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Electrostatic fields due to distributions of electrons

JACOB KOREVAAR⁽¹⁾

1. Introduction

Working in \mathbb{R}^s ($s \geq 2$) with the classical potential, we let K denote a compact set (“conductor”) of positive capacity. By ω we denote the unique distribution of positive charge on K of total charge 1 with minimal potential energy. This probability measure defines the so-called classical equilibrium distribution for K , whose support belongs to the outer boundary $\partial_0 K$, cf. Frostman [5]. We wish to approximate ω by distributions (probability measures) $\mu_N = \mu_N(x_1, \dots, x_N)$ which consist of N point masses or charges $1/N$ (“electrons”) at points x_1, \dots, x_N of K . If one imposes the condition of minimal potential energy on such discrete measures, one obtains what we call a “Fekete equilibrium distribution” ω_N . Its support is a set of N th order “Fekete points” f_{N1}, \dots, f_{NN} for K , which are located on $\partial_0 K$. For planar sets, such points were introduced by Fekete in 1923 [4]. Instead of minimizing the energy, he (equivalently) maximized the product

$$\prod_{1 \leq j < k \leq N} |x_j - x_k|^2, \quad x_1, \dots, x_N \in K.$$

The quality of the approximation to ω by μ_N can be measured in different ways. One may estimate the differences $\omega(E) - \mu_N(E)$ for suitably regular sets E , or one may compare the potentials U^ω and U^{μ_N} or the electrostatic fields \mathcal{E}^ω and \mathcal{E}^{μ_N} . The paper surveys results on the following main problems.

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PROBLEM 1. — *It should be of physical interest to compare the classical equilibrium field with “Fekete fields” for large N . How small are the differences $\mathcal{E}^\omega - \mathcal{E}^{\omega_N}$ away from the outer boundary $\partial_0 K$?*

One knows that $\mathcal{E}^\omega = 0$ throughout the interior of the conductor K (Faraday cage phenomenon of electrostatics). Question: How small is \mathcal{E}^{ω_N} inside K for large N ? In other words, how well can one explain the Faraday cage phenomenon on the basis of a model, in which the total charge 1 on the conductor is made up of a large number of equal point charges?

PROBLEM 2. — *How small can one make $\mathcal{E}^\omega - \mathcal{E}^{\mu_N}$ for large N if one allows arbitrary distributions μ_N of N point charges $1/N$ on $\partial_0 K$?*

Beginning in 1885, STIELTJES devoted a number of papers to equilibrium problems for point charges on a segment in the plane and related matters, see [29]–[32] and cf. Van Assche [34]. Among other things STIELTJES’ work contains a description of the Fekete points for the case where K is the interval $[-1, 1]$, cf. the Examples 2.1 below.

For a conductor K given by an analytic or $C^{3,\alpha}$ Jordan curve Γ in the plane, Pommerenke ([24], [25]) and Korevaar and Kortram ([11], [15]) have obtained close approximations to the Fekete points. For very smooth Γ , the approximations show that $\omega(E) - \omega_N(E) = \mathcal{O}(1/N)$, uniformly for the subarcs $E \subset \Gamma$. Via a STIELTJES integral for the potential difference $U^\omega - U^{\omega_N}$, the approximations imply that $\mathcal{E}^\omega - \mathcal{E}^{\omega_N}$ is at most of order $1/N$ at distance $\geq \epsilon > 0$ from the curve, see Korevaar and coauthors Geveci and Kortram ([11], [14, [15])). This order is sharp except when Γ is a circle.

For less smooth conductors in the plane (such as a square) and for conductors in higher dimensions, there are separation results for the points in Fekete N -tuples (Kövari and Pommerenke [19], [20]; Dahlberg [3]), but only the beginnings of good approximations, cf. Sjögren [28]. Without explicit information about the Fekete points, Korevaar and his student Monnerie have recently obtained rather precise estimates for $\mathcal{E}^\omega - \mathcal{E}^{\omega_N}$ in the case of convex or smoothly bounded sets K . In \mathbb{R}^3 the basic order is $1/\sqrt{N}$. The precise results will be stated and the various steps in the proof will be sketched in Section 3.

On Problem 2 it is known that at least for smooth Jordan curves in the plane different from circles, the Fekete fields give much worse approximations to the classical equilibrium field than the fields due to certain other N -tuples of point charges $1/N$, cf. Korevaar and Geveci [14] for the case of analytic curves. In the present paper we will restrict ourselves

to the case of the unit sphere S in \mathbb{R}^3 where the situation is unclear. For the sphere, Problem 2 is of interest because of its relation to Chebyshev-type quadrature formulas, that is, quadrature formulas in which all N nodes carry the same weight. Very good N -tuples of Chebyshev nodes on S correspond to N -tuples of point charges $1/N$ on the sphere for which the electrostatic field is extremely small on compact subsets of the unit ball, see Section 4 and Korevaar and Meyers [16]. The optimal order of smallness lies between $\exp(-cN^{1/3})$ and $\exp(-cN^{1/2})$ [16].

It is conjectured that the latter order can be achieved. A proof may be derived from a plausible (but unproved) separation result for the N th order Fekete points on the sphere relative to the nonstandard potential given by (2.4) below, see Theorem 4.3 and cf. Korevaar [13].

