

THE POLARIZATION PROBLEM FOR THE HONEYCOMB STRUCTURE

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ABSTRACT. We study the polarization problem in dimension 2 for the honeycomb structure and compare it to the maximal polarization lattice, the hexagonal lattice. As expected, the hexagonal lattice has higher polarization than the honeycomb at all densities.

1. INTRODUCTION AND NOTATION

The *polarization problem* has its origin in potential analysis and the study of Chebyshev constants and the work of Fekete [17] and Polyá and Szegő [22]. It has been intensively studied in recent years for the Riesz potential on the (d -dimensional) sphere, see, e.g., [1], [9], [10], [12], [19], to name just a few articles. We consider the problem for periodic point configurations in the plane and for exponential potentials of squared distance, i.e., Gaussians. A problem for potentials $f(r^2)$ with $f : \mathbb{R}_+ \rightarrow \mathbb{R}_+$, being decreasing and convex was formulated for lattices by Hardin, Petrache and Saff [20] and answered by Bétermin, Faulhuber, and Steinerberger [8]. Most recently, Bachoc, Moustrou, Vallentin, and Zimmermann characterized *cold spots* of many root lattices [2], which is a first step towards tackling the polarization problem in $\mathbb{R}^d$.

We say a function $f : \mathbb{R}_+ \rightarrow \mathbb{R}$, $r \mapsto f(r)$ is completely monotone if $(-1)^k f^{(k)}(r) \geq 0$. We will consider the following problem:

$$(1.1) \quad \max_{\Gamma \subset \mathbb{R}^d} \min_{z \in \mathbb{R}^d} \sum_{\gamma \in \Gamma} f(|\gamma - z|^2).$$

This is known as the polarization problem in Euclidean space $\mathbb{R}^d$. The minimum depends generally on the geometry and density (defined below) of Γ , and the potential f . The maximizer among (periodic) point configurations Γ is sought for a fixed density of Γ . In rare cases, a maximizer may be optimal among all densities (scales), in which case it becomes a universal polarization maximizer, much like universally optimal energy minimizers in the sense of Cohn and Kumar [13]. For energy minimization, solutions have been derived in dimensions 8 and 24 by Cohn, Kumar, Miller, Radchenko, and Viazovska [14]. The energy minimization problem in dimension 2 was solved among lattices by Montgomery [21]. For polarization, we only know that the hexagonal lattice Λ_2 (the A_2 root lattice) is a universal polarization maximizer among lattices (of any fixed density) and completely monotone potentials of squared distance [8]. In this note we prove the following polarization result.

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Theorem 1.1. *Denote the hexagonal lattice by Λ_2 and the honeycomb structure by Γ_2 , both of density 1. For an arbitrary but fixed density $\rho > 0$ and any completely monotone potential $f : \mathbb{R}_+ \rightarrow \mathbb{R}$ (of sufficient decay at infinity) of squared distance, the hexagonal lattice of density ρ has higher polarization than the honeycomb structure of density ρ :*

$$\min_z \sum_{\lambda \in \rho^{-1/2}\Lambda_2} f(|\lambda - z|^2) > \min_z \sum_{\gamma \in \rho^{-1/2}\Gamma_2} f(|\gamma - z|^2).$$

By the Bernstein-Widder theorem [5], [23], a completely monotone function of squared distance can be written as

$$(1.2) \quad f(r^2) = \int_{\mathbb{R}_+} e^{-\alpha r^2} d\mu_f(\alpha),$$

for a non-negative Borel measure μ_f . In accordance with [2], we say a structure Γ has a cold spot in z_0 if (fix f for the moment) z_0 is a minimizer in (1.1). It is a universal cold spot if it does not depend on the density of Γ . For the potential $\phi_\alpha(r^2) = e^{-\pi\alpha r^2}$, if a Γ solve (1.1) for any fixed density (which corresponds to being a maximizer at density 1 and all scales $\alpha > 0$ of the Gaussian), then it is a universal polarization maximizer for all completely monotone functions of squared distance $f(r^2)$ (given fast enough decay of f). In this case the universal cold spot is also independent of f . Yet, the existence of a universally polarization maximizers is open, except for lattices in dimension 2 [8].

