M}(f; N) = V_f\, N^2 - \frac{2}{|\Gamma|}N^2 \sum_{n=0}^{q} a_n \frac{a^{1-s_n}}{1-s_n} - \mathcal{A}_p(S_q; N) + \mathcal{B}_p(f; N)
$$

$$
\begin{aligned}
&+ \mathcal{R}_p(S_q; N) + \widetilde{\mathfrak{R}}_p(f - S_q; N) \\
&= V_f\, N^2 + \sum_{n=0}^{q} a_n \left\{ \frac{2}{|\Gamma|} N^2 \frac{a^{1-s_n}}{s_n - 1} - \mathcal{A}_p(x^{-s_n}; N) + \mathcal{R}_p(x^{-s_n}; N) \right\} \\
&+ \mathcal{B}_p(f; N) + \widetilde{\mathfrak{R}}_p(f - S_q; N).
\end{aligned}
$$

Furthermore, using (21a), (21c) and Definition 22, we can write the expression in curly brackets above as follows:

$$
\begin{aligned}
\frac{2}{|\Gamma|} N^2 \frac{a^{1-s_n}}{s_n - 1} - \mathcal{A}_p(x^{-s_n}; N) + \mathcal{R}_p(x^{-s_n}; N) &= \frac{2}{|\Gamma|} N^2 \frac{a^{1-s_n}}{s_n - 1} \\
&- \frac{2}{|\Gamma|} N^2 \sum_{r=1}^{2p} \frac{B_r(\omega)}{r!} \left(|\Gamma| / N \right)^r \left\{ t^{-s_n} \right\}^{(r-1)} \Big|_{t=a} \\
&+ 2N \frac{\left(|\Gamma| / N \right)^{2p+1}}{(2p+1)!} \int_{1-\omega}^{N/2} C_{2p+1}(x) \left\{ t^{-s_n} \right\}^{(2p+1)} \Big|_{t = x |\Gamma| / N} \, dx \\
&= \frac{2}{|\Gamma|} N^2 \left(|\Gamma| / N \right)^{1-s_n} \left\{ \frac{(1-\omega)^{1-s_n}}{s_n - 1} \right. \\
&+ \sum_{r=1}^{2p} \frac{B_r(\omega)}{r!} (-1)^r (s_n)_{r-1} (1-\omega)^{1-s_n-r} \\
&\left. - \frac{(s_n)_{2p+1}}{(2p+1)!} \int_{1-\omega}^{N/2} C_{2p+1}(x)\, x^{-s_n-1-2p} \, dx \right\} \\
&= \frac{2}{|\Gamma|} N^2 \left(|\Gamma| / N \right)^{1-s_n} \zeta_p(\omega, N/2; s_n).
\end{aligned}
$$

Hence, we arrive at the formula

$$
\mathcal{M}(f; N) = V_f\, N^2 + \sum_{n=0}^{q} a_n \frac{2\, \zeta_p(\omega, N/2; s_n)}{|\Gamma|^{s_n}} N^{1+s_n} + \mathcal{B}_p(f; N) + \widetilde{\mathfrak{R}}_p(f - S_q; N).
$$

For $\mathfrak{R}_p(\Gamma, f; N)$ defined by (6) we have

$$
\mathfrak{R}_p(\Gamma, f; N) = \sum_{n=0}^{q} a_n \frac{2\, \zeta_p(\kappa/2, N/2; s_n) - 2\, \zeta(s_n)}{|\Gamma|^{s_n}} N^{1+s_n} + \widetilde{\mathfrak{R}}_p(f - S_q; N). \tag{23}
$$