2. Basic notions and results from potential theory

Throughout the paper, μ stands for an *arbitrary probability measure* on the compact set $K \subset \mathbb{R}^s$. It is convenient to start with general (repulsive) potentials of the form

$$U^\mu(x) = \int_K \Phi(|x - y|) d\mu(y), \quad (2.1)$$

where $\Phi(r)$ is smooth on $(0, \infty)$ and strictly decreasing. The field and the potential energy are given by

$$\mathcal{E}^\mu(x) = -\text{grad } U^\mu(x), \quad I(\mu) = \int_{K \times K} \Phi(|x - y|) d\mu(x) d\mu(y). \quad (2.2)$$

We are primarily interested in the classical potential for \mathbb{R}^s which corresponds to

$$\Phi(r) = \begin{cases} 1/r^{s-2} & \text{if } s > 2, \\ \log(1/r) & \text{if } s = 2. \end{cases} \quad (2.3)$$

For $\Phi(r) = 1/r^\alpha$ ($0 < \alpha < s$) one obtains the Riesz potentials. In \mathbb{R}^3 another interesting potential is given by

$$\Phi(r) = 1/\sqrt{r^2 + a^2} \quad (a > 0). \quad (2.4)$$

Let us first assume $\inf_\mu I(\mu) < \infty$. For the classical potential Frostman [5] proved that there is a unique probability measure μ on K with minimal

potential energy, the “equilibrium distribution” ω for K with the following properties:

$$I(\omega) = V = V_K \stackrel{\text{def}}{=} \min I(\mu),$$

$$U^\omega \leq V \text{ throughout } \mathbb{R}^s,$$

$$U^\omega = V \text{ inside } K \text{ and quasi everywhere on } \partial_0 K,$$

so that $\mathcal{E}^\omega = 0$ inside K . If $\inf I(\mu) = \infty$ one sets $V = \infty$. The constant $V = V_K$ is called “Robin’s constant” (after the mathematical physicist Robin [26]). It is customary to define

$$\text{cap } K = \Phi^{-1}(V_K), \tag{2.5}$$

so that the capacity has the dimension of a length. The expression “quasi everywhere” above means: everywhere outside an exceptional set of (outer) capacity zero. The preceding results extend to the Riesz potentials with $s - 2 < \alpha < s$, cf. Frostman [5].

We return to the classical case, in which $\text{supp } \omega \subset \partial_0 K$. If the outer boundary $\partial_0 K$ is such that its exterior K^∞ relative to $\mathbb{R}^s \cup \{\infty\}$ is regular for the Dirichlet problem for harmonic functions, there is no exceptional set. In that case one may define a Green’s function $G(y, \infty)$ for K^∞ with pole at ∞ as follows. Excluding the case $s = 2$ for a moment, $G(y, \infty)$ is the harmonic function on $K^\infty - \{\infty\}$ with boundary values 0 on $\partial K^\infty = \partial_0 K$ and 1 at ∞ . Thus for $s \geq 3$,

$$\begin{aligned} G(y, \infty) &= 1 - U^\omega(y)/V \quad \text{for } y \in K^\infty \\ &= 1 - \left(\frac{\text{cap } K}{|y|} \right)^{s-2} + \mathcal{O} \left(\frac{1}{|y|^{s-1}} \right) \quad \text{as } y \rightarrow \infty. \end{aligned} \tag{2.6}$$

In the case $s = 2$ one has $G(y, \infty) = V - U^\omega(y)$. For well-behaved outer boundary $\partial_0 K$ one can express the equilibrium measure in terms of the normal derivative $(\partial G / \partial n_y)(y, \infty)$, see Theorem 6.3.

As stated in the Introduction, we also consider *special discrete probability measures*

$$\mu_N = \mu_N(x_1, \dots, x_N) \quad (N \geq 2)$$

given by charges $1/N$ at points $x_1, \dots, x_N \in K$. The corresponding potential and *discrete energy* are

$$U^{\mu_N}(x) = \frac{1}{N} \sum_{k=1}^N \Phi(|x - x_k|), \quad I^*(\mu_N) = \frac{1}{N^2} \sum_{j,k=1, j \neq k}^N \Phi(|x_j - x_k|). \tag{2.7}$$

(Observe that the “ordinary” energy $I(\mu_N)$ may be equal to ∞ .)

Any μ_N with minimal discrete energy will be denoted by ω_N and called an N th order *Fekete measure* on K . The carrying points are N th order Fekete points f_{N1}, \dots, f_{NN} . For the classical potential they lie on $\partial_0 K$. Fekete N -tuples need *not* be *unique*.

Examples 2.1. — On the unit circle or the closed unit disc in the plane, the Fekete N -tuples are given by the N th roots of unity or their rotations through a fixed angle, cf. Schur [27].

For the segment $[-1, 1]$ in the plane, STIELTJES' results of 1885-86 imply that the Fekete points are the zeros of $(1 - x^2)P'_{N-1}(x)$, where P_k denotes the Legendre polynomial of degree k , cf. Stieltjes [29]–[32], Schur [27], Szegő's book [33, Sect. 6.7] and Van Assche [34].

In the case of the unit sphere in \mathbb{R}^3 , we will also be interested in the Fekete points for the potential given by (2.4).

It follows from Frostman's work that for the classical potentials (as well as the Riesz potentials with $s - 2 < \alpha < s$) and every compact set K of positive capacity,

$$\omega_N \rightarrow \omega \quad \text{in weak* sense as } N \rightarrow \infty, \quad (2.8)$$

cf. Frostman [5, pp. 47 and 10].