A (full-rank) lattice Λ in $\mathbb{R}^d$ is a discrete co-compact subgroup (see [15] for a full introduction) and its density is the average number of lattice points per volume, given by

$$\rho(\Lambda) = 1/\text{vol}(\mathbb{R}^d/\Lambda).$$

A periodic configuration is the union of relatively shifted copies of a lattice $\Lambda \subset \mathbb{R}^d$;

$$\Gamma = \bigcup_{n=1}^N (\Lambda + x_n), \quad x_m - x_n \notin \Lambda, m \neq n.$$

The density of Γ is then given by $\rho(\Gamma) = N/\text{vol}(\mathbb{R}^d/\Lambda)$ (cf. [13, Sec. 9]).

2. UNIVERSAL COLD SPOTS AND THE HONEYCOMB STRUCTURE

The honeycomb Γ_2 structure is the union of two hexagonal lattices, relatively shifted by a deep hole z_0 . A deep hole of a lattice is a point in $\mathbb{R}^d$ maximizing the distance to the closest lattice point(s). For the hexagonal lattice, it is the circumcenter of the equilateral (fundamental) triangle formed by 3 lattice points (see Fig. 1).

The hexagonal lattice of density 1 is, up to rotational equivalence, explicitly given by

$$\Lambda_2 = \sqrt{\frac{1}{\sin(\pi/3)}} \begin{pmatrix} 1 & \cos(\pi/3) \\ 0 & \sin(\pi/3) \end{pmatrix} \mathbb{Z}^2 = \sqrt{\frac{2}{\sqrt{3}}} \begin{pmatrix} 1 & \frac{1}{2} \\ 0 & \frac{\sqrt{3}}{2} \end{pmatrix} \mathbb{Z}^2$$

The honeycomb structure of unity density is given by

$$(2.1) \quad \Gamma_2 = \sqrt{2} (\Lambda_2 \cup (\Lambda_2 + z_0)).$$

The factor $\sqrt{2}$ scales Γ_2 appropriately and we always write z_0 for the deep hole(s) of Λ_2 .

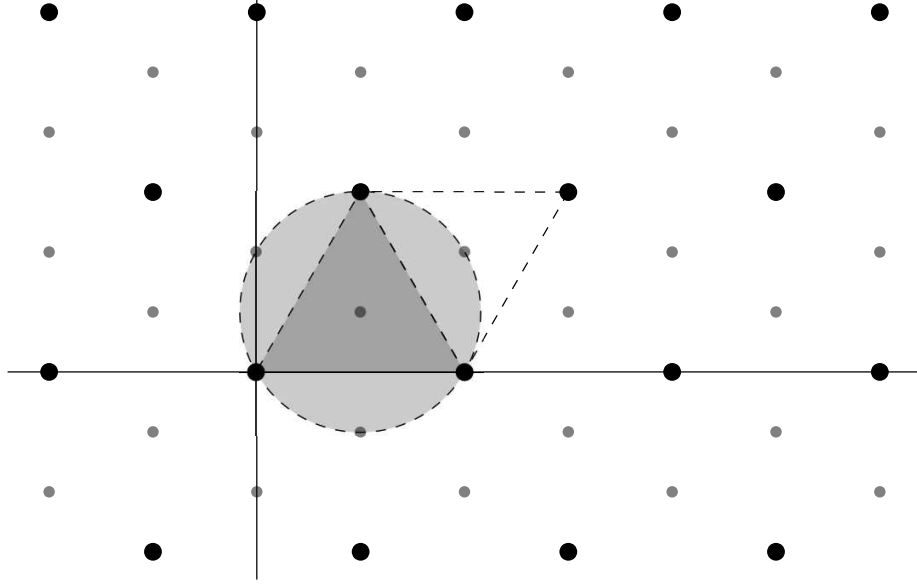


Figure 1. A part of the hexagonal lattice Λ_2 with its fundamental cell, a fundamental triangle, and a covering circle centered at a deep hole. The large black dots are the lattice points and the smaller gray dots are deep holes.