Furthermore, it follows from Lemma 21 that $\widetilde{\mathfrak{R}}_p(f - S_q; N) = \mathcal{O}(N^{1-\delta+s_q}) + \mathcal{O}(N^{1-2p})$ if $2p \neq \delta - \operatorname{Re} s_q$ and $\widetilde{\mathfrak{R}}_p(f - S_q; N) = \mathcal{O}(N^{1-\delta+s_q}) + \mathcal{O}(N^{1-2p} \log N)$

if $2p = \delta - \operatorname{Re} s_q$. Finally, using (22) and Proposition 23 we obtain the estimate

$$\begin{aligned}
&\left| \sum_{n=0}^{q} a_n \frac{\zeta_p(\kappa/2, N/2, s_n) - \zeta(s_n)}{|\Gamma|^{s_n}} N^{1+s_n} \right| \\
&\qquad \leq 2\,(N/2)^{1-2p} \sum_{n=0}^{q} \left| a_n \frac{B_{2p}}{(2p)!} (s_n)_{2p} \frac{2p + s_n}{2p + \operatorname{Re} s_n} \right| (|\Gamma|/2)^{-\operatorname{Re} s_n} .
\end{aligned}$$

Note that, whenever $s_n = -k$ for some $k = 0, 1, \dots, 2p$, then the corresponding terms on both sides of the estimate above are not present. Also, from Definition 4 it follows that $2p + \operatorname{Re} s_n > 0$ for $n = 0, \dots, q-1$ and that either $\operatorname{Re} s_q + 2p > 0$ or $s_q = -2p$. In either case the sum on the left-hand side above is of order $\mathcal{O}(N^{1-2p})$. Hence, we have from (23) that $\mathfrak{R}_p(\Gamma, f; N) = \mathcal{O}(N^{1-\delta+s_q}) + \mathcal{O}(N^{1-2p})$ if $2p \neq \delta - \operatorname{Re} s_q$ and $\mathfrak{R}_p(\Gamma, f; N) = \mathcal{O}(N^{1-\delta+s_q}) + \mathcal{O}(N^{1-2p} \log N)$ if $2p = \delta - \operatorname{Re} s_q$. □

Proof of Theorem 6. Proceeding as in the proof of Theorem 5 the remainder term now takes the form

$$\begin{aligned}
\mathfrak{R}_p(\Gamma, f; N) = {} & \frac{2}{|\Gamma|} N^2 a_{q'} \left(\Psi_p(\kappa/2, N/2) - \gamma \right) \\
& + \sum_{\substack{n=0,\\ n \neq q'}}^{q} a_n \frac{2\,\zeta_p(\kappa/2, N/2, s_n) - 2\,\zeta(s_n)}{|\Gamma|^{s_n}} N^{1+s_n} \\
& - N^2 \frac{2}{|\Gamma|} \int_0^{(1-\omega)|\Gamma|/N} (f - S_q)(y)\, dy \\
& - \mathcal{A}_p(\Gamma, f - S_q; N) + \mathcal{R}_p(\Gamma, f - S_q; N).
\end{aligned}$$

Using Lemma 21, Proposition 23, and the inequality

$$\left| \frac{2}{|\Gamma|} N^2 a_{q'} \left(\Psi_p(\kappa/2, N/2) - \gamma \right) \right| \leq 4 \frac{2}{|\Gamma|} \left| a_{q'} B_{2p} \right| (N/2)^{1-2p},$$

we get the estimate $\mathfrak{R}_p(\Gamma, f; N) = \mathcal{O}(N^{1-2p}) + \mathcal{O}(N^{1-\delta+s_q})$ if $2p \neq \delta - \operatorname{Re} s_q$ and $\mathfrak{R}_p(\Gamma, f; N) = \mathcal{O}(N^{1-2p} \log N)$ if $2p = \delta - \operatorname{Re} s_q$. □

Next, we prove the results related to particular types of kernel functions.

Proof of Theorem 7. The Laplace transform $f(x) := \int_0^\infty e^{-xt}\, d\mu(t)$ of a signed measure μ on $[0, \infty)$ satisfying $\int_0^\infty t^m\, d|\mu|(t) < \infty$ for every $m = 0, 1, 2, \dots$ has derivatives of all orders on $(0, \infty)$. For q a positive integer let $S_q(x)$ be defined by $S_q(x) := \sum_{n=0}^{q} \frac{\mu_n}{n!}(-x)^n$. For every $0 \leq m \leq q$ we can write