3. Fekete fields in \mathbb{R}^s : new results

In the following, Σ will be a bounded closed (hyper)surface whose complement has two components. The interior domain will be called Ω , while the exterior domain – including the point at ∞ – is denoted by Ω^∞ . It will be convenient to think of K as $\text{clos } \Omega$. We use the classical potentials here.

THEOREM 3.1 (Korevaar and Monterie [17], cf. Monterie [21]). — *For $\Omega \subset \mathbb{R}^s$ convex or $\Sigma = \partial\Omega$ of class $C^{1,\alpha}$, and at distance $\geq \epsilon > 0$ from Σ , there are uniform estimates*

$$U^\omega - U^{\omega_N} = \mathcal{O}\left(\frac{1}{N^{1/(s-1)}}\right), \quad \mathcal{E}^\omega - \mathcal{E}^{\omega_N} = \mathcal{O}\left(\frac{1}{N^{1/(s-1)}}\right) \quad \text{if } s \geq 3,$$

$$U^\omega - U^{\omega_N} = \mathcal{O}\left(\frac{\log N}{N}\right), \quad \mathcal{E}^\omega - \mathcal{E}^{\omega_N} = \mathcal{O}\left(\frac{\log N}{N}\right) \quad \text{if } s = 2 \quad (N \geq 2).$$

Since the proof has not appeared in a journal we will present an outline here, and provide additional technical details in Sections 5 and 6. For the time being *we take* $s \geq 3$.

Step 1. — In order to manufacture a positive potential, we introduce a *lower bound* for the difference $U^{\omega_N} - U^\omega$ on K or Σ . Here $U^\omega \equiv V$, the Robin constant for K . Setting

$$\min_{x \in \Sigma} \{U^{\omega_N}(x) - U^\omega(x)\} = -\delta(\omega_N), \quad (3.1)$$

it is easy to see that $\delta(\omega_N) > 0$. Indeed, by Fubini's theorem,

$$\int_{\Sigma} (U^{\omega_N} - U^\omega) d\omega = \int_{\Sigma} U^\omega d\omega_N - \int_{\Sigma} U^\omega d\omega = V - V = 0.$$

Hence $U^{\omega_N} - U^\omega$, which is positive near the Fekete points, must be negative somewhere on Σ (the support of ω is all of Σ).

We now form the auxiliary potential

$$T(x) \stackrel{\text{def}}{=} U^{\omega_N}(x) - \{1 - \delta(\omega_N)/V\}U^\omega(x) = U^{\rho_N}(x), \quad (3.2)$$

$$\rho_N \stackrel{\text{def}}{=} \omega_N - \{1 - \delta(\omega_N)/V\}\omega, \quad \text{supp } \rho_N \subset \Sigma.$$

By (3.1), $T(x) \geq 0$ on Σ , hence $T(x) > 0$ throughout $\mathbb{R}^s - \Sigma$ (minimum principle for harmonic functions).

Step 2. — If Σ is the unit sphere, $V = 1/\text{cap } \Sigma = 1$, so that $T(0) = \delta(\omega_N)$. One may then use the Poisson integral or Harnack's inequality to prove that T , and hence $U^{\omega_N} - U^\omega < T$, is $\leq \mathcal{O}(\delta(\omega_N))$ away from the surface, cf. Korevaar [12] for $s = 3$.

In the general case there is usually no finite center where one has information about the value of T . However, *we do have information at infinity*:

$$L(T) \stackrel{\text{def}}{=} \lim_{x \rightarrow \infty} |x|^{s-2}T(x) = \delta(\omega_N)/V, \quad (3.3)$$

since $\lim |x|^{s-2}U^\mu(x) = 1$ for all probability measures μ .

For x in the exterior domain Ω^∞ one may now use a Harnack-type inequality around ∞ to conclude that for the positive harmonic function T ,

$$|x|^{s-2}T(x) \leq c(d_x)L(T), \quad d_x = d(x, \Sigma). \quad (3.4)$$

To verify this one may apply Kelvin inversion with center $0 \in \Omega$; for finite domains there is a general Harnack inequality in Gilbarg and Trudinger [8]. In our case, $c(d_x)$ turns out to be $\leq c_1(1 + 1/d_x^{s-1})$, cf. Korevaar and Monterie [17] for $s = 3$.

Step 3.— We next take x in the interior domain Ω . For our kind of domains, there are integrals for $T(x)$ and $L(T)$ over Σ in terms of normal derivatives of Green's functions, as well as certain useful inequalities for those derivatives, see Section 6. Using suitably normalized area measure σ , these tools enable us to estimate as follows:

$$\begin{aligned} T(x) &= \int_{\Sigma} T(y) \frac{\partial G}{\partial n_y}(y, x) d\sigma(y) \leq M(d_x) \int_{\Sigma} T(y) d\sigma(y) \\ &\leq \frac{M(d_x)}{m(\infty)} \int_{\Sigma} T(y) \frac{\partial G}{\partial n_y}(y, \infty) d\sigma(y) = \frac{M(d_x)}{m(\infty)} L(T) \\ &\leq \frac{c_2}{d_x^{s-1}} L(T). \end{aligned} \quad (3.5)$$

Indeed, $(\partial G/\partial n_y)(y, x)$ will be bounded above by a constant $M(d_x) \leq c/d_x^{s-1}$ for $x \in \Omega$ and $y \in \Sigma$, while $(\partial G/\partial n_y)(y, \infty)$ is bounded from below by a positive constant $m(\infty)$ (Section 6).

