SHARP $N^{3/4}$ LAW FOR THE MINIMIZERS OF THE EDGE-ISOPERIMETRIC PROBLEM ON THE TRIANGULAR LATTICE

ELISA DAVOLI, PAOLO PIOVANO, AND ULISSE STEFANELLI

Abstract. We investigate the Edge-Isoperimetric Problem (EIP) for sets of n points in the triangular lattice by emphasizing its relation with the emergence of the Wulff shape in the crystallization problem. By introducing a suitable notion of perimeter and area, EIP minimizers are characterized as extremizers of an isoperimetric inequality: they attain maximal area and minimal perimeter among connected configurations. The maximal area and minimal perimeter are explicitly quantified in terms of n. In view of this isoperimetric characterizations EIP minimizers M_n are seen to be given by hexagonal configurations with some extra points at their boundary. By a careful computation of the cardinality of these extra points, minimizers M_n are estimated to deviate from such hexagonal configurations by at most $K_t\, n^{3/4} + \mathrm{o}(n^{3/4})$ points. The constant K_t is explicitly determined and shown to be sharp.

1. Introduction

This paper is concerned with the *Edge-Isoperimetric Problem* (EIP) in the triangular lattice

$$\mathcal{L}_t := \{m\boldsymbol{t}_1 + n\boldsymbol{t}_2 \;:\; m,n \in \mathbb{Z}\} \quad \text{for } \boldsymbol{t}_1 := (1,0) \text{ and } \boldsymbol{t}_2 := \left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right).$$

Let $\mathcal{C}_n$ be the family of sets C_n containing n distinct elements $x_1, \cdots, x_n$ in $\mathcal{L}_t$. The *edge perimeter* $|\Theta(C_n)|$ of a set $C_n \in \mathcal{C}_n$ is the cardinality of the *edge boundary* Θ of C_n defined by

$$\Theta(C_n) := \{(x_i, x_j) \;:\; |x_i - x_j| = 1,\, x_i \in C_n \text{ and } x_j \in \mathcal{L}_t \setminus C_n\}. \tag{1}$$

Note that, with a slight abuse of notation, the symbol $|\cdot|$ denotes, according to the context, both the cardinality of a set and the euclidean norm in $\mathbb{R}^2$. The EIP over the family $\mathcal{C}_n$ consists in characterizing the solutions to the minimum problem:

$$\theta_n := \min_{C_n \in \mathcal{C}_n} |\Theta(C_n)|. \tag{2}$$

Our main aim is to provide a characterization of the minimizers M_n of (2) as extremizers of a suitable isoperimetric inequality (see Theorem 1.1) and to show that there exists a *hexagonal Wulff shape* in $\mathcal{L}_t$ from which M_n differs by at most

$$K_t\, n^{3/4} + \mathrm{o}(n^{3/4}) \tag{3}$$

2010 *Mathematics Subject Classification.* 82D25.
Key words and phrases. Edge-isoperimetric problem, edge perimeter, triangular lattice, isoperimetric inequality, Wulff shape, $N^{3/4}$ law.

points (see Theorem 1.2). A crucial issue of our analysis is that both the the exponent and the constant in front of the leading term in (3) are explicitly determined and optimal (see Theorem 1.3).

The EIP is a classical combinatorial problem. We refer to [2, 5] for the description of this problem in various settings and for a review of the corresponding results available in the literature. The importance of the EIP is however not only theoretical, since the edge perimeter (and similar notions) bears relevance in problems from *machine learning*, such as classification and clustering (see [12] and references therein).

We shall emphasize the link between the EIP and the *Crystallization Problem* (CP). For this reason we will often refer to the sets $C_n \in \mathcal{C}_n$ as *configurations of particles* in $\mathcal{L}_t$ and to minimal configurations as *ground states*. The CP consists in analytically explaining why particles at low temperature arrange in periodic lattices by proving that the minima of a suitable *configurational energy* are subsets of a regular lattice. At low temperatures particle interactions are expected to be essentially determined by particle positions. In this classical setting, all available CP results in the literature with respect to a finite number n of particles are in two dimensions for a phenomenological energy E defined from $\mathbb{R}^{2n}$, the set of possible particle positions, to $\mathbb{R} \cup \{+\infty\}$. In [6, 10] the energy E takes the form

$$E(\{y_1, \dots, y_n\}) := \frac{1}{2} \sum_{i \neq j} v_2(|y_i - y_j|) \tag{4}$$

for a potential $v_2 : [0, \infty) \to \mathbb{R} \cup \{+\infty\}$ that accounts for two-body interactions, while in [7, 8, 9] additional three-body interaction terms were included in the energy. We also refer the reader to [3] for a general review of the CP results.

The link between the EIP on $\mathcal{L}_t$ and the CP resides on the fact that when only two-body and short-ranged interactions are considered the minima of E are expected to be subsets of a triangular lattice. The fact that ground states are subsets of $\mathcal{L}_t$ has been analytically shown in [6] and [10] for specific choices of the two-body interaction potential v_2, i.e. for the *sticky-disc* and *soft-disc* interaction potentials (see [6, 10] for more details), for which in particular we have that

$$E(C_n) = -|B(C_n)| \tag{5}$$

for every $C_n \in \mathcal{C}_n$. Here, the set

$$B(C_n) := \{(x_i, x_j) \ : \ |x_i - x_j| = 1, \, i < j, \text{ and } x_i, x_j \in C_n\}$$

represents the *bonds* of $C_n \in \mathcal{C}_n$. The number of bonds of C_n with an endpoint in x_i will be instead denoted by

$$b(x_i) = |\{j \in \{1, \cdots, n\} \ : \ (x_i, x_j) \in B(C_n)\}| \tag{6}$$

for every $x_i \in C_n$. The link between the EIP and the CP consists in the fact that by (1), (5), and (6) we have that

$$\begin{aligned} |\Theta(C_n)| &= \sum_{i=1}^{n} (6 - b(x_i)) = 6n - \sum_{i=1}^{n} b(x_i) \\ &= 6n \, - \, 2|B(C_n)| = 6n \, + \, 2E(C_n) \end{aligned} \tag{7}$$

for every $C_n \in \mathcal{C}_n$, since the degree of $\mathcal{L}_t$ is 6.

In view of (7) minimizing E among configurations in $\mathcal{C}_n$ is equivalent to the EIP (2), and since by [6, 10] ground states belong to $\mathcal{C}_n$, the ground states of the CP correspond to the minimizers of the EIP. Furthermore, in [6, 10] the energy of ground states with n particles has been also explicitly quantified in terms of n to be equal to

$$e_n := -\lfloor 3n - \sqrt{12n-3} \rfloor = -3n + \lceil \sqrt{12n-3} \rceil \tag{8}$$

where $\lfloor x \rfloor := \max\{z \in \mathbb{Z} : z \leq x\}$ and $\lceil x \rceil := \min\{z \in \mathbb{Z} : x \leq z\}$ denote the standard right- and left-continuous functions, respectively. Therefore, (7) and (8) entails also a characterization of θ_n in terms of n, i.e.,

$$\theta_n = 6n + 2e_n = 2\lceil \sqrt{12n-3} \rceil. \tag{9}$$

A first property of the minimizers of (2) has been provided in [5, Theorem 7.2] where it is shown that the EIP has the *nested-solution property*, i.e. there exists a total order $\tau : \mathbb{N} \to \mathcal{L}_t$ such that for all $n \in \mathbb{N}$ the configuration

$$D_n := \{x_{\tau(1)}, \dots, x_{\tau(n)}\}$$

is a solution of (2) (see Proposition 2.1 and the discussion below for the definition of τ). Given the symmetry of the configurations D_n, we will refer to them as *daisies* in the following. Since solutions of the EIP are in general nonunique, the aim of this paper is to characterize them all.

In this paper we provide a first characterization of the minimizers M_n of the EIP by introducing an isoperimetric inequality in terms of suitable notions of *area* and *perimeter* of configurations in $\mathcal{C}_n$ and by showing that the connected minimizers M_n of the EIP are optimal with respect to it. We refer here the reader to (19) and (20) for the definition of the area $A(C_n)$ and the perimeter $P(C_n)$ of a configuration $C_n \in \mathcal{C}_n$. Note also that we say that a configuration C_n is connected if given any two points $x_i, x_j \in C_n$ then there exists a sequence y_k of points in C_n with $k = 1, \dots, K$ for some $K \in \mathbb{N}$ such that $y_1 = x_i$, $y_K = x_j$, and either (y_k, y_{k+1}) or (y_{k+1}, y_k) is in $B(C_n)$ for every $k = 1, \dots, K-1$. It easily follows that minimizers of the EIP need to be connected. Our isoperimetric characterization reads as follows.