$$f^{(m)}(x) = (-1)^m \int_0^\infty e^{-xt} t^m \, d\mu(t) = (-1)^m \sum_{n=m}^{q} \frac{\mu_n}{(n-m)!}(-x)^{n-m} + (f - S_q)^{(m)}(x), \qquad x > 0,$$

where, using a finite section of the Taylor series expansion of $h(x) = e^{-xt}$ with integral remainder term, we have that

$$\begin{aligned}(f - S_q)^{(m)}(x) &= f^{(m)}(x) - S_q^{(m)}(x) \\ &= (-1)^m \int_0^\infty \left\{ e^{-xt} - \sum_{n=0}^{q-m} \frac{(-xt)^n}{n!} \right\} t^m \, d\mu(t) \\ &= \frac{(-1)^{q+1}}{(q-m)!} \int_0^\infty \left\{ \int_0^x e^{-ut} \, (x-u)^{q-m} \, du \right\} t^{q+1} \, d\mu(t), \quad x > 0.\end{aligned}$$

For $x > 0$ we have the following bound:

$$\left| (f - S_q)^{(m)}(x) \right| \leq \frac{x^{q+1-m}}{(q+1-m)!} \int_0^\infty t^{q+1} \, d|\mu|(t), \qquad m = 0, 1, \dots, q.$$

Since $S_q^{(q+1)}(x) = 0$ for all x, it is immediate that the last estimate also holds for $m = q+1$. It follows that f is admissible in the sense of Definition 4 with $q = 2p$, $\delta = 1$. The result follows from Theorem 5, after observing that

$$V_f(\Gamma) = \frac{2}{|\Gamma|} \int_0^{|\Gamma|/2} f(x) \, dx = \frac{2}{|\Gamma|} \int_0^{|\Gamma|/2} \int_0^\infty e^{-xt} \, d\mu(t) \, dx.$$

□

In the case that f is a completely monotonic function on $(0, \infty)$ (that is, μ is a positive measure), it is possible to improve the estimate for $\mathcal{R}_p(\Gamma, f; N)$ in (21c).

P r o o f o f T h e o r e m 8. Let f be analytic in a disc with radius $|\Gamma|/2 + \varepsilon$ ($\varepsilon > 0$) centered at the origin. Then $f(z) = \sum_{n=0}^{\infty} a_n z^n$ for $|z| < |\Gamma|/2 + \varepsilon$ and f is admissible in the sense of Definition 4 for any positive integers p and $q = 2p$, where $S_{2p}(z) = \sum_{n=0}^{2p} a_n z^n$ and $\delta = 1$. The asymptotic expansion follows from Theorem 5 on observing that with $s_n = -n$ ($n = 0, \dots, 2p$), one has

$$V_f(\Gamma) = \frac{2}{|\Gamma|} \sum_{n=0}^{2p} a_n \int_0^{|\Gamma|/2} x^n \, dx + \frac{2}{|\Gamma|} \int_0^{|\Gamma|/2} \big(f - S_{2p}\big)(x) \, dx = \frac{2}{|\Gamma|} \int_0^{|\Gamma|/2} f(x) \, dx.$$

Moreover, since $s_q = -2p$ and $\delta = 1$, it follows that $\mathfrak{R}_p(\Gamma, f; N) = \mathcal{O}_{p,|\Gamma|,f}(N^{1-2p})$ as $N \to \infty$. □

P r o o f o f T h e o r e m 10. Suppose f has a pole of integer order $K \geq 1$ at zero and is analytic in the annulus $0 < |z| < |\Gamma|/2 + \varepsilon$ ($\varepsilon > 0$) with series expansion $f(z) = \sum_{n=-K}^{\infty} a_n z^n$. Then f is admissible in the sense of Definition 4 for any positive integers p and $q = 2p$ with $S_{2p}(z) = \sum_{n=-K}^{2p} a_n z^n$ and $\delta = 1$. In the case (i) Theorem 5 is applied and in the case (ii) Theorem 6 is applied. The expressions for $V_f(\Gamma)$ follow from termwise integration in (7) and (8). Since $1 - \delta + s_q = -2p$, the remainder terms are $\mathfrak{R}_p(\Gamma, f; N) = \mathcal{O}_{p,|\Gamma|,f}(N^{1-2p})$ as $N \to \infty$. □