Step 4.— Comparison of $U^{\omega_N} - U^{\omega}$ on K or Σ with a difference of energies will show that under the hypotheses of Theorem 3.1,

$$\delta(\omega_N) \leq \frac{c_3}{N^{1/(s-1)}}, \quad (3.6)$$

see Section 5.

Step 5.— The end result from (3.1)–(3.6) is that for $N \geq 2$ and all $x \notin \Sigma$,

$$-\frac{c_3}{N^{1/(s-1)}} < U^{\omega_N}(x) - U^{\omega}(x) < T(x) < \frac{c_4(1 + d_x)}{d_x^{s-1}} \frac{1}{N^{1/(s-1)}} \quad (s \geq 3) \quad (3.7)$$

where $d_x = d(x, \Sigma)$ and the constants c_j depend only on Ω .

An upper bound for $|\mathcal{E}^{\omega} - \mathcal{E}^{\omega_N}|$ may be obtained from (3.7) with the aid of the Poisson integral. The result is that for $N \geq 2$ and all $x \notin \Sigma$,

$$|\mathcal{E}^{\omega}(x) - \mathcal{E}^{\omega_N}(x)| < \frac{c_5(1 + d_x)}{d_x^s} \frac{1}{N^{1/(s-1)}} \quad (s \geq 3). \quad (3.8)$$

Remarks

In the case of dimension $s = 2$ one would define $T(x) = U^{\omega_N}(x) - U^\omega(x) + \delta(\omega_N)$. Here the method of Section 5 will give $\delta(\omega_N) = \mathcal{O}((\log N)/N)$, hence the disappointing estimate for $s = 2$ in Theorem 3.1. One has the feeling that the logarithm should not be there, cf. the known result for very smooth curves! In fact, in the degenerate case of the interval $[-1, 1]$, direct computation of the difference of the potentials also gives an estimate $\mathcal{O}(1/N)$. On the other hand it may be remarked that a related older result of Pommerenke for (simply connected) exterior domains also contains a logarithm [23].

In a way it is encouraging that the present method gives a result for smooth curves which is close to best possible. Thus the following conjecture appears to be reasonable.

CONJECTURE 3.2. — *The order $1/N^{1/(s-1)}$ for dimensions $s \geq 3$ in Theorem 3.1 is sharp except possibly for the case where Σ is a sphere.*

4. Small fields due to electrons on the sphere

For the unit circle $C = C(0, 1)$ in the plane, the Fekete N -tuples are given by the N th roots of unity or their rotations through a fixed angle. Here $|\mathcal{E}^\omega(x) - \mathcal{E}^{\omega_N}(x)|$ will become exponentially small outside a fixed neighborhood of C as $N \rightarrow \infty$. Restricting oneself to the interior of C , one finds that

$$\sup_{|x| \leq r} |\mathcal{E}^{\omega_N}(x)| = \frac{r^{N-1}}{1 - r^N} \quad \text{for } 0 < r < 1.$$

For smooth Jordan curves other than circles, very small electrostatic fields \mathcal{E}^{μ_N} are associated with charges at the images of N th roots of unity under an exterior conformal map rather than Fekete points, cf. Korevaar and Geveci [14]. In a sense this is true even for the outer boundary of an arbitrary connected compact set, see Korevaar [10].

The unit sphere $S = S(0, 1) \subset \mathbb{R}^3$

Preliminary numerical results of Kuijlaars and Voogd in Amsterdam suggest that for the sphere S , the *Fekete* fields \mathcal{E}^{ω_N} do not become extremely

small on interior balls $B(0, r)$ as $N \rightarrow \infty$. But *how small* can one make the fields \mathcal{E}^{μ_N} on such balls if one allows *arbitrary* N -tuples of point charges $1/N$ on S ?

It will be convenient to introduce some new notation. In the following $Z_N = (\zeta_1, \dots, \zeta_N)$ stands for an N -tuple of points on S . The corresponding N -tuple μ_N of point charges $1/N$ will be denoted by $\mu(Z_N)$. For the potential U^{μ_N} and the electrostatic field \mathcal{E}^{μ_N} we will write $U(\cdot, Z_N)$ and $\mathcal{E}(\cdot, Z_N)$.

THEOREM 4.1 (Korevaar and Meyers [16]). — *On the unit sphere S there are special N -tuples of points Z_N such that for $N \rightarrow \infty$, the differences*

$$\mathcal{E}^\omega(x) - \mathcal{E}(x, Z_N) \tag{4.1}$$

become as small as $\mathcal{O}(e^{-cN^{1/3}})$ outside any given neighborhood of S (with $c > 0$ depending on the neighborhood). However, the differences can not become of smaller order than $e^{-cN^{1/2}}$.

The proof depends on the close relation between the electrostatic field $\mathcal{E}(\cdot, Z_N)$ inside S and Chebyshev-type quadrature on S with nodes Z_N mentioned in the Introduction. Good N -tuples Z_N will be described below when we discuss Chebyshev-type quadrature. As to the second part, it was shown in [16] that for *every* N -tuple Z_N on S ,

$$\sup_{|x|=r} |\mathcal{E}(x, Z_N)| > \frac{r^{2\sqrt{N}}}{4(\sqrt{N} + 1)^3}, \quad 0 < r < 1.$$

CONJECTURE 4.2. — *We conjecture that for suitably chosen families of N -tuples Z_N on S , where $N \rightarrow \infty$, the associated differences (4.1) become as small as $\mathcal{O}(e^{-cN^{1/2}})$ outside any given neighborhood of S (with $c > 0$ again depending on the neighborhood).*

The following conditional result describes candidate N -tuples Z_N for the conjecture.