For the hexagonal lattice Λ_2 and the potential $\phi_\alpha(r) = e^{-\pi\alpha r}$ (the π in the exponent is for technical reasons, due to our normalization (3.2) of the Fourier transform) we have

$$(2.2) \quad \sum_{\lambda \in \Lambda_2} \phi_\alpha(|\lambda - z_0|^2) \leq \sum_{\lambda \in \Lambda_2} \phi_\alpha(|\lambda - z|^2), \quad \forall \alpha > 0, z \in \mathbb{R}^2.$$

This result is due to Baernstein [3] and shows that deep holes are universal cold spots of the hexagonal lattice. Note that if $z_0 \in \mathbb{R}^2/\Lambda_2$ is a deep hole, then $2z_0 \notin \Lambda_2 + z_0$ is also a deep hole. These two deep holes are inequivalent; all other deep holes can be reached from these by translation by Λ_2 . For the honeycomb structure Γ_2 , we have, by setting $\tilde{z} = \sqrt{2}z$,

$$(2.3) \quad \begin{aligned} \sum_{\gamma \in \Gamma_2} \phi_\alpha(|\gamma - \tilde{z}|^2) &= \sum_{\lambda \in \Lambda_2} \phi_\alpha(2|\lambda - z|^2) + \sum_{\lambda \in \Lambda_2} \phi_\alpha(2|\lambda + z_0 - z|^2) \\ &= \sum_{\lambda \in \Lambda_2} \phi_{2\alpha}(|\lambda - z|^2) + \sum_{\lambda \in \Lambda_2} \phi_{2\alpha}(|\lambda + z_0 - z|^2). \end{aligned}$$

Note that scaling the arguments is necessary, due to (2.1). The scaling is put into the parameter α of the Gaussian $\phi_\alpha(r^2)$. This will also happen in sequential computations.

As $2z_0$ is a deep hole of Λ_2 and of $\Lambda_2 + z_0$ (corresponding to z_0 of Λ_2) we have by (2.2)

$$\sum_{\gamma \in \Gamma_2} \phi_\alpha(|\gamma - 2\tilde{z}_0|^2) \leq \sum_{\gamma \in \Gamma_2} \phi_\alpha(|\gamma - z|^2), \quad \forall \alpha > 0, z \in \mathbb{R}^2,$$

where $\tilde{z}_0 = \sqrt{2}z_0$ is a deep hole of the scaled hexagonal lattice $\sqrt{2}\Lambda_2$.