Theorem 1.1 (Isoperimetric characterization)**.** *Every connected configuration $C_n \in \mathcal{C}_n$ satisfies*

$$\sqrt{A(C_n)} \leq k_n P(C_n), \tag{10}$$

where

$$k_n := \frac{\sqrt{-2\theta_n + 8n + 4}}{\theta_n - 6}\,. \tag{11}$$

Moreover, connected minimizers $M_n \in \mathcal{C}_n$ of the EIP correspond to those configurations for which (10) holds with the equality. Equivalently, connected minimizers attain the maximal area $a_n := -\theta_n/2 + 2n + 1$ and the minimal perimeter $p_n := \theta_n/2 - 3$.

Notice that a similar isoperimetric result has been already achieved in the square lattice in [8] with a different method, based on introducing a rearrangement of the configurations. Theorem 1.1 is proved here by assigning to each element x of a configuration $C_n \in \mathcal{C}_n$ a weight $\omega_{C_n}(x)$ that depends on C_n and on the above-mentioned order τ (see (26)).

In [5] it is observed that when $n := 1 + 3s + 3s^2$ for some $s \in \mathbb{N}$ the daisy $D_{1+3s+3s^2}$ is the unique minimizer of the EIP. Note that in the following we will often refer to lattice translations of $D_{1+3s+3s^2}$ as *hexagonal configurations with radius* $s \in \mathbb{N}$ since each configuration $D_{1+3s+3s^2}$ can be seen as the intersection of $\mathcal{L}_t$ and a regular hexagon with side s. In order to further characterize the solution of the EIP we associate to every minimizer M_n a maximal hexagonal configuration $H_{r_{M_n}}$ that is contained in M_n and we evaluate how much M_n differs from $H_{r_{M_n}}$ (see Section 3).

In view of the isoperimetric characterization of the ground states provided by Theorem 1.1, we are able to sharply estimate the *distance* of M_n to $H_{r_{M_n}}$ both in terms of the cardinality of $M_n \setminus H_{r_{M_n}}$ and by making use of empirical measures. We associate to every configuration $C_n = \{x_1, \dots, x_n\}$ the empirical measure denoted by $\mu_{C_n} \in M_b(\mathbb{R}^2)$ (where $M_b(\mathbb{R}^2)$ is the set of bounded Radon measures in $\mathbb{R}^2$) of the rescaled configuration $\{x_1/\sqrt{n}, \dots, x_n/\sqrt{n}\}$, i.e.,

$$\mu_{C_n} := \frac{1}{n} \sum_i \delta_{x_i/\sqrt{n}}\,,$$

and we denote by $\|\cdot\|$ and $\|\cdot\|_{\mathrm{F}}$ the total variation norm and the *flat norm*, respectively (see (65) for the definition of flat norm). Our second main result is the following.

Theorem 1.2 (Convergence to the Wulff shape)**.** *For every sequence of minimizers M_n in $\mathcal{L}_t$ there exists a sequence of suitable translations M_n' such that*

$$\mu_{M_n'} \rightharpoonup^* \frac{2}{\sqrt{3}}\chi_W \quad \textit{weakly* in the sense of measures},$$

where χ_W is the characteristic function of the regular hexagon W defined as the convex hull of the vectors

$$\left\{\pm\frac{1}{\sqrt{3}}\boldsymbol{t}_1,\, \pm\frac{1}{\sqrt{3}}\boldsymbol{t}_2,\, \pm\frac{1}{\sqrt{3}}(\boldsymbol{t}_2 - \boldsymbol{t}_1)\right\}.$$

Furthermore, the following assertions hold true:

$$\left|M_n \setminus H_{r_{M_n}}\right| \le K_t n^{3/4} + \mathrm{o}(n^{3/4}), \tag{12}$$

$$\left\|\mu_{M_n} - \mu_{H_{r_{M_n}}}\right\| \le K_t n^{-1/4} + \mathrm{o}(n^{-1/4}), \tag{13}$$

and

$$\left\|\mu_{M_n'} - \frac{2}{\sqrt{3}}\chi_W\right\|_{\mathrm{F}} \le K_t n^{-1/4} + \mathrm{o}(n^{-1/4}), \tag{14}$$

where $H_{r_{M_n}}$ is the maximal hexagon associated to M_n, and

$$K_t := \frac{2}{3^{1/4}}. \tag{15}$$

The proof of Theorem 1.2 is based on the isoperimetric characterization of the minimizers provided by Theorem 1.1 and relies in a fundamental way on the maximality of the radius r_{M_n} of the maximal hexagonal configuration $H_{r_{M_n}}$. The latter is essential to carefully estimate the number of particles of M_n that reside outside $H_{r_{M_n}}$ in terms of r_{M_n} itself and the minimal perimeter p_n. Thanks to this fine estimate we are able to find a lower bound on r_{M_n} in terms of n only (see (61)). In particular, the method provides a lower bound for the radius r_{M_n} that allows us to also show that

$$d_{\mathcal{H}}(M_n, H_{r_{M_n}}) \le \mathrm{O}(n^{1/4}),$$

where $d_{\mathcal{H}}$ is the Hausdorff distance.

The previous result appears to be an extension of analogous results obtained in [1, 11] by using a completely different method hinged on Γ-convergence. In that context the set W is the asymptotic *Wulff shape* and we will also often refer to W in this way. More precisely the minimization problem (4) is reformulated in [1, 11] in terms of empirical measures by introducing the energy functional

$$\mathcal{E}_n(\mu) := \begin{cases} \displaystyle\int_{\mathbb{R}^2\setminus\mathrm{diag}} \frac{n}{2} v_2(\sqrt{n}|x-y|)\,\mathrm{d}\mu\otimes\mathrm{d}\mu & \mu=\mu_{C_n} \text{ for some } C_n\in\mathcal{C}_n, \\ \infty & \text{otherwise} \end{cases} \tag{16}$$

defined on the set of nonnegative Radon measures in $\mathbb{R}^2$ with mass 1, where v_2 is (a quantified small perturbation of) the sticky-disc potential [6]. In [1, 11] it is proved that the rescaled sequence of functionals $n^{-1/2}(2\mathcal{E}_n + 6n)$ Γ-converges with respect to the weak* convergence of measures to the anisotropic perimeter

$$\mathcal{P}(\mu) := \begin{cases} \displaystyle\int_{\partial^* S} \varphi(\nu_S)\,\mathrm{d}\mathcal{H}^1 & \text{if } \mu = \frac{2}{\sqrt{3}}\chi_S \text{ for some set } S \text{ of finite perimeter} \\ & \text{and such that } \mathcal{L}^2(S) := \sqrt{3}/2, \\ \infty & \text{otherwise} \end{cases} \tag{17}$$

where $\partial^* S$ is the reduced boundary of S, ν_S is the outward-pointing normal vector to S, $\mathcal{L}^2(S)$ is the two-dimensional Lebesgue measure of S, $\mathcal{H}^1$ is the one dimensional measure, and the anisotropic density φ is defined by

$$\varphi(\nu) := 2\left(\nu_2 - \frac{\nu_1}{\sqrt{3}}\right)$$

for every $\nu = (\nu_1, \nu_2)$ with $\nu_1 = -\sin\alpha$ and $\nu_2 = \cos\alpha$ for $\alpha \in [0, \pi/6]$.

Let us note here that the Γ-convergence result provided in [1] can be restated as a Γ-convergence result for the edge perimeter. In fact, since the energy functional $\mathcal{E}_n$ is such that

$$\mathcal{E}_n(\mu_{C_n}) = E(C_n) \tag{18}$$

for every $C_n \in \mathcal{C}_n$, by (7) we have that the functional $\mathcal{T}_n := \mathcal{E}_n(\mu) + 6n$ is such that

$$\mathcal{T}_n(\mu_{C_n}) = |\Theta(C_n)|$$

and $n^{-1/2}\mathcal{T}_n$ Γ-converges with respect to the weak* convergence of measures to the anisotropic perimeter $\mathcal{P}(\mu)$.

Besides the completely independent method, the main achievement of this paper with respect to [1, 11] is that of sharply estimating the constant K_t in formulas (12), (13), and (14). The deviation of the minimizers from the Wulff-shape of order $n^{3/4}$ was exhibited in [11] and referred to as the $n^{3/4}$*-law*. Here we sharpen the result from [11] by determining the optimal constant in estimates (12), (13), and (14). We have the following.

Theorem 1.3 (Sharpness of the estimates)**.** *A sequence of minimizers M_{n_i} satisfying* (12) – (14) *with equalities can be explicitly constructed for $n_i := 2 + 3i + 3i^2$ with $i \in \mathbb{N}$.*

Finally, we notice that our method appears to be implementable in other settings possibly including three-body interactions. This is done for the crystallization problem in the hexagonal lattice $\mathcal{L}_h$ in a companion paper [4]. Furthermore, we observe that analogous results to Theorem 1.2 were obtained in the context of the crystallization problem in the square lattice in [8, 9] with a substantially different method (even though also based on an isoperimetric characterization of the minimizers) resulting only in suboptimal estimates.