P r o o f o f E x a m p l e s 11 a n d 12. If f has an essential singularity at 0 and is analytic in the annulus $0 < |z| < |\Gamma|/2 + \varepsilon$ ($\varepsilon > 0$), then for positive integers p one has $f(z) = S_{2p}(z) + F_{2p}(z)$, where

$$S_{2p}(z) := \sum_{n=-\infty}^{2p} a_n z^n, \qquad F_{2p}(z) := \sum_{n=2p+1}^{\infty} a_n z^n = \mathcal{O}(z^{2p+1}) \text{ as } z \to 0.$$

Clearly, the function $f(z)$ satisfies Item (i) of Definition 4 and both functions $f(z)$ and $S_{2p}(z)$ satisfy an extended version of item (ii) of Definition 4 suitable for an infinite series $S_{2p}(z)$. Since termwise integration and differentiation of $S_{2p}(z)$ are justified by the theory for Laurent series, Theorems 5 and 6 can be extended for such kernel functions f. In this case all formulas in Theorems 5 and 6 still hold provided the index n starts with $-\infty$. In particular, we note that the infinite series $\sum_{n=-\infty, n\neq -1}^{2p} a_n \, \zeta(-n) \, |\Gamma|^n \, N^{1-n}$ appearing in the asymptotics of $\mathcal{M}(\Gamma, f; N)$ converges for every N, since $\zeta(m) \leq \zeta(2)$ for all integers $m \geq 2$.

Example 11 follows from the extended version of Theorem 6.

To justify Example 12 let λ be a zero of the Bessel function J_{-1}. The extended version of Theorem 5 with $a_n = \mathrm{J}_n(\lambda)$ gives that for integers $p \geq 2$ and $m \geq 2$

$$\begin{aligned}
\mathcal{M}(\Gamma, f; N) &= V_f(\Gamma)\, N^2 + 2 \sum_{\substack{n=-2p,\\ n\neq \pm 1}}^{\infty} \mathrm{J}_{-n}(\lambda)\, \zeta(n)\, |\Gamma|^{-n}\, N^{1+n} \\
&\quad + \mathcal{B}_p(\Gamma, f; N) + \mathcal{O}(N^{1-2p}) \\
&= 2N \sum_{n=m}^{\infty} \mathrm{J}_{-n}(\lambda)\, \zeta(n) (N/|\Gamma|)^n + 2 \sum_{n=2}^{m-1} \mathrm{J}_{-n}(\lambda)\, \zeta(n)\, |\Gamma|^{-n}\, N^{1+n} \\
&\quad + V_f(\Gamma)\, N^2 + |\Gamma|\, B_2(\frac{\kappa}{2}) f'(\frac{|\Gamma|}{2}) + 2 \sum_{k=2}^{2p} J_k(\lambda)\, \zeta(-k)\, |\Gamma|^k\, N^{1-k} \\
&\quad + \sum_{n=2}^{p} \frac{2 B_{2n}(\kappa/2)}{(2n)!\, |\Gamma|^{1-2n}} f^{(2n-1)}(|\Gamma|/2) N^{2-2n} + \mathcal{O}(N^{1-2p}),
\end{aligned}$$

where

$$V_f(\Gamma) = \frac{2}{|\Gamma|} \sum_{\substack{n=-\infty,\\ n\neq\pm1}}^{\infty} \mathrm{J}_n(\lambda) \frac{(|\Gamma|/2)^{1+n}}{1+n}.$$

In the above we used relation (5). Observe that $\zeta(-k) = 0$ for $k = 2, 4, 6, \dots$. $\square$