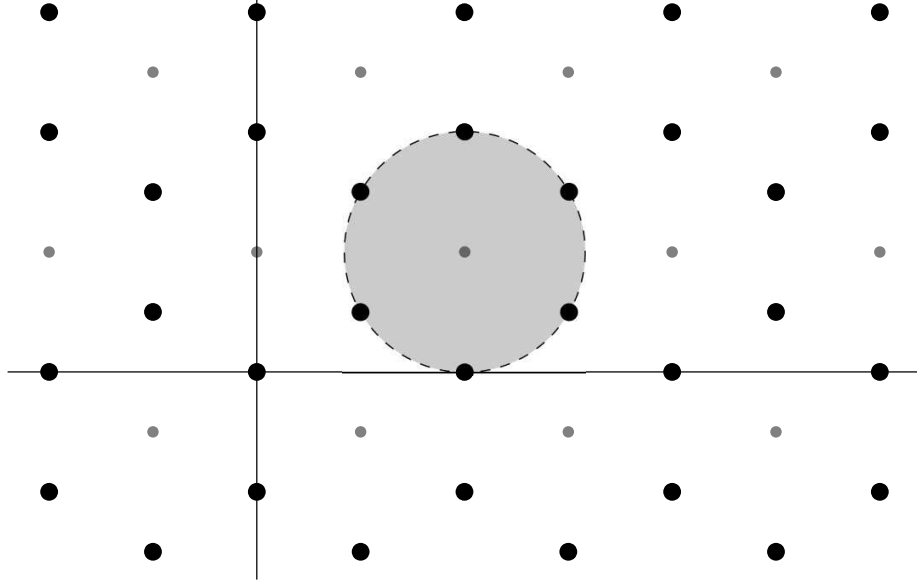


Figure 2. The honeycomb structure Γ_2 is a union of the hexagonal lattice and a copy shifted by a deep hole. The second, inequivalent deep hole of Λ_2 is a deep hole of Γ_2 . The big black dots are points of Γ_2 while the smaller gray dots are its deep holes.

3. PROOF OF THEOREM 1.1

Most methods we use are basic, the Poisson summation formula being already an advanced technique. However, we build on deep insights by Baernstein [3] on the universality of cold spots in the hexagonal lattice. At one point we will use a result of Ramanujan (see [4, Chap. 33]), put on solid mathematical ground by Borwein and Borwein [11].

By (1.2) it suffices to consider the potential $\phi_\alpha(|r^2|)$ and to show that

$$(3.1) \quad \sum_{\gamma \in \Gamma_2} \phi_\alpha(|\gamma - 2\tilde{z}_0|^2) < \sum_{\lambda \in \Lambda_2} \phi_\alpha(|\lambda - z_0|^2), \quad \forall \alpha > 0,$$

in order to prove Theorem 1.1. We start with noting that

$$\sum_{\lambda \in \Lambda_2} \phi_\alpha(|\lambda - 2z_0|^2) = \sum_{\lambda \in \Lambda_2} \phi_\alpha(|\lambda - z_0|^2),$$

as both z_0 and $2z_0$ are deep holes of Λ_2 and, thus, universal cold spots [3]. We rewrite the entities from (3.1) over the integer lattice $\mathbb{Z}^2$ by a linear coordinate change (cf. [8], [21]):

$$\begin{aligned} \sum_{\lambda \in \Lambda_2} \phi_\alpha(|\lambda - z_0|^2) &= \sum_{(k,l) \in \mathbb{Z}^2} e^{-\frac{2\pi\alpha}{\sqrt{3}}((k-1/3)^2 + (k-1/3)(l-1/3) + (l-1/3)^2)}, \\ \sum_{\gamma \in \Gamma_2} \phi_\alpha(|\gamma - 2\tilde{z}_0|^2) &= \sum_{\lambda \in \Lambda_2} \phi_{2\alpha}(|\lambda - 2z_0|^2) + \sum_{\lambda \in \Lambda_2} \phi_{2\alpha}(|\lambda - z_0|^2) = 2 \sum_{\lambda \in \Lambda_2} \phi_{2\alpha}(|\lambda - z_0|^2) \\ &= 2 \sum_{(k,l) \in \mathbb{Z}^2} e^{-\frac{4\pi\alpha}{\sqrt{3}}((k-1/3)^2 + (k-1/3)(l-1/3) + (l-1/3)^2)}. \end{aligned}$$

To split the series for the honeycomb we used (2.3). It is not hard to observe that

$$\min_{(k,l) \in \mathbb{Z}^2} ((k-1/3)^2 + (k-1/3)(l-1/3) + (l-1/3)^2) = 1/3,$$

which is achieved if and only if

$$(k, l) \in \{(0, 0), (1, 0), (0, 1)\}.$$

As a next step, we note that for $x \in \mathbb{R}_+$

$$e^{-x} > 2e^{-2x} \iff x > \log(2).$$

This particularly implies that for all $(k, l) \in \mathbb{Z}^2$

$$\begin{aligned} e^{-\frac{2\pi\alpha}{\sqrt{3}}((k-1/3)^2 + (k-1/3)(l-1/3) + (l-1/3)^2)} &> e^{-\frac{4\pi\alpha}{\sqrt{3}}((k-1/3)^2 + (k-1/3)(l-1/3) + (l-1/3)^2)} \\ \iff \frac{2\pi\alpha}{3\sqrt{3}} &> \log(2) \\ \iff \alpha > \frac{3\sqrt{3}\log(2)}{2\pi} &\approx 0.573228. \end{aligned}$$