The paper is organized as follows. In Section 2 we introduce the notions of area A and perimeter P of configurations $C_n \in \mathcal{C}_n$, we define the order τ in $\mathcal{L}_t$, and we introduce the notion of weight ω_{C_n}. Furthermore, in Subsection 2.1 we provide the proof of Theorem 1.1. In Section 3 we introduce the notion of maximal hexagons $H_{r_{M_n}}$ associated to minimizers M_n of (2) and we carefully estimate r_{M_n} from below in terms of n. In Section 4 we use the latter lower bound in order to study the convergence to the Wulff shape by providing the proof of Theorems 1.2 and 1.3 in Subsections 4.1 and 4.2, respectively.

2. Isoperimetric Inequality

In this section we introduce the notion of area and perimeter of a configuration in $\mathcal{C}_n$ and we deduce various relations between its area, perimeter, energy and its edge boundary including a isoperimetric inequality.

We define the area A of a configuration $C_n \in \mathcal{C}_n$ by

$$A(C_n) := \frac{1}{6}|T(C_n)| \tag{19}$$

where $T(C_n)$ is the family of triples of elements in C_n forming triangles with unitary edges, i.e.,

$$T(C_n) := \{(x_{i_1}, x_{i_2}, x_{i_3}) \ : \ x_{i_1}, x_{i_2}, x_{i_3} \in C_n \text{ and } |x_{i_j} - x_{i_k}| = 1 \text{ for } j \neq k\}.$$

In order to introduce the perimeter of a configuration in $\mathcal{C}_n$ let us denote by $F(C_n) \subset \mathbb{R}^2$ the closure of the union of the regions enclosed by the triangles with vertices in $T(C_n)$, and by $G(C_n) \subset \mathbb{R}^2$ the union of all bonds which are not included in $F(C_n)$. The *perimeter* P of a regular configuration $C_n \in \mathcal{C}_n$ is defined as

$$P(C_n) := \mathcal{H}^1(\partial F(C_n)) + 2\mathcal{H}^1(G(C_n))\,, \tag{20}$$

where $\mathcal{H}^1$ is the one-dimensional Hausdorff measure. Note in particular that

$$P(C_n) = \lim_{\varepsilon \searrow 0} \mathcal{H}^1\Big(\partial\big(\partial F(C_n) \cup G(C_n) + B_\varepsilon\big)\Big)$$

where $B_\varepsilon = \{y \in \mathbb{R}^2 \ : \ |y| \leq \varepsilon\}$.

Since every triangle with vertices in $T(C_n)$ contributes with 3 bonds to $B(C_n)$, by (5) and (19) we have that

$$\begin{aligned} 3A(C_n) &= 2\,|B(C_n \cap F(C_n))| \,-\, |B(C_n \cap \partial F(C_n))| \\ &= -2\,E(C_n \cap F(C_n)) - \mathcal{H}^1(\partial F(C_n)). \end{aligned} \tag{21}$$

Thus, by recalling (20) and (21) the equality

$$\mathcal{H}^1(G(C_n)) = |B(C_n \cap G(C_n))| = -E(C_n \cap G(C_n))$$

yields

$$\begin{aligned} P(C_n) &= -2E(C_n \cap F(C_n)) \,-\, 3A(C_n) - 2E(C_n \cap G(C_n)) \\ &= -2E(C_n) \,-\, 3A(C_n), \end{aligned}$$

and we conclude that

$$E(C_n) = -\frac{3}{2}A(C_n) \,-\, \frac{1}{2}P(C_n). \tag{22}$$

Notice that (22) allows to express the energy of a configuration C_n as a linear combinations of its area and its perimeter, and that by (7) an analogous relation can be deduced for the edge boundary, namely

$$|\Theta(C_n)| = 6n - 3A(C_n) - P(C_n). \tag{23}$$

As already discussed in the introduction, in view of (7) we are able to combine the exact quantification of the ground-state energy E established in [6, 10] with the nested-solution property provided by [5, Theorem 7.2]. We record this fact in the following result that we state here without proof.

Proposition 2.1. *There exists a total order $\tau : \mathbb{N} \to \mathcal{L}_t$ such that for all $n \in \mathbb{N}$ the configuration D_n defined by $D_n := \{x_{\tau(1)}, \dots, x_{\tau(n)}\}$ which we refer to as* daisy *with n points, is a solution of* (2)*, i.e.*

$$|\Theta(D_n)| = \min_{C_n \in \mathcal{L}_t} |\Theta(C_n)| = \theta_n, \tag{24}$$

where θ_n is given by (9)*.*

We remark that the sequence of daisy ground states $\{D_n\}$ satisfies the property that

$$D_{n+1} = D_n \cup \{x_{\tau(n+1)}\}.$$

In particular, within the class of daisy configurations one can pass from a ground state to another by properly adding atoms at the right place, determined by the order τ.

The total order provided by Theorem 2.1 is not unique. We will consider here the total order τ on $\mathcal{L}_t$ defined by moving clockwise on concentric daisies centered at a fixed point, as the radius of the daisies increases. To be precise, let $x_{\tau(1)}$ be the origin $(0,0)$ and let $x_{\tau(2)}$ be a point in $\mathcal{L}_t$ such that there is an active bond between $x_{\tau(2)}$ and $x_{\tau(1)}$. For $i = 3, \cdots, 7$, we define the points $x_{\tau(i)} \in \mathcal{L}_t$ as the vertices of the hexagon H_k with center $x_{\tau(1)}$ and radius 1, numbered clockwise starting from $x_{\tau(2)}$. We then consider the regular hexagons H_k that are centered at $x_{\tau(1)}$, and have radius k and one side parallel to the vector $x_{\tau(2)} - x_{\tau(1)}$, and proceed by induction on the radius $k \in \mathbb{N}$. To this aim, notice that the number of points of $\mathcal{L}_t$ contained in H_k is $n_k := 1+3k+3k^2$. Assume that all the points $x_{\tau(i)}$, with $i \le n_k$, have been identified. We define $x_{\tau(1+n_k)}$ as the point $p \in \mathcal{L}_t \cap \ell_k$ such that $|p - x_{\tau(n_k)}| = 1$ and $p \neq x_{\tau(n_k-1)}$, where ℓ_k denotes the line parallel to the vector $x_{\tau(2)} - x_{\tau(1)}$, and passing through the point $x_{\tau(n_k)}$. For $i \in (n_k + 1, n_{k+1}]$ we then define $x_{\tau(i)}$ by clockwise numbering the points of $\mathcal{L}_t$ on the boundary of H_k (see Figure 1).

We will write $x <_\tau y$ referring to the total order τ described above. A weight function ω is defined on $\mathcal{L}_t$ by the following

$$\omega(x) := |\{y \in \mathcal{L}_t \ : \ |x - y| = 1 \text{ and } y <_\tau x\}|,$$

for every $x \in \mathcal{L}_t$. We observe that ω assumes value 0 at the point $x_{\tau(1)}$, value 1 at $x_{\tau(2)}$ (that is a point bonded to $x_{\tau(1)}$), and values 2 or 3 at all the other points in $\mathcal{L}_t$ (see Figure 2). Furthermore, we have that

$$E(D_n) = -\sum_{i=1}^{n} \omega(x_{\tau(i)}) \quad \text{for every } n \in \mathbb{N}. \tag{25}$$

and that $\mathcal{L}_t = \{x_1, x_2\} \cup \Omega_2 \cup \Omega_3$ with

$$\Omega_2 := \{x \in \mathcal{L}_t \, : \, \omega(x) = 2\} \quad \text{and} \quad \Omega_3 := \{x \in \mathcal{L}_t \, : \, \omega(x) = 3\}.$$

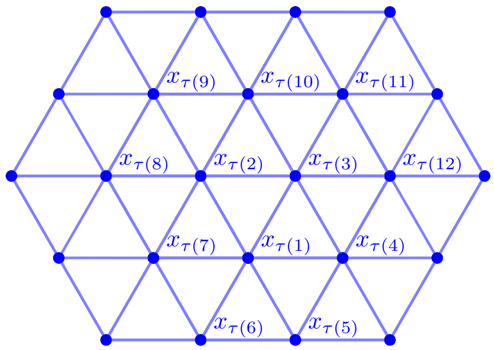

FIGURE 1. The total order τ is defined by considering the concentric hexagons centered in $x_{\tau(1)}$ with increasing radii, and by ordering the points clockwise within each hexagon.

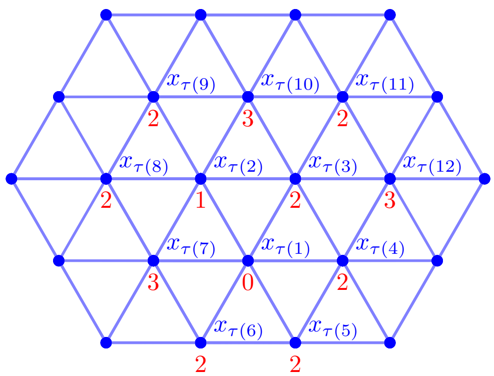

FIGURE 2. The first elements of $\mathcal{L}_t$ with respect to the order τ are shown with their weight assigned by the value of the function ω appearing below them.