Proof of Theorem 13. The asymptotics and the remainder estimates follow from Theorem 5 on observing that $f_s^w(x)$ has derivatives of all orders in $(0, |\Gamma|/2 + \varepsilon)$, $S_q(x) = \sum_{n=0}^{q} a_n x^{n-s}$, and $\delta = 1$. The constraints on $s_q = s - q$ imply that the positive integers q, p and $s \in \mathbb{C}$ satisfy $q - 2p < \operatorname{Re} s < 2 + q$ or $s = q - 2p$. For $0 < s < 1$ we have (see (7))

$$V_{f_s^w}(\Gamma) = \frac{2}{|\Gamma|} \int_0^{|\Gamma|/2} f_s^w(x)\, dx = \frac{2}{|\Gamma|} \sum_{n=0}^{\infty} a_n \frac{(|\Gamma|/2)^{1+n-s}}{1+n-s}$$

and the right-hand side as a function of s is analytic in $\mathbb{C}$ except for poles at $s = 1 + n$ ($n = 0, 1, 2, \dots$) provided $a_n \neq 0$. $\square$

Using the same method of proof as in [21] for the Hurwitz zeta function, we obtain the following two propositions, which will be used in the proofs of Theorems 16 and 17.

Proposition 24. *Let $q \geq 1$ and $\alpha = 1/2$ or $\alpha = 1$. For $x > 0$ and $s \in \mathbb{C}$ with $s \neq 1$ and $\operatorname{Re} s + 2q + 1 > 0$ the* Hurwitz zeta function *defined by the series $\zeta(s, a) := \sum_{k=0}^{\infty} (k + a)^{-s}$ for $\operatorname{Re} s > 1$ and $a \neq 0, -1, -2, \dots$ has the following representation*

$$\zeta(s, x + \alpha) = \frac{x^{1-s}}{s-1} - B_1(\alpha)\, x^{-s} + \sum_{n=1}^{q} \frac{B_{2n}(\alpha)}{(2n)!} (s)_{2n-1} x^{1-s-2n} + \rho_q(s, x, \alpha).$$

The remainder term is given by

$$\rho_q(s, x, \alpha) = \frac{1}{2\pi i} \int_{\gamma_q - i\infty}^{\gamma_q + i\infty} \frac{\Gamma(-w)\, \Gamma(s+w)}{\Gamma(s)} \zeta(s+w, \alpha) x^w \, dw = \mathcal{O}_{s,q}(x^{-1-\operatorname{Re} s - 2q})$$

as $N \to \infty$, where $-1 - \operatorname{Re} s - 2q < \gamma_q < -\operatorname{Re} s - 2q$.

By the well-known relation $\log[\Gamma(x+\alpha)/\sqrt{2\pi}] = \frac{\partial}{\partial s} \zeta(s, x+\alpha)|_{s=0}$ one obtains the next result from Proposition 24.

Proposition 25. *Let $q \geq 1$ and $\alpha = 1/2$ or $\alpha = 1$. For $x > 0$*

$$\log \frac{\Gamma(x+\alpha)}{\sqrt{2\pi}} = (x + \alpha - 1/2) \log x - x + \sum_{n=1}^{q} \frac{B_{2n}(\alpha)}{(2n-1)\, 2n} x^{1-2n} + \rho_q(x, \alpha).$$

The remainder term is given by

$$\rho_q(x,\alpha) = \frac{1}{2\pi i} \int_{\gamma_q - i\infty}^{\gamma_q + i\infty} \Gamma(-w)\,\Gamma(w)\,\zeta(w,\alpha) x^w \, dw = \mathcal{O}_q(x^{-1-2q})$$

as $N \to \infty$, *where* $-1-2q < \gamma_q < -2q$.

In the proofs of Theorems 16 and 17 we make use of the observation that for $N = 2M + \kappa$ with $M \geq 1$ and $\kappa = 0, 1$ formula (4) simplifies to

$$\mathcal{M}_s(\Gamma; N) = \frac{2}{|\Gamma|^s} N^{1+s} \sum_{k=1}^{\lfloor N/2 \rfloor} \frac{1}{k^s} - \frac{1-\kappa}{(|\Gamma|/2)^s} N, \tag{24}$$

which involves the *generalized harmonic numbers* $H_n^{(s)} := \sum_{k=1}^{n} k^{-s}$.