It readily follows that (3.1) holds for α large enough:

$$\sum_{\lambda \in \Lambda_2} \phi_\alpha(|\lambda - z_0|^2) > \sum_{\gamma \in \Gamma_2} \phi_\alpha(|\gamma - \tilde{z}_0|^2), \quad \forall \alpha > \frac{3\sqrt{3}\log(2)}{2\pi}.$$

To show that the polarization of Λ_2 is larger than that of Γ_2 on small scales α (equivalently for high densities), we employ the Poisson summation formula as usual in such situations.

We recall that the dual lattice Λ^* is characterized by $\Lambda^* = \{\lambda^* \in \mathbb{R}^d \mid \lambda \cdot \lambda^* \in \mathbb{Z} \forall \lambda \in \Lambda\}$, the dot $\cdot$ denoting the Euclidean inner product. We denote the Fourier transform of f by

$$(3.2) \quad \widehat{f}(y) = \int_{\mathbb{R}^d} f(x) e^{-2\pi i x \cdot y} dx.$$

The Poisson summation formula, in this case, reads

$$\sum_{\lambda \in \Lambda} f(\lambda + z) = \frac{1}{\text{vol}(\mathbb{R}^d/\Lambda)} \sum_{\lambda^* \in \Lambda^*} \widehat{f}(\lambda^*) e^{2\pi i \lambda^* \cdot z}, \quad z \in \mathbb{R}^d.$$

Our situation is special; any lattice $\Lambda \subset \mathbb{R}^2$ (of density 1) is self-dual. More precisely, if $\Lambda \subset \mathbb{R}^2$, $\text{vol}(\mathbb{R}^2/\Lambda) = 1$, then $\Lambda^* = J\Lambda$ (cf. [8, App. A]), where

$$J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

is a rotation by 90 degrees. Generally, the Gaussian $x \mapsto e^{-\pi|x|^2}$, $x \in \mathbb{R}^d$, is an eigenfunction of the Fourier transform. In particular, we have [18, App. A]

$$\widehat{\phi_\alpha}(y^2) = \alpha^{-d/2} \phi_{1/\alpha}(y^2), \quad y \in \mathbb{R}^d.$$

So, in our very particular situation, we have (note that $-\lambda \in \Lambda$ for any lattice)

$$\sum_{\lambda \in \Lambda_2} \phi_\alpha(|\lambda - z_0|^2) = \sum_{\lambda \in \Lambda_2} \phi_\alpha(|\lambda + z_0|^2) = \alpha^{-1} \sum_{\lambda \in \Lambda_2} \phi_{1/\alpha}(|\lambda|^2) e^{2\pi i (J\lambda) \cdot z_0}.$$

We used the symmetry of Λ_2 , the Poisson summation formula, the fact that $\text{vol}(\mathbb{R}^2/\Lambda_2) = 1$, that $\Lambda_2^* = J\Lambda_2$, and that $\phi_\alpha(|r|^2)$ is rotational invariant. Note that the left side is real-valued, so the right side must also be real-valued. With the same arguments, we obtain a dual formula for the polarization of Γ_2 :

$$\sum_{\gamma \in \Gamma_2} \phi_\alpha(|\gamma - 2\tilde{z}_0|^2) = 2 \sum_{\lambda \in \Lambda_2} \phi_{2\alpha}(|\lambda + z_0|^2) = \alpha^{-1} \sum_{\lambda \in \Lambda_2} \phi_{1/(2\alpha)}(|\lambda|^2) e^{2\pi i(J\lambda) \cdot z_0}.$$