Moreover, for every configuration C_n we introduce a weight function ω_{C_n} defined by

$$\omega_{C_n}(x) := |\{y \in C_n \ : \ |x-y| = 1 \text{ and } y <_\tau x\}|, \tag{26}$$

for every $x \in C_n$ (and thus depending on C_n). In this way C_n can be rewritten as the union

$$C_n = \bigcup_{k=0}^{3} C_n^k$$

where

$$C_n^k := \{x \in C_n \ : \ \omega_{C_n}(x) = k\}$$

for $k = 0, \ldots, 3$. We notice that $\omega_{C_n}(x) \leq \omega(x)$ for every $x \in C_n$ and that $|C_n^0|$ is the number of connected components of C_n.

In order to prove the isoperimetric inequality (10), we first express the energy, the perimeter, the edge perimeter, and the area of a regular configuration C_n as a function of the cardinality of the sets C_n^k.

Proposition 2.2. *Let C_n be a regular configuration in $\mathcal{L}_t$. Then*

$$E(C_n) = -|C_n^1| - 2|C_n^2| - 3|C_n^3|, \tag{27}$$

$$A(C_n) = |C_n^2| + 2|C_n^3|, \tag{28}$$

$$P(C_n) = 2|C_n^1| + |C_n^2|, \tag{29}$$

$$|\Theta(C_n)| = 6|C_n^0| + 4|C_n^1| + 2|C_n^2|, \tag{30}$$

for every $n \in \mathbb{N}$.

Proof. Fix $n \in \mathbb{N}$, and let C_n be a regular configuration in $\mathcal{L}_t$. In analogy to (25) there holds

$$E(C_n) = -\sum_{i=1}^{n} \omega_{C_n}(x_i).$$

For $i = 0, \cdots, n-1$, denote by C_i the subset of C_n containing the first i points of C_n, according to the total order τ. If $x_{\tau(i)} \in C_n^0$, then

$$A(C_i) - A(C_{i-1}) = 0, \quad P(C_i) - P(C_{i-1}) = 0 \quad \text{and} \quad |\Theta(C_i)| - |\Theta(C_{i-1})| = 6; \tag{31}$$

if $x_{\tau(i)} \in C_n^1$, then

$$A(C_i) - A(C_{i-1}) = 0, \quad P(C_i) - P(C_{i-1}) = 2 \quad \text{and} \quad |\Theta(C_i)| - |\Theta(C_{i-1})| = 4; \tag{32}$$

if $x_{\tau(i)} \in C_n^2$, then

$$A(C_i) - A(C_{i-1}) = 1, \quad P(C_i) - P(C_{i-1}) = 1 \quad \text{and} \quad |\Theta(C_i)| - |\Theta(C_{i-1})| = 2; \tag{33}$$

whereas, if $x_{\tau(i)} \in C_n^3$, we have

$$A(C_i) - A(C_{i-1}) = 2, \quad P(C_i) - P(C_{i-1}) = 0 \quad \text{and} \quad |\Theta(C_i)| - |\Theta(C_{i-1})| = 0. \tag{34}$$

In view of (31)–(34), we obtain (27)–(30). □

We notice that from (27),(28), and (29) we also recover (22), which in turn, together with (30), yields

$$E(C_n) = -\frac{3}{2}A(C_n) - \frac{1}{4}|\Theta(C_n)| + \frac{3}{2}|C_n^0| \tag{35}$$

for every configuration C_n. Moreover, from the equality

$$\sum_{i=0}^{3} |C_n^i| = n,$$

(28), and (29) it follows that

$$A(C_n) = 2n - 2|C_n^0| - P(C_n). \tag{36}$$

Note that in particular if $C_n = D_n$ then $\omega_{C_n}(x) = \omega(x)$. Furthermore, $D_n^0 = \{x_{\tau(1)}\}$, $D_n^1 = \{x_{\tau(2)}\}$, $D_n^2 = \Omega_2 \cap D_n$, and $D_n^3 = \Omega_3 \cap D_n$. Therefore, (27)–(35) yield

$$E(D_n) = -1 - 2|\Omega_2 \cap D_n| - 3|\Omega_3 \cap D_n|, \tag{37}$$

$$A(D_n) = |\Omega_2 \cap D_n| + 2|\Omega_3 \cap D_n|, \tag{38}$$

$$P(D_n) = 2 + |\Omega_2 \cap D_n|, \tag{39}$$

$$|\Theta(D_n)| = 10 + 2|\Omega_2 \cap D_n|, \tag{40}$$

and by (35) and (36) we obtain

$$E(D_n) = -\frac{3}{2}A(D_n) - \frac{1}{4}|\Theta(D_n)| + \frac{3}{2},$$

and

$$A(D_n) = 2n - 2 - P(D_n)$$

for every $n > 1$.

Proposition 2.3. *The following assertions are equivalent and hold true for every connected configuration C_n:*

(i) $|\Theta(D_n)| \leq |\Theta(C_n)|$;
(ii) $P(D_n) \leq P(C_n)$;
(ii) $A(D_n) \geq A(C_n)$.

Proof. The first assertion follows directly from (24), and is equivalent to the second by (29) and (30). The second assertion is equivalent to the third by (23) and (24). □

2.1. **Proof of Theorem 1.1.** In this subsection we prove Theorem 1.1 by characterizing the minimizers of EIP as the solutions of a discrete isoperimetric problem. We proceed in two steps.

Step 1. We claim that

$$\sqrt{A(D_n)} = k_n P(D_n). \tag{41}$$

Indeed, by (24), (37), and Theorem 2.1 there holds

$$\frac{\theta_n}{2} - 3n = e_n = E(D_n) = -1 - 2|\Omega_2 \cap D_n| - 3|\Omega_3 \cap D_n|. \tag{42}$$

Equalities (7) and (40) yield

$$\theta_n = |\Theta(D_n)| = 10 + 2|\Omega_2 \cap D_n|. \tag{43}$$

Theorefore, by (8), (42) and (43), we have

$$|\Omega_2 \cap D_n| = \frac{\theta_n}{2} - 5, \tag{44}$$

and

$$|\Omega_3 \cap D_n| = -\frac{\theta_n}{2} + n + 3. \tag{45}$$

Claim (41) follows now by (38), (39), (44) and (45), and by observing that

$$\begin{aligned}\sqrt{A(D_n)} &= \sqrt{|\Omega_2 \cap D_n| + 2|\Omega_3 \cap D_n|} = \sqrt{\theta_n/2 - 5 + 2(-\theta_n/2 + n + 3)} \\ &= \sqrt{-\theta_n/2 + 2n + 1} = k_n(\theta_n/2 - 3) = k_n(|\Omega_2 \cap D_n| + 2) = k_n P(D_n).\end{aligned}$$

Inequality (10) is a direct consequence of (41) and Proposition 2.3. By Proposition 2.3 we also deduce that the maximal area and the minimal perimeter among connected configurations are realized by $A(D_n) = -\theta_n/2+2n+1$ and $P(D_n) = \theta_n/2-3$, respectively.

Step 2. We prove the characterization statement of Theorem 1.1. Let C_n be a connected configuration satisfying

$$\sqrt{A(C_n)} = k_n P(C_n). \tag{46}$$

We claim that C_n is a minimizer. In fact, the claim follows from

$$\begin{aligned}|\Theta(D_n)| \le |\Theta(C_n)| &= 6n - 3A(C_n) - P(C_n)\\ &= 6n - 3(k_n)^2(P(C_n))^2 - P(C_n)\\ &\le 6n - 3(k_n)^2(P(D_n))^2 - P(D_n)\\ &= 6n - 3A(D_n) - P(D_n) = |\Theta(D_n)|\end{aligned}$$

where we used (24) in the first inequality, (23) in the first and last equality, (22) in the second, (46) in the third, Proposition 2.3 in the second inequality, and (41) in the third equality.

Viceversa, let M_n be a connected minimizer. By (7), (29), and (30), $P(M_n) = P(D_n)$; by (22), $A(M_n) = A(D_n)$. Thus (10) holds with the equality by (41). This concludes the proof of the theorem. □

3. Maximal hexagons associated to EIP minimizers

In this section we introduce the notion of maximal hexagons $H_{r_{M_n}}$ associated to minimizers M_n and we provide a uniform lower estimate of r_{M_n} in terms of n (see (61)).

Fix a minimizer M_n. Let $\mathcal{H}_s^{M_n}$ be the family of the configurations contained in M_n that can be seen as translations in $\mathcal{L}_t$ of daisy configurations $D_{1+3s+3s^2}$ for some $s \in \mathbb{N} \cup \{0\}$, i.e.,

$$\mathcal{H}_s^{M_n} := \{H_s \subset \mathcal{L}_t \ : \ H_s := D_{1+3s+3s^2} + q \text{ for some } q \in \mathcal{L}_t \text{ and } H_s \subset M_n\}, \tag{47}$$

and choose $H_{r_{M_n}}$ to be a configuration in $\mathcal{H}_{r_{M_n}}^{M_n}$ where

$$r_{M_n} := \max\{s \in \mathbb{N} \cup \{0\} \ : \ \mathcal{H}_s^{M_n} \neq \emptyset\}. \tag{48}$$

We will refer to $H_{r_{M_n}}$ as the *maximal hexagon associated to* M_n. Notice that the number of atoms of M_n contained in $H_{r_{M_n}}$ is

$$n(r_{M_n}) := 1 + 3\,r_{M_n} + 3\,(r_{M_n})^2\,. \tag{49}$$

In the following we will often denote the minimal regular hexagon containing $H_{r_{M_n}}$ by $\hat{H}_{r_{M_n}}$, i.e.,

$$\hat{H}_{r_{M_n}} := F(H_{r_{M_n}})$$

(see Figure 3).