P r o o f o f T h e o r e m 16. Differentiating (24) with respect to s and taking the limit $s \to 0$ yields

$$\mathcal{M}_{\log}(\Gamma; N) = N\,(N-\kappa) \log \frac{N}{|\Gamma|} - 2N \log \Gamma(\lfloor N/2 \rfloor + 1) - (1-\kappa)\, N \log(N/2).$$

The asymptotic expansion of the theorem now follows by applying Proposition 25 with $x = N/2$, $\alpha = (2-\kappa)/2$. Note that $B_{2n}(\alpha) = B_{2n}(1-\kappa/2) = B_{2n}(\kappa/2)$. □

P r o o f o f T h e o r e m 17. Starting with Theorem 5, we obtain an asymptotic formula of the form (14) but with error estimate $\mathcal{O}(N^{1-2q})$.[‡‡] On the other hand, substitution of the identity $\sum_{k=1}^{n} k^{-s} = \zeta(s) - \zeta(s, n+1)$ into (24) gives the exact formula

$$\mathcal{M}_s(\Gamma; N) = \frac{2\,\zeta(s)}{|\Gamma|^s} N^{1+s} - \frac{2}{|\Gamma|^s} N^{1+s}\, \zeta(s, \lfloor N/2 \rfloor + 1) - \frac{1-\kappa}{(|\Gamma|/2)^s} N.$$

Then the asymptotic relation (14) with error term of order $\mathcal{O}(N^{-2q})$ follows by applying Proposition 24 with $x = N/2$, $\alpha = (2-\kappa)/2$. This expansion holds for s with $\operatorname{Re} s + 2q + 1 > 0$, $q \geq 1$. □

P r o o f o f P r o p o s i t i o n 18. Using Jacob Bernoulli's celebrated summation formula ([1, Eq. (23.1.4)]) $1^p + 2^p + \cdots + n^p = (B_{p+1}(n+1) - B_{p+1})/(p+1)$ in (24), one gets

$$\mathcal{M}_{-p}(\Gamma; N) = 2\,|\Gamma|^p\, \frac{B_{p+1}((N+\kappa)/2) - B_{p+1}}{p+1} N^{1-p} + (1-\kappa)\,(|\Gamma|/2)^p\, N.$$

Use of the addition theorem for Bernoulli polynomials (see [1, Eq. (23.1.7)]) yields the result. □

[‡‡]If $\operatorname{Re} s = -2q$ and $s \neq 2q$, then a factor $\log N$ must be included.

Proof of Theorem 19. An asymptotic formula with error bound $\mathcal{O}(N^{1-2p})$ follows from Theorem 6; see also the second remark after Theorem 6. However, by substituting into (24) with $\omega = \kappa/2$ ($\kappa = 0, 1$) the following relation

$$\begin{aligned} H_n = \sum_{k=1}^{n} \frac{1}{k} = \log(n+\omega) + \gamma - \frac{B_1(\omega)}{n+\omega} - \sum_{k=1}^{q} \frac{B_{2k}(\omega)/(2k)}{(n+\omega)^{2k}} \\ \pm \theta_{q,N,\kappa} \frac{B_{2q+2}(\omega)/(2q+2)}{(n+\omega)^{2q+2}}, \end{aligned} \tag{25}$$

where $0 < \theta_{q,N,\kappa} < 1$, and collecting terms we get the asymptotic formula (16) with improved error estimate. The plus sign in (25) is taken if $\omega = 1/2$ and the negative sign corresponds to $\omega = 0$. We remark that the representation (25) is given in [12] if $\omega = 1/2$ and can be obtained as an application of the Euler-MacLaurin summation formula if $\omega = 0$ (see, for example, [3]). We leave the details to the reader. □

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J. S. Brauchart
School of Mathematics and Statistics,
University of New South Wales,
Sydney, NSW, 2052,
Australia
E-mail: j.brauchart@unsw.edu.au

D. P. Hardin and E. B. Saff
Center for Constructive Approximation,
Department of Mathematics,
Vanderbilt University,
Nashville, TN 37240,
USA
E-mail: Doug.Hardin@Vanderbilt.Edu
Edward.B.Saff@Vanderbilt.Edu