Thus, by making the substitution $\alpha \mapsto \alpha^{-1}$, we seek to show that

$$\sum_{\lambda \in \Lambda_2} \phi_\alpha(|\lambda|^2) e^{2\pi i(J\lambda) \cdot z_0} > \sum_{\lambda \in \Lambda_2} \phi_{\alpha/2}(|\lambda|^2) e^{2\pi i(J\lambda) \cdot z_0}, \quad \alpha > \frac{2\pi}{3\sqrt{3}\log(2)} \approx 1.74451.$$

By splitting the complex exponential into its real and imaginary parts and using the linear coordinate change from before, we actually obtain (cf. [6])

$$\begin{aligned} \sum_{\lambda \in \Lambda_2} \phi_\alpha(|\lambda|^2) e^{2\pi i(J\lambda) \cdot z_0} &= \sum_{\lambda \in \Lambda_2} \phi_\alpha(|\lambda|^2) \cos(2\pi(J\lambda) \cdot z_0) \\ &= \sum_{(k,l) \in \mathbb{Z}^2} e^{-\frac{2\pi\alpha}{\sqrt{3}}(k^2+kl+l^2)} \cos(2\pi(k-l)/3) \end{aligned}$$

Note that $\cos(2\pi(k-l)/3) \in \{-1/2, 1\}$ for all $(k, l) \in \mathbb{Z}^2$. Also, the way in which the values are taken is determined by the quadratic form $q(k, l) = k^2 + kl + l^2$ and

$$\lim_{R \rightarrow \infty} \frac{|\{(k, l) \in \mathbb{Z}^2 \mid \cos(2\pi(k-l)/3) = -1/2\} \cap [-R, R]^2|}{|\{(k, l) \in \mathbb{Z}^2 \mid \cos(2\pi(k-l)/3) = 1\} \cap [-R, R]^2|} = 2.$$

So we have twice as many negative signs with weight $1/2$ in the series as positive signs (with weight 1), leading to an overall “neutral charge” of Λ_2 (cf. [7]). In fact, we can decompose Λ_2 into 3 relatively shifted copies (shifted by deep holes), 2 copies having negative signs with half weights, and 1 copy with positive signs (and full weights) (cf. [6]). This is the geometric interpretation (cf. [16]) of the *arithmetic part* of the cubic AGM of Browein and Borwein [11]: for a complex number q with $|q| < 1$ set

$$a(q) = \sum_{(k,l) \in \mathbb{Z}^2} q^{k^2+kl+l^2} \quad \text{and} \quad b(q) = \sum_{(k,l) \in \mathbb{Z}^2} q^{k^2+kl+l^2} e^{2\pi i \frac{k-l}{3}}.$$

Then

$$3a(q^3) = a(q) + 2b(q).$$

Setting $q = e^{-\frac{2\pi\alpha}{\sqrt{3}}} < 1$, $\alpha > 0$, we have

$$\sum_{\lambda \in \Lambda_2} \phi_\alpha(|\lambda|^2) e^{2\pi i(J\lambda) \cdot z_0} = b(q) = \frac{3a(q^3) - a(q)}{2},$$

and

$$\sum_{\lambda \in \Lambda_2} \phi_{\alpha/2}(|\lambda|^2) e^{2\pi i(J\lambda) \cdot z_0} = b(q^{1/2}) = \frac{3a(q^{3/2}) - a(q^{1/2})}{2}.$$