With the same notation as in Section 2, we decompose M_n as

$$M_n = \bigcup_{k=0}^{3} M_n^k.$$

For every k there holds $M_n^k = (\Omega_k \cap H_{r_{M_n}}) \bigcup (M_n^k \setminus H_{r_{M_n}})$. In the following proposition we observe that if $n > 6$, then there exists a non-degenerate maximal hexagon for every minimizer.

Proposition 3.1. *For $n \le 6$, then the maximal hexagon $H_{r_{M_n}}$ is degenerate for every minimizer M_n of (2). If $n > 6$, then the maximal radius r_{M_n} of every minimizer M_n of (2) satisfies $r_{M_n} \ge 1$.*

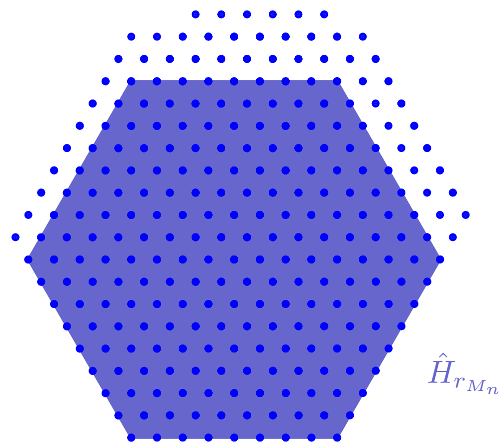

FIGURE 3. A minimizer M_n is represented by the set of dots and its maximal hexagon $H_{r_{M_n}}$ is given by the intersection of M_n with the regular hexagon $\hat{H}_{r_{M_n}}$ which is drawn in dark color (blue).

Proof. It is immediate to check that for $n = 1$, $|M_n^1| = 0$, and for $n = 2$ or $n = 3$, $|M_n^1| = 1$. A direct analysis of the cases in which $n = 4, 5, 6$, shows that $2 \geq |M_n^1| \geq 1$. It is also straightforward to observe that for $n = 0, \cdots, 6$, there holds $r = 0$.

We claim that for $n \geq 7$ the radius r_{M_n} satisfies $r_{M_n} \geq 1$. Indeed, assume that M_n is such that $r_{M_n} = 0$. Then M_n does not contain any hexagon with radius 1 and hence, for every $x \in M_n$ we have that

$$b(x) \leq 5. \tag{50}$$

Property (50) is equivalent to claiming that every element of M_n contributes to the overall perimeter of M_n, and the contribution of each element is at least 1. Therefore,

$$P(M_n) \geq n.$$

By Theorem 1.1, it follows that

$$\frac{\theta_n}{2} - 3 \geq n, \tag{51}$$

which in turn by (9) implies

$$\sqrt{12n-3} - 2 \geq \lceil \sqrt{12n-3} \rceil - 3 \geq n,$$

that is

$$n^2 - 8n + 7 \leq 0,$$

which finally yields $1 \leq n \leq 7$. To conclude, it is enough to notice that for $n = 7$, $\theta_n/2 - 3 = 6$, thus contradicting (51). □

In view of Proposition 3.1 for every minimizer M_n with $n > 6$ we can fix a vertex V_0 of its (non-degenerate) hexagon $\hat{H}_{r_{M_n}}$ and denote by $V_1, \ldots, V_5$ the other vertices of $\hat{H}_{r_{M_n}}$ numbered counterclockwise starting from V_0. For $k = 0, \cdots, 4$, let us also denote by s_k the line passing through the side of $\hat{H}_{r_{M_n}}$ with endpoints V_k and V_{k+1}, and let s_5 be the line passing through V_5 and V_0.

In the following we will need to consider the number of *levels* of atoms in $\mathcal{L}_t$ around $H_{r_{M_n}}$ containing at least one element of M_n. Denote by $\mathbf{e}_k$ the outer unit normal to the side s_k of $\hat{H}_{r_{M_n}}$ and define

$$\lambda_k := \max\{j \in \mathbb{N} \, : \, s_k^j \cap M_n \neq \emptyset\} \tag{52}$$

where s_k^j are the lines of the lattice $\mathcal{L}_t$ parallel to s_k and not intersecting $H_{r_{M_n}}$, namely

$$s_k^j := s_k + \frac{\sqrt{3}}{2} j \mathbf{e}_k$$

for $j \in \mathbb{N}$. Let also π_k be the open half-plane with boundary s_k and not intersecting the interior of $\hat{H}_{r_{M_n}}$.

We first show that M_n satisfies a connectedness property with respect to the directions determined by the lattice $\mathcal{L}_t$. To this purpose, we introduce the notion of *3-connectedness with respect to* $\mathcal{L}_t$.

Definition 3.2. We recall that

$$\boldsymbol{t}_1 := (1,0)\,, \quad \boldsymbol{t}_2 := \left(\frac{1}{2}, \frac{1}{2\sqrt{3}}\right), \quad \text{and define} \quad \boldsymbol{t}_3 := \boldsymbol{t}_2 - \boldsymbol{t}_1.$$

We say that a set $S \subset \mathcal{L}_t$ is *3-connected* if for every $p, q \in S$ such that $q := m\boldsymbol{t}_i + p$ for some $m \in \mathbb{N}$ and $i \in \{1,2,3\}$ one has that $q' := m'\boldsymbol{t}_i + p \in S$ for every integer $m' \in (0, m)$. Furthermore, we refer to the lines

$$\ell_i^p := \{q \in \mathbb{R}^2 \, : \, q = r\boldsymbol{t}_i + p \text{ for some } r \in \mathbb{R}\}$$

as the *lines of the lattice* $\mathcal{L}_t$ *at* p.

Note that by Definition 3.2 a set S is 3-connected if there is no line ℓ_i^p of the lattice $\mathcal{L}_t$ at a point $p \in \mathcal{L}_t \setminus M_n$ that is separated by p in two half-lines both containing points of the set S.

Proposition 3.3. *Let M_n be a minimizer. Then M_n is 3-connected.*

Proof. For the sake of contradiction assume that the minimizer M_n is a not 3-connected. Then there exist a point $p \in \mathcal{L}_t \setminus M_n$ and $i \in \{1,2,3\}$ such that the line ℓ_i^p (see Definition 3.2) is divided by p in two half-lines both containing points of M_n. We claim that we can rearrange the n points of M_n in a new 3-connected configuration $\tilde{M}_n$ such that $|\Theta(\tilde{M}_n)| < |\Theta(M_n)|$ thus contradicting optimality.

Denote for simplicity $\ell_0 := \ell_i^p$ and let $\ell_1, \cdots, \ell_m$ be all the other lines parallel to ℓ_0 that intersect M_n. Furthermore, let $c_k = |M_n \cap \ell_k|$ for $k = 1, \cdots, m$. Starting from the elements of the set $\{c_k\}$ we rearrange them in a decreasing order, constructing another set $\{d_k\}$ with the property that $d_0 \geq d_1 \geq \cdots \geq d_m$. Finally, we separate the elements of $\{d_k\}$ having odd indexes from those having even indexes and we rearrange them in a new set $\{f_k\}$ obtained by first considering the elements of $\{d_k\}$ with even indexes, in decreasing order with respect to their indexes, and then the elements of $\{d_k\}$ having odd indexes, with increasing order with respect to their indexes. The set $\{f_k\}$ constructed as above has the property that the two central elements have the maximal value, and the values of the elements decrease in an alternated way by moving toward the sides of the ordered set. Let $\bar{k}$ be the index corresponding to the central element of the set $\{f_k\}$, if m is even, and to the maximum between the two central elements of $\{f_k\}$, if m is odd.

As an example, if we start with a set $\{c_k\} = \{9, 4, 2, 5, 3, 1, 17\}$, the sequence $\{d_k\}$ is given by $\{17, 9, 5, 4, 3, 2, 1\}$ and the sequence $\{f_k\}$ by $\{1, 3, 5, 17, 9, 4, 2\}$. Here $\bar{k} = 4$.