THEOREM 4.3 (cf. Korevaar [13]). — *Let the N -tuples $Z_N = (\zeta_1, \dots, \zeta_N)$, with $\zeta_k = \zeta_k^{(N)}$, $N \geq 2$ be Fekete N -tuples on S for the potential $\Phi(r) = 1/\sqrt{r^2 + a^2}$ where $a > 0$ is arbitrary. In other words, for each N , the N -tuple of points ζ_1, \dots, ζ_N minimizes the corresponding function*

$$\sum_{j,k=1}^N \frac{1}{\sqrt{|x_j - x_k|^2 + a^2}}, \quad x_1, \dots, x_N \in S.$$

If it is true [as we conjecture] that the points in the minimizing N -tuples are well-separated, that is, if

$$|\zeta_j^{(N)} - \zeta_k^{(N)}| \geq \frac{\delta}{\sqrt{N}}, \quad j \neq k \quad (4.4)$$

for some constant $\delta > 0$ independent of N , then the corresponding differences (4.1) are of order $\mathcal{O}(e^{-cN^{1/2}})$ at distance $\geq \epsilon > 0$ from S as $N \rightarrow \infty$.

The proof is quite technical. It makes essential use of the fact that a bounded analytic function of two complex variables with many zeros is small provided the zeros are well-separated. If an analytic function of one complex variable on the unit disc is bounded by 1 and has N zeros on a concentric disc of radius $r_0 < 1$, the function will be $\mathcal{O}(e^{-cN})$ on the latter disc. For a related result in $q \geq 2$ complex variables one needs separated zeros and then the order of smallness is $\mathcal{O}(e^{-cN^{1/q}})$, cf. [13].

Chebyshev-type quadrature on S

The existence of special N -tuples Z_N on S with very small differences (4.1) is important for Chebyshev-type quadrature on the sphere.

Relative to normalized area measure $\sigma = \lambda/4\pi$, the Chebyshev-type quadrature formula for S with nodes at the points ζ_1, \dots, ζ_N of Z_N has the form

$$\int_S f(\zeta) d\sigma(\zeta) \approx \frac{1}{N} \sum_{k=1}^N f(\zeta_k). \quad (4.5)$$

The difference between the two members is the quadrature remainder,

$$R(f, Z_N) = \int_S f(\zeta) d\sigma(\zeta) - \frac{1}{N} \sum_{k=1}^N f(\zeta_k). \quad (4.6)$$

The quadrature formula (4.5) is called (polynomially) exact to degree p if $R(f, Z_N) = 0$ for all polynomials $f(x) = f(x_1, x_2, x_3)$ of degree $\leq p$.

We will call $Z_N = (\zeta_1, \dots, \zeta_N)$ a “good” N -tuple of nodes if formula (4.5) is exact to relatively high degree $p = p_N$, or if at least the remainder (4.6) is very small for such polynomials.

Observe that $U^\omega(x) - U(x, Z_N)$ can be interpreted as a quadrature remainder. For $|x| < 1$,

$$U^\omega(x) - U(x, Z_N) = \int_S \frac{1}{|x - \zeta|} d\sigma(\zeta) - \frac{1}{N} \sum_{k=1}^N \frac{1}{|x - \zeta_k|} = 1 - U(x, Z_N). \quad (4.7)$$

This fact was used by Korevaar and Meyers [16], cf. Korevaar [13], to derive the following

Equivalence principle

Z_N forms a good N -tuple of nodes for Chebyshev-type quadrature on S if and only if the corresponding distribution $\mu(Z_N)$ of charges $1/N$ gives a nearly constant potential $U(\cdot, Z_N)$ or a small electrostatic field $\mathcal{E}(\cdot, Z_N)$ on a ball (or on all balls) $B(0, r)$ with $0 < r < 1$. (The differences (4.1) will then also be small for $|x| > R > 1$.)

Some precise forms are the following.

THEOREM 4.4. — *The Chebyshev-type quadrature formula (4.5) for S corresponding to the N -tuple Z_N is polynomially exact to degree p if and only if*

$$\mathcal{E}(x, Z_N) = \mathcal{O}(|x|^p) \quad \text{for } 0 \leq |x| \leq c < 1. \quad (4.8)$$

THEOREM 4.5. — *The following two statements, involving a constant $\alpha > 0$ and a family of N -tuples Z_N on S with $N \rightarrow \infty$, are equivalent:*

- (i) *For some (or every) $r \in (0, 1)$ there are positive constants $c_1(r)$ and $c_2(r)$ such that*

$$\sup_{|x| \leq r} |\mathcal{E}(x, Z_N)| \leq c_1(r) \exp(-c_2(r)N^\alpha) \quad (N \rightarrow \infty). \quad (4.9)$$

- (ii) *There are positive constants c_3, c_4, c_5 such that*

$$|R(f, Z_N)| \leq c_3 \exp(-c_4 N^\alpha) \sup_S |f| \quad (4.10)$$

for all polynomials f of degree $\leq c_5 N^\alpha$.

N -tuples Z_N for which formula (4.5) is exact to degree $p \approx cN^{1/3}$ have been described by Korevaar and Meyers in [16], cf. Korevaar [13]. Starting point was the following existence theorem of S. N. Bernstein [1].