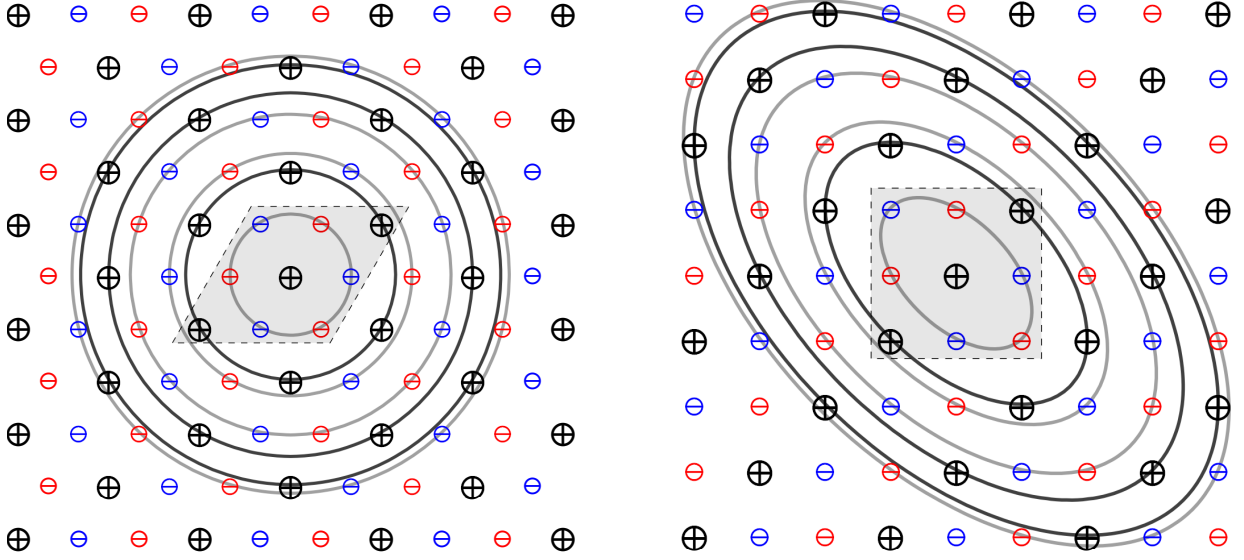


Figure 3. Left: After performing a Poisson summation the polarization problem becomes a question on charged ionic crystals. The hexagonal lattice can then be decomposed into 3 (shifted) hexagonal lattices, each of third the density, 2 having negative charges of half weights and one having positive charges.

Right: After a linear change of coordinates, the hexagonal setup is transferred to an anisotropic interaction problem on $\mathbb{Z}^2$. The anisotropic interaction is determined via the quadratic form $q(k, l) = k^2 + kl + l^2$. In the square $[-1, 1]^2$ we find twice as many negative charges of half weights as positive ones.

Similar to before, we make an auxiliary computation. We seek to find $x \in \mathbb{R}_+$ such that

$$3e^{-3x} - e^{-x} > 3e^{-\frac{3x}{2}} - e^{-\frac{x}{2}}.$$

Substituting $s = e^{-x/2}$, this leads to finding $s \in [0, 1]$ such that

$$3s^6 - 3s^3 - s^2 + s = s(3s^5 - 3s^2 - s + 1) = s g(s) > 0.$$

Clearly, the value of $g(s)$ at $s = 0$ is $g(0) = 1$. Moreover, $g(1/5) = 2128/15625 > 0$. We check the sign of the derivative. We have

$$g'(s) = 15s^4 - 6s - 1.$$

For $0 < s < 1/5$ we have $15s^4 = 3/125 < 1$ and so $g'(s) < 0$ on $(0, 1/5)$. Thus $g(s)$ is positive on the interval $(0, 1/5)$ and, ultimately,

$$s g(s) > 0, \quad s \in (0, 1/5) \quad \Longleftrightarrow \quad 3e^{-3x} - e^{-x} > 3e^{-\frac{3x}{2}} - e^{-\frac{x}{2}}, \quad x \in (2 \log(5), \infty).$$

We note that our estimates are far from optimal, but they imply

$$\frac{3a(q^3) - a(q)}{2} > \frac{3a(q^{3/2}) - a(q^{1/2})}{2}, \quad q = e^{-\frac{2\pi\alpha}{\sqrt{3}}}, \quad \alpha > \frac{2 \log(5) \sqrt{3}}{2\pi} \approx 0.88733,$$

by comparing for all $(k, l) \in \mathbb{Z}^2 \setminus \{(0, 0)\}$. Note that the value at the origin adds 1 to both sides of the inequality. Thus, the proof of Theorem 1.1 is finished. $\square$

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