Fix a point $p_{\bar{k}} \in \mathcal{L}_t$ and an angular sector S of amplitude $2\pi/3$, with vertex in $p_{\bar{k}}$, and whose sides σ_1 and σ_2 lay on the two lines departing from $p_{\bar{k}}$ and which are not parallel to ℓ_0. Consider the points $p_0, \cdots, p_{\bar{k}-1} \in \sigma_1 \cap G_n$, such that

$$|p_k - p_{\bar{k}}| = \bar{k} - k \quad \text{for } k = 0, \cdots \bar{k} - 1.$$

Analogously, consider the points $p_{\bar{k}+1}, \cdots, p_m \in \sigma_2 \cap G_n$, satisfying

$$|p_k - p_{\bar{k}}| = k - \bar{k} \quad \text{for } k = \bar{k} + 1, \cdots, m.$$

For $k = 0, \cdots, m$, let $\tilde{\ell}_k$ be the line parallel to ℓ_0 and passing through p_k. To construct the set $\tilde{M}_n$ we consider f_k consecutive points on each line $\tilde{\ell}_k$, starting from p_k. The set $\tilde{M}_n$ is clearly 3-connected, $|\tilde{M}_n| = |M_n| = n$, the number of bonds in each line parallel to ℓ_0 has increased, and the number of bonds between different lines has not decreased. Hence,

$$|\Theta(\tilde{M}_n)| < |\Theta(M_n)|,$$

providing a contradiction to the optimality of M_n. □

Since every minimizer M_n is 3-connected, the quantity λ_k introduced in (52) for $k = 0, \cdots, 5$ provides the number of non-empty levels of atoms in $M_n \cap \pi_k$ for $n > 6$. In fact, by the definition of τ each partially full level contains at least one point in $(M_n^1 \cup M_n^2) \setminus H_{r_{M_n}}$. Hence,

$$\sum_{k=0}^{5} \lambda_k \leq |M_n^1 \setminus H_{r_{M_n}}| + |M_n^2 \setminus H_{r_{M_n}}|. \tag{53}$$

On the other hand,

$$2|M_n^1 \setminus H_{r_{M_n}}| + |M_n^2 \setminus H_{r_{M_n}}| = P(M_n) - P(H_{r_{M_n}}) = p_n - 6\, r_{M_n}. \tag{54}$$

Therefore, by (53) and (54),

$$\sum_{k=0}^{5} \lambda_k \leq p_n - 6\, r_{M_n}. \tag{55}$$

In the remaining part of this section we provide a characterization of the geometry of $M_n \setminus H_{r_{M_n}}$ for $n > 6$, by subdividing this set into *good* polygons P_k and *bad* polygons T_k, and by showing that the cardinality of $M_n \setminus H_{r_{M_n}}$ is, roughly speaking, of the same order of magnitude as the one of the union of *good* polygons.

Given a minimizer M_n and its maximal hexagon $H_{r_{M_n}}$, we denote by $H_{r_{M_n}+1}$ the hexagon with side $r_{M_n} + 1$ and having the same center as $H_{r_{M_n}}$. In the following we denote the hexagon containing $H_{r_{M_n}+1}$ by

$$\hat{H}_{r_{M_n}+1} := F(H_{r_{M_n}+1}).$$

We first show that, by the optimality of $H_{r_{M_n}}$, there exists an angular sector of $2\pi/3$, and centered in one of the vertices of $\hat{H}_{r_{M_n}+1}$, which does not intersect M_n. To this end, we denote by V_i', $i = 0, \cdots, 5$ the vertices of the hexagon $\hat{H}_{r_{M_n}+1}$, with the convention that V_i' lies on the half-line starting from the center of $H_{r_{M_n}}$ and passing through V_i.

Lemma 3.4. *Let M_n be a minimizer with $r_{M_n} > 0$. Then* *(i)* *The hexagon* $\hat{H}_{r_{M_n}+1}$ *presents at least a vertex, say* V_j' *with* $j \in \{0,\dots,5\}$*, that does not belong to* M_n*.*

(ii) *There exists* $k \in \{0,\dots,5\}$ *such that the open angular sector* S_k *of amplitude* $2\pi/3$*, centered in* V_k'*, and with sides* s_k^1 *and* s_{k-1}^1 *(with the convention that* $s_{-1}^1 := s_5^1$*) is such that* $\overline{S_k} \cap M_n = \emptyset$*.*

(iii) *Every translation* $\hat{H}$ *of* $\hat{H}_{r_{M_n}+1}$ *by a vector* $\boldsymbol{t} := n\boldsymbol{t}_1 + m\boldsymbol{t}_2$ *with* $n, m \in \mathbb{Z}$ *that has a vertex* $v \notin M_n$ *admits an open angular sector* S *of amplitude* $2\pi/3$ *and centered in* v *such that* $\overline{S} \cap M_n = \emptyset$*.*

Proof. We begin by showing assertion (i). In view of the maximality of $H_{r_{M_n}}$ there exists a point $p \in \mathcal{L}_t$ on the boundary of $\hat{H}_{r_{M_n}+1}$ such that $p \notin M_n$. Either p is already a vertex of $\hat{H}_{r_{M_n}+1}$ or p is an internal point on the side of $\hat{H}_{r_{M_n}+1}$ parallel to s_j for some j. In this latter case, by the 3-connectedness of M_n, either V_j' or V_{j+1}' does not belong to M_n and hence, also in this case assertion (i) holds true.

We now denote by V_j' the missing vertex of the hexagon $\hat{H}_{r_{M_n}+1}$ and prove assertion (ii). Let us consider the two half-lines in which V_j' divides the line s_j^1. By the 3-connectedness of M_n at least one of them does not intersect M_n. Analogously, if we consider the two half-lines in which V_j' divides the line s_{j-1}^1, by the 3-connectedness of M_n at least one of them does not intersect M_n. Finally, if we consider the line s' passing through the center of $H_{r_{M_n}}$ and V_j', the 3-connectedness of M_n implies that the points of s' whose distance from the center of $H_{r_{M_n}}$ is bigger than $r_{M_n}+1$ do not belong to M_n. In view of the geometric position of such three half-line departing from V_j' we can conclude that the claim holds true by using once again the 3-connectedness of M_n.

Let us conclude by observing that assertion (iii) directly follows by applying the same argument used to prove assertion (ii) to every translation $\hat{H}$ of $\hat{H}_{r_{M_n}+1}$. ☐

In the following we assume without loss of generality that the vertex V_0 has been chosen so that the index k in assertion (ii) of Lemma 3.4 is 0. Therefore by assertion (ii) of Lemma 3.4 we obtain that the open angular sector S_0 of $2\pi/3$, centered in V_0', and with sides s_0^1 and s_5^1 is such that $\overline{S_0} \cap M_n = \emptyset$.

Let us use the definition of the levels λ_k for $k = 0,\dots,5$ introduced in (52) to define a region $\hat{R}$ that contains all extra points of M_n, i.e., points of M_n not contained in $H_{r_{M_n}}$. We already know that we can take $\hat{R} \subset (\mathbb{R}^2 \setminus \hat{H}_{r_{M_n}}) \cap (\mathbb{R}^2 \setminus S_0)$. We define the region $\hat{R}$ as follows:

$$\hat{R} := \Big(\bigcup_{j=0}^{5} \hat{P}_j\Big) \bigcup \Big(\bigcup_{j=1}^{5} \hat{T}_j\Big) \tag{56}$$

(see Figure 4). The set $\hat{P}_0$ in (56) is the polygon delimited by the lines $s_5, s_0^1, s_0^{\lambda_0}, s_5^{-r+1}$ and the sets $\hat{P}_k$ in (56) is defined by

$$\hat{P}_k := \begin{cases} \hat{P}_k^1(\lambda_k) & \text{if } \lambda_k \le \lambda_{k-1}+1, \\ \hat{P}_k^1(\lambda_k - \lambda_{k-1}+1) \cup \hat{P}_k^2(\lambda_k - \lambda_{k-1}+1) & \text{if } \lambda_k > \lambda_{k-1}+1, \end{cases}$$

for every $k = 1,\dots,5$, where for every $a \in [-2\,r_{M_n}, 2\,r_{M_n}]$ we denote by $\hat{P}_k^1(a)$ the polygon contained between s_k^1, s_k^a, s_{k+1}, s_{k+1}^{-r+1}, and by $\hat{P}_k^2(a)$ the set delimited by s_k^a,

$s_k^{\lambda_k}$, $s_{k-1}^{\lambda_{k-1}-r+1}$, $s_{k-1}^{\lambda_{k-1}}$. Finally the sets $\hat{T}_k$ are the *region* between $\hat{P}_{k-1}$ and $\hat{P}_k$ or, more precisely,

$$\begin{aligned}\hat{T}_k := &\{x \in R :\, x \in s_{k-1}^{j_{k-1}} \cap s_k^{j_k}, \text{ with } 1 \le j_{k-1} \le \lambda_{k-1},\, 1 \le j_k \le \lambda_k,\, j_{k-1} \ge j_k \\ &\text{and, if } \lambda_{k-1} > \lambda_{k-2}+1,\, j_{k-1} \le j_k + \lambda_{k-1} - \lambda_{k-2}\}.\end{aligned} \tag{57}$$