PROPOSITION 4.6. — For odd $p = 2q - 1 \geq 1$, let M be even and

$$\geq N_1(p) = 2 \left[2\sqrt{2}(q+1)(q+4) + 1 \right]$$

where $[\cdot]$ denotes integral part. Then there exist points $z_1 > z_2 > \dots > z_p$, $z_{2q-j} = -z_j$ and positive integral weights $m_j = m_{2q-j}$, $\sum_{j=1}^p m_j = M$ such that for all polynomials $g(z)$ of degree $\leq p$,

$$\int_{-1}^1 g(z) \frac{1}{2} dz = \frac{1}{M} \sum_{j=1}^p m_j g(z_j).$$

On the sphere, it is now convenient to use coordinates x, y, z as follows:

$$x = \sin \theta \cos \phi, \quad y = \sin \theta \sin \phi, \quad z = \cos \theta, \quad 0 \leq \theta \leq \pi, \quad 0 \leq \phi < 2\pi,$$

with normalized area element

$$d\sigma(x, y, z) = \frac{1}{4\pi} \sin \theta d\theta d\phi = \frac{1}{4\pi} |dz| d\phi.$$

COROLLARY 4.7. — For $p = 2q - 1 \geq 1$ we set $N(p) = (p+1)N_1(p)$ with $N_1(p)$ as above. Let $z_1 > z_2 > \dots > z_p$ and the positive integers m_1, \dots, m_p also be as in Proposition 4.6 and set

$$\phi_{j,k} = (k-1) \frac{2\pi}{(p+1)m_j}, \quad j = 1, \dots, p, \quad k = 1, \dots, (p+1)m_j.$$

Then for all polynomials $f(x, y, z) \simeq F(z, \phi)$ of degree $\leq p$.

$$\int_S f d\sigma = \frac{1}{4\pi} \int_{-1}^1 \int_0^{2\pi} F(z, \phi) dz d\phi = \frac{1}{N(p)} \sum_{j=1}^p \sum_{k=1}^{(p+1)m_j} F(z_j, \phi_{j,k}).$$

In other words, the Chebyshev-type quadrature formula for S with the $N = N(p) \approx \sqrt{2}p^3$ distinct nodes

$$\zeta_{j,k} \simeq (z_j, \phi_{j,k}), \quad 1 \leq j \leq p, \quad 1 \leq k \leq (p+1)m_j$$

is exact to degree $p \approx cN^{1/3}$. It follows that parts (ii) and (i) in Theorem 4.5 are true with $\alpha = 1/3$.

Theorem 4.3 describes N -tuples Z_N for which the two parts of Theorem 4.5 will hold with $\alpha = 1/2$ provided the conjectured separation condition (4.4) is satisfied.

We end with a strong conjecture about Chebyshev-type quadrature on S .

CONJECTURE 4.8 (Korevaar and Meyers [16]). — *There exist a constant $c > 0$ and special N -tuples Z_N of distinct nodes, $N \rightarrow \infty$ for which formula (4.5) for S is polynomially exact to degree $p_N \approx c\sqrt{N}$. Such N -tuples Z_N on S are sometimes called spherical p_N -designs. Using that terminology, our conjecture asserts that for $p \rightarrow \infty$, there exist spherical p -designs consisting of $\mathcal{O}(p^2)$ points.*

5. Technical results: comparing energies and potentials

Let K be any compact set in \mathbb{R}^s of positive capacity. The weak* convergence $\omega_N \rightarrow \omega$ may be derived from the following comparison of energies:

$$0 < (1 - 1/N)I(\omega) - I^*(\omega_N) \rightarrow 0, \quad (5.1)$$

cf. Frostman [5].

For the proof of Theorem 3.1 we need an explicit upper bound in (5.1). The basic ingredients used in the derivation below may be found in the classical work of Pólya and Szegő [22], cf. the author's report [12]. For $\rho > 0$ we let K_ρ denote the closed ρ -neighborhood of K .

PROPOSITION 5.1. — *In terms of Robin constants $V(\cdot)$ one has for $N \geq 2$ and all $\rho > 0$,*

$$0 < \left(1 - \frac{1}{N}\right) I(\omega) - I^*(\omega_N) < \left(1 - \frac{1}{N}\right) V(K) - V(K_\rho) + \frac{1}{N} \Phi(\rho). \quad (5.2)$$

Proof

(i) The first inequality. By the definition of ω_N ,

$$I^*(\omega_N) \leq \frac{1}{N^2} \sum_{\substack{j,k=1 \\ j \neq k}}^N \Phi(|x_j - x_k|), \quad \forall x_1, \dots, x_N \in K.$$

Hence by N -fold integration, recalling that $\omega(K) = 1$,

$$\begin{aligned}
 I^*(\omega_N) &= \int_{K \times \dots \times K} I^*(\omega_N) d\omega(x_1) \cdots d\omega(x_N) \\
 &< \frac{1}{N^2} \sum_{\substack{j,k=1 \\ j \neq k}}^N \int_{K \times K} \Phi(|x_j - x_k|) d\omega(x_j) d\omega(x_k) \cdot \omega(K)^{N-2} \quad (5.3) \\
 &= \frac{N-1}{N} I(\omega).
 \end{aligned}$$

(ii) The second inequality. Let ω_N^ρ be the probability measure on K_ρ , obtained from ω_N on K by distributing the charges $1/N$ at the Fekete points f_{Nk} uniformly over the spheres $S(f_{Nk}, \rho)$ of radius ρ , centered at those points. The potential U_{Nk} of the resulting measure ω_{Nk}^ρ on $S(f_{Nk}, \rho)$ satisfies the relations

$$U_{Nk}(x) = \frac{1}{N} \min \{ \Phi(\rho), \Phi(|x - f_{Nk}|) \} \leq \frac{1}{N} \Phi(|x - f_{Nk}|).$$

Thus for $j \neq k$,

$$\begin{aligned}
 \int U_{Nj} d\omega_{Nk}^\rho &\leq \frac{1}{N} \int \Phi(|x - f_{Nj}|) d\omega_{Nk}^\rho(x) = \frac{1}{N} U_{Nk}(f_{Nj}) \\
 &\leq \frac{1}{N^2} \Phi(|f_{Nj} - f_{Nk}|),
 \end{aligned}$$

while for $j = k$,

$$\int U_{Nk} d\omega_{Nk}^\rho = \frac{1}{N^2} \Phi(\rho).$$

Adding up all the terms $\int U_{Nj} d\omega_{Nk}^\rho$, it follows that

$$I(\omega_N^\rho) \leq \frac{1}{N^2} \sum_{\substack{j,k=1 \\ j \neq k}}^N \Phi(|f_{Nj} - f_{Nk}|) + \frac{1}{N} \Phi(\rho) = I^*(\omega_N) + \frac{1}{N} \Phi(\rho). \quad (5.4)$$

Finally observing that $I(\omega_N^\rho) > V(K_\rho)$, one obtains (5.2).

The minimum property of the Fekete N -tuples may be used to compare U^{ω_N} on K with $I^*(\omega_N)$, cf. Sjögren [28]:

PROPOSITION 5.2.— *One has*

$$\left(1 - \frac{1}{N}\right) U^{\omega_N}(x) \geq I^*(\omega_N), \quad \forall x \in K. \quad (5.5)$$

Indeed, for $x \in K$ and each j , by the minimum property mentioned above,

$$\sum_{k=1, k \neq j}^N \Phi(|x - f_{Nk}|) \geq \sum_{k=1, k \neq j}^N \Phi(|f_{Nj} - f_{Nk}|). \quad (5.6)$$

Summing over $j = 1, \dots, N$ one finds that $N(N-1)U^{\omega_N}(x) \geq N^2 I^*(\omega_N)$.

Combination with Proposition 5.1 gives

PROPOSITION 5.3.— *One has*

$$\begin{aligned} \delta(\omega_N) &\stackrel{\text{def}}{=} \sup_{x \in K} \{U^\omega(x) - U^{\omega_N}(x)\} \\ &< V(K) - \frac{1}{N-1} \{NV(K_\rho) - \Phi(\rho)\}, \quad \forall \rho > 0, \quad N \geq 2. \end{aligned} \quad (5.7)$$

(Recall for the proof that $U^\omega(x) \leq V(K) = I(\omega)$ on K .)

We wish to minimize the final member of (5.7) in the case where K is the closure of a well-behaved domain Ω . What we need here is

PROPOSITION 5.4 (cf. Korevaar and Monterie [17], Monterie [21]).— *If Ω is convex or $\Sigma = \partial\Omega$ is of class $C^{1,\alpha}$ and $K = \text{clos } \Omega$, there are positive constants A and B such that*

$$\text{cap } K_\rho \leq \text{cap } K + A\rho, \quad V(K_\rho) \geq V(K) - B\rho, \quad \forall \rho > 0. \quad (5.8)$$

Proof. — In the convex case we may take the origin at the center of a maximal ball in Ω . Denoting the ball by $B(0, r)$, one may use geometric arguments to show that K_ρ is contained in the set $(1 + \rho/r)K$, hence $\text{cap } K_\rho \leq (1 + \rho/r) \text{cap } K$.

In the $C^{1,\alpha}$ case one may use the level surfaces of the Green's function $G = G(y, \infty)$ for K^∞ with pole at ∞ . These must be "well-separated" since $|\text{grad } G|$ will be bounded by a constant C on K^∞ , cf. Widman ([35], [36]). In particular K_ρ will (for small ρ) be enclosed by the level

surface $\Sigma_\delta: \{G = \delta\}$ with $\delta = C\rho$. Now for $s \geq 3$, the exterior of Σ_δ will have Green's function with pole at ∞ equal to $(G - \delta)/(1 - \delta)$, hence by (2.6), $(\text{cap } \Sigma_\delta)^{s-2} = (\text{cap } K)^{s-2}/(1 - \delta)$. Conclusion: $\text{cap } K_\rho \leq (\text{cap } K)/(1 - C\rho)^{1/(s-2)}$. For $s = 2$, one finds that $V(K_\rho) \geq V(K) - C\rho$.

To complete the proof one uses the relation between the capacity and the Robin constant, cf. (2.5).

Combining Propositions 5.3 and 5.4 we can prove the crucial estimate (3.6) required for the proof of Theorem 3.1:

PROPOSITION 5.5 (cf. Korevaar and Monterie [17]). — *Under the conditions on Ω given in Theorem 3.1 or Proposition 5.4, there is a constant c depending only on Ω such that*

$$\delta(\omega_N) \leq \begin{cases} \frac{c}{N^{1/(s-1)}} & \text{if } s \geq 3, \\ \frac{c \log N}{N} & \text{if } s = 2. \end{cases} \quad (N \geq 2). \quad (5.9)$$

The proof is by minimization of the final member in (5.7) with respect to ρ , after one has replaced $V(K_\rho)$ by its minorant $V(K) - B\rho$ from (5.8).