Furthermore, we consider the configurations $P_k := \hat{P}_k \cap \mathcal{L}_t$ for $k = 0, \dots, 5$, $T_k := \hat{T}_k \cap \mathcal{L}_t$ for $k = 1, \dots, 5$, and $R := \hat{R} \cap \mathcal{L}_t$. We notice that $M_n \subset H_{r_{M_n}} \cup R$ and that

$$n = |H_{r_{M_n}}| + |R| - |R \setminus M_n|,$$

where $|H_{r_{M_n}}| = 1 + 3\, r_{M_n} + 3\, (r_{M_n})^2$, and

$$|R| = \sum_{k=0}^{5} |P_k| + \sum_{k=1}^{5} |T_k| = r_{M_n} \sum_{k=0}^{5} \lambda_k + \sum_{k=1}^{5} |T_k|$$

where in the last equality we used that $|P_k| = r_{M_n} \lambda_k$ for $k = 0, \dots, 5$. Furthermore, for every $x \in R$ and every $k = 0, \cdots, 5$ there exists $j_k \in [-\lambda_{k'} - 2r, \lambda_k]$ with $k' := (k+3)_{\mathrm{mod}\ 6}$ and $k' \in \{0, \dots, 5\}$ such that $x \in s_k^{j_k}$. Hence, in particular, every $x \in R$ is uniquely determined by a pair of indexes $(j_k, j_{k'})$, with $k' \neq k+3$ in $\mathbb{Z}_6$.

Proposition 3.5. *Let $\mathcal{H}$ be the family of the configurations that can be seen as translations in $\mathcal{L}_t$ of the daisy configuration $D_{1+3s+3s^2}$ for $s := r_{M_n} + 1$ and that are contained in $H_{r_{M_n}} \cup R$, i.e.,*

$$\mathcal{H} := \{H \subset H_{r_{M_n}} \cup R \,:\, H = D_{1+3s+3s^2} + q \textit{ for } s := r_{M_n} + 1 \textit{ and some } q \in \mathcal{L}_t\}.$$

Then there holds

$$|R \setminus M_n| \ge |\mathcal{H}|.$$

Proof. Let $h := |\mathcal{H}|$. We show by induction on $m = 1, \dots, h$ that for every family $\mathcal{H}_m \subset \mathcal{H}$ with $|\mathcal{H}_m| = m$, there exists a set $V_{\mathcal{H}_m} \subset R \setminus M_n$ with $|V_{\mathcal{H}_m}| = m$, such that the correspondence that associates to each $v \in V_{\mathcal{H}_m}$ a hexagon $H \in \mathcal{H}_m$ if v is a vertex of $\hat{H} := F(H)$, is a bijection.

We remark that the thesis will follow once we prove the assertion for $m = h$. The claim holds for $m = 1$ by reasoning in the same way as in the first assertion of Lemma 3.4. Assume now that the claim is satisfied for $m = \bar{m}$. Consider a family $\mathcal{H}_{\bar{m}+1} = \{H_1, \dots, H_{\bar{m}+1}\} \subset \mathcal{H}$, and the polygon

$$\mathcal{P}_{\bar{m}+1} := \bigcup_{i=1}^{\bar{m}+1} H_i \subset H_{r_{M_n}} \cup R.$$

Furthermore, let us define

$$\hat{\mathcal{P}}_{\bar{m}+1} := F(\mathcal{P}_{\bar{m}+1}).$$

We subdivide the remaining part of the proof into 4 steps.

Step 1. There exists a vertex $\tilde{v}$ of $\hat{\mathcal{P}}_{\bar{m}+1}$ that is not in M_n. Indeed, if all vertices of $\hat{\mathcal{P}}_{\bar{m}+1}$ belong to M_n, by 3-connectedness $\mathcal{P}_{\bar{m}+1} \subset M_n$, and hence $H_{\bar{m}+1} \subset \mathcal{P}_{\bar{m}+1} \subset M_n$, which would contradict the maximality of r_{M_n}.

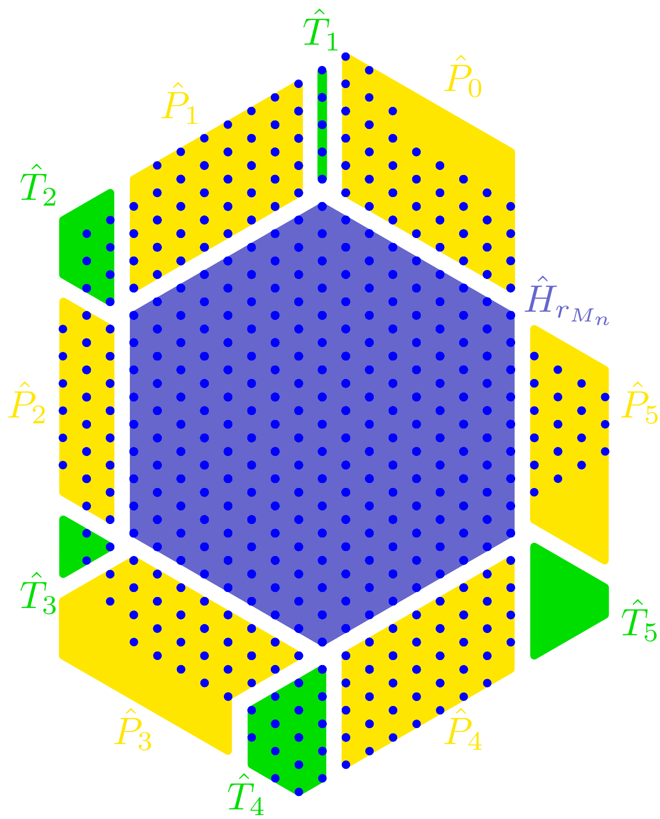

FIGURE 4. Representation of the region $\hat{R}$ given by the union of the polygons $\hat{P}_j$ with $j = 0, \ldots, 5$ drawn in the lightest color (yellow) and the polygons $\hat{T}_j$ with $j = 1, \ldots, 5$ drawn in the middle color (green). Note that this picture has a mere illustrative purpose (the configuration is not a EIP minimizer).

Step 2. By assertion (*iii*) of Lemma 3.4 there exists an open angular sector S centered in $\tilde{v}$, amplitude $2\pi/3$, and sides $\sigma_1, \sigma_2 \subset \mathcal{L}_t$ such that $\bar{S} \cap M_n = \emptyset$.

Step 3. There exists a vertex v of $\hat{\mathcal{P}}_{\bar{m}+1}$ that is not in M_n and that corresponds to an interior angle of $\hat{\mathcal{P}}_{\bar{m}+1}$ of $2\pi/3$. In fact, $\hat{\mathcal{P}}_{\bar{m}+1}$ can have vertices with angles of $2\pi/3$, $4\pi/3$, and $5\pi/3$ only. If the vertex $\tilde{v}$ detected in Step 2 corresponds to an angle of $2\pi/3$, there is nothing to prove. If $\tilde{v}$ corresponds to an angle of $4\pi/3$ or $5\pi/3$, then we have two cases.

Case 1: the intersection between S and the closure of $\hat{\mathcal{P}}_{\bar{m}+1}$ is empty. Then, for every $j = 1, 2$, there exists $v_j \in \sigma_j$ such that the segment with endpoints $\tilde{v}$ and v_j denoted by $\tilde{v}v_j$ is contained in $\partial\hat{\mathcal{P}}_{\bar{m}+1}$ and v_j is a vertex of $\hat{\mathcal{P}}_{\bar{m}+1}$. Furthermore, $v_j \notin M_n$ because $v_j \in S$, and v_j is associated to an angle of $2\pi/3$, since $S \cap \bar{\mathcal{P}}_{\bar{m}+1} = \emptyset$. The proof follows by taking $v = v_1$.

Case 2: the intersection between S and the closure of $\hat{\mathcal{P}}_{\bar{m}+1}$ is nonempty. Without loss of generality, we can assume that the two sides of the angular sector S are given by

$$\sigma_1 = \Big\{(\alpha,\beta) \in \mathbb{R}^2 :\, \beta = \alpha \boldsymbol{t}_1 + \tilde{v},\, \alpha > 0\Big\}$$

and

$$\sigma_2 = \Big\{(\alpha,\beta) \in \mathbb{R}^2 :\, \beta = -\alpha \boldsymbol{t}_2 + \tilde{v},\, \alpha > 0\Big\}.$$

Define

$$\sigma_1^k := \sigma_1 - \frac{\sqrt{3}}{2} k\,(0,1) \quad \text{and} \quad \sigma_2^k := \sigma_2 + k\,\boldsymbol{t}_1,$$

for $k \in \mathbb{N}$. Since $\mathcal{P}_{\bar{m}+1} \cap S$ is bounded, we can find

$$k_1 := \max\{k \in \mathbb{N} :\, \sigma_1^k \cap \mathcal{P}_{\bar{m}+1} \cap S \neq \emptyset\}$$

and

$$k_2 := \max\{k \in \mathbb{N} :\, \sigma_2^k \cap \mathcal{P}_{\bar{m}+1} \cap S \neq \emptyset\}.$$

For $j = 1, 2$, the intersection $\sigma_j^{k_j} \cap \partial\hat{\mathcal{P}}_{\bar{m}+1} \cap S$ is either a vertex of $\hat{\mathcal{P}}_{\bar{m}+1}$ associated to an angle of $2\pi/3$, or a segment with at least one endpoint $v \in S$ corresponding to a vertex of $\partial\hat{\mathcal{P}}_{\bar{m}+1}$ associated to an angle of $2\pi/3$.