6. Additional technical results: integral representations and inequalities

The convex or $C^{1,\alpha}$ domains Ω of Theorem 3.1 are special cases of Lipschitz domains: bounded domains Ω with Lipschitz boundary Σ . For such domains Dahlberg has proved an important result on harmonic measure. To simplify the corresponding representations, we divide the Lebesgue measure λ on the boundary surface Σ by the area $\lambda(S)$ of the unit sphere $S \subset \mathbb{R}^s$. The *adjusted area measure* will be $\sigma(y) = \lambda(y)/\lambda(S)$.

THEOREM 6.1 (Dahlberg [2], theorem 3). — *Let Ω be a Lipschitz domain and let $G(y) = G(y, x)$ be the Green's function for Ω with pole at x . Then the inward unit normal n_y and the corresponding normal derivative*

$$\frac{\partial G}{\partial n_y}(y) = \lim_{\epsilon \downarrow 0} G(y + \epsilon n_y)$$

exist for almost all $y \in \Sigma = \partial\Omega$ relative to σ . The function $\partial G/\partial n_y$ is positive a.e. and integrable over Σ . For the measurable subsets $E \subset \Sigma$, the harmonic measure

$$\omega_x(E) \text{ equals } \int_E \frac{\partial G}{\partial n_y}(y, x) d\sigma(y). \quad (6.1)$$

Not only is ω_x absolutely continuous with respect to σ , but the converse is also true.

By the definition of harmonic measure, Theorem 6.1 implies a representation formula for harmonic functions which are continuous up to the boundary. In the case of *convex* or $C^{1,\alpha}$ domains this formula can be extended to potentials of measures on the boundary by a limit process involving monotone or dominated convergence. The result is given in Theorem 6.2.

There are corresponding results for the exterior domain Ω^∞ of Σ . In the special case of the Green's function $G(y, \infty)$ with pole at ∞ one will thus obtain a representation for $L(u) = \lim |z|^{s-2} u(z)$ at ∞ . Observe that normals must always point into the domain considered, hence for the exterior domain one uses the outward normal to Σ .

THEOREM 6.2 (cf. Korevaar and Monterie [17]).— *For convex or $C^{1,\alpha}$ domains Ω as in Theorem 3.1 and for harmonic functions u on Ω or Ω^∞ that are continuous up to the boundary Σ , and also for potentials $u = U^\rho$ with $\text{supp } \rho \subset \Sigma$,*

$$\begin{aligned} u(x) &= \int_\Sigma u(y) \frac{\partial G}{\partial n_y}(y, x) d\sigma(y), \quad x \in \Omega, \\ L(u) &\stackrel{\text{def}}{=} \lim_{z \rightarrow \infty} |z|^{s-2} u(z) = \int_\Sigma u(y) \frac{\partial G}{\partial n_y}(y, \infty) d\sigma(y). \end{aligned} \quad (6.2)$$

As a by-product of our proof for the second formula (6.2) we have obtained the following representation for the equilibrium measure.

THEOREM 6.3 (cf. Korevaar and Monterie [17]).— *If K is the closure of a Lipschitz domain Ω , the equilibrium measure ω for K on $\Sigma = \partial\Omega$ has the representation*

$$d\omega(y) = \begin{cases} V \frac{\partial G}{\partial n_y}(y, \infty) d\sigma(y) & \text{if } s \geq 3, \\ \frac{\partial G}{\partial n_y}(y, \infty) d\sigma(y) & \text{if } s = 2. \end{cases} \quad (6.3)$$

For the application of Theorem 6.2 in the proof of Theorem 3.1 we need bounds on the normal derivatives of the Green's functions. Let us first suppose that $\Sigma = \partial\Omega$ is of class $C^{1,\alpha}$ and that $x \in \Omega$. Then the following results are known from the work of Lyapunov, Eydus and Widman, cf. Widman ([35], [36]) who actually considered somewhat more general Lyapunov-Dini domains Ω . The normal derivative $(\partial G/\partial n_y)(y, x)$ is continuous on Σ and strictly positive, and

$$\frac{\partial G}{\partial n_y}(y, x) \leq \frac{c}{|x-y|^{s-1}} \leq \frac{c}{d_x^{s-1}}, \quad \forall y \in \Sigma. \quad (6.4)$$

(As before, $d_x = d(x, \Sigma)$.) One may use Kelvin inversion to obtain related results for exterior Green's functions $G(y, x)$. In particular the derivative $(\partial G/\partial n_y)(y, \infty)$ will be continuous on Σ and strictly positive.

Next let Σ , or more precisely Ω , be *convex*. In this case the level surfaces for the interior Green's functions $G(y, x)$ and for the exterior Green's function $G(y, \infty)$ are also convex. This was proved by Gabriel ([6], [7]) for $s = 3$ but his proof readily extends to other dimensions (the case $s = 2$ is classical). (There is an extensive literature on convexity of level sets, cf. Kawohl [9] and N. J. Korevaar [18] for references.) As a corollary one may deduce that the normal derivative $(\partial G/\partial n_y)(y, x)$ is bounded above on Σ by a constant $A_x \leq M(d_x)$ and that the derivative $(\partial G/\partial n_y)(y, \infty)$ is bounded from below by a positive constant $m(\infty)$, cf. Korevaar and Monerie [17]. Comparison of Ω with a half-space readily shows that one may take $M(d_x) = 2(s-2)/d_x^{s-1}$ if $s \geq 3$, $M(d_x) = 2/d_x$ if $s = 2$.

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