Step 4. Let v be the vertex provided by Step 3. Then, there exists a unique $\hat{H}_{\bar{j}} \in \mathcal{H}_{\bar{m}+1}$ having v among his vertices. By the induction hypothesis on $\{\hat{H}_1, \ldots, \hat{H}_{\bar{m}+1}\} \setminus \{\hat{H}_{\bar{j}}\}$ there exists a family of vertices $\{v_j\}_{j=1,\ldots,\bar{m}+1,\, j\neq\bar{j}} \subset R \setminus M_n$ such that v_j is a vertex of $\hat{H}_j$ and for every $i \neq j$, v_j is not a vertex of $\hat{H}_i$. The thesis follows then by setting $v_{\bar{j}} = v$, and by taking $V_{\mathcal{H}_{\bar{m}+1}} = \{v_1, \ldots, v_{\bar{m}+1}\}$. □

In view of Proposition 3.5 in order to estimate from below the cardinality of $R \setminus M_n$ it suffices to estimate the cardinality of $\mathcal{H}$. To this end we denote in the following by $\hat{U}_k$ the closure of the region in $\mathbb{R}^2$ containing $H_{r_{M_n}}$ and delimited, respectively, by s_3, s_4, and s_5 for $k = 2$, s_4, s_5, and s_0 for $k = 3$, s_5, s_0, and s_1 for $k = 4$, and s_0, s_1, and s_2 for $k = 5$. Notice that $T_k \subset \hat{U}_k$ (see Figure 5).

Lemma 3.6. *There holds*

$$|\mathcal{H}| \geq \sum_{j=2}^{5} |T_j| - \lambda_1 - 2\lambda_2 - 2\lambda_3 - 2\lambda_4 - \lambda_5 + 4. \tag{58}$$

Proof. For notational simplicity we will omit in the rest of this proof the dependence of the radius r_{M_n} on the minimizer M_n. We begin by noticing that

$$|\mathcal{H}| \geq \sum_{k=2}^{5} |\mathcal{H}_k| \tag{59}$$

where

$$\mathcal{H}_k := \{H \in \mathcal{H} :\, H \subset \hat{U}_k \text{ and has a vertex in } T_k\}$$

for $k = 2, 3, 4, 5$. We claim that

$$|\mathcal{H}_k| \geq |T_k| - \lambda_k - \lambda_{k-1} + 1 \tag{60}$$

and we observe that (58) directly follows from (59) and (60).

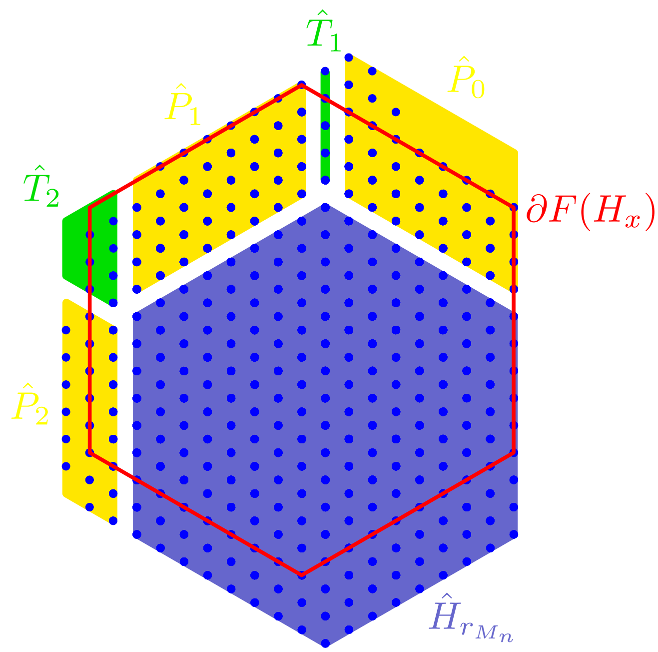

FIGURE 5. The region $\hat{U}_2$ is shown and the boundary $\partial F(H_x)$ of a hexagon $H_x \in \mathcal{H}_2$ with vertex $x \in T_2$ is represented by a continuous (red) line. Note that this picture has a mere illustrative purpose (the configuration is not a EIP minimizer).

The rest of the proof is devoted to show (60). Let $x \in T_k$ and consider (j_k, j_{k-1}, j_{k-2}) such that $x \in s_k^{j_k} \cap s_{k-1}^{j_{k-1}} \cap s_{k-2}^{j_{k-2}}$. In the following we identify x with the triple of indexes (j_k, j_{k-1}, j_{k-2}), and we write $x = (j_k, j_{k-1}, j_{k-2})$. Let H_x be the hexagon with vertices x,

$$\begin{aligned}
v_1 &:= (j_k - (r+1), j_{k-1}, j_{k-2} + (r+1)),\\
v_2 &:= (j_k - 2(r+1), j_{k-1} - (r+1), j_{k-2} + (r+1)),\\
v_3 &:= (j_k - 2(r+1), j_{k-1} - 2(r+1), j_{k-2}),\\
v_4 &:= (j_k - (r+1), j_{k-1} - 2(r+1), j_{k-2} - (r+1)),\\
v_5 &:= (j_k, j_{k-1} - (r+1), j_{k-2} - (r+1))
\end{aligned}$$

(see Figure 5 for an example of an hexagon $H_x \in \mathcal{H}_2$ with $x \in T_2$).

H_x is contained in $\hat{U}_k$ if for every $j = 0, \ldots, 5$ there holds $v_j \in \hat{U}_k$. This latter condition is equivalent to checking that the following inequalities are satisfied

$$\begin{aligned}
&j_k - 2(r+1) \geq -2r, \quad j_k \leq \lambda_k,\\
&j_{k-1} - 2(r+1) \geq -2r, \quad j_{k-1} \leq \lambda_{k-1},\\
&j_{k-2} - (r+1) \geq -2r, \quad j_{k-2} + (r+1) \leq \lambda_{k-2}.
\end{aligned}$$

Hence, if $x=(j_j,j_{k-1},j_{k-2})\in T_k$ is such that

$$\begin{aligned}&2\leq j_k\leq\lambda_k,\\&2\leq j_{k-1}\leq\lambda_{k-1},\\&-r+1\leq j_{k-2}\leq\lambda_{k-2}-(r+1),\end{aligned}$$

then $H_x\subset\hat{U}_k$. By the definition of the sets T_k (see (57)), the previous properties are fulfilled by every $x\in T_k$, apart from those points belonging to the portion of the boundary of $\hat{T}_k$ which is adjacent either to $\hat{P}_{k-1}$ or to $\hat{P}_k$. Denoting by $\tilde{T}_k$ this latter set, claim (60) follows once we observe that

$$|\tilde{T}_k|=|T_k|-\lambda_k-\lambda_{k-1}+1.$$ □

Moving from Proposition 3.5 and Lemma 3.6, we deduce the lower estimate on the maximal radii r_{M_n} of the minimizers M_n of (2).

Proposition 3.7. *Let M_n be a minimizer of (2) with maximal radius r_{M_n}. Then*

$$r_{M_n}\geq\frac{\lceil\alpha_n\rceil}{6}-2-\frac{1}{6}\sqrt{\lceil\alpha_n\rceil^2-(\alpha_n)^2+75}\tag{61}$$

with

$$\alpha_n:=\sqrt{12n-3}\,.\tag{62}$$

Proof. For the sake of notational simplicity we will omit in the rest of this proof the dependence of the maximal radius r_{M_n} from M_n. By Proposition 3.5 and Lemma 3.6 we have

$$|R\setminus M_n|\geq\sum_{j=2}^{5}|T_j|-\lambda_1-2\lambda_2-2\lambda_3-2\lambda_4-\lambda_5+4,$$

and so, by (55) and $|T_1|=\min\{\lambda_0,\lambda_1\}$, we obtain

$$\begin{aligned}n&=|H_{r_{M_n}}|+|R|-|R\setminus M_n|\\&\leq 1+3r^2+3r+\sum_{j=0}^{5}|P_j|+\sum_{j=1}^{5}|T_j|-\sum_{j=2}^{5}|T_j|+\lambda_1+2\lambda_2+2\lambda_3+2\lambda_4+\lambda_5-4\\&\leq 1+3r^2+3r+r\sum_{j=0}^{5}\lambda_j+|T_1|+\lambda_1+2\lambda_2+2\lambda_3+2\lambda_4+\lambda_5-4\\&\leq 1+3r^2+3r+(r+2)\sum_{j=0}^{5}\lambda_j-4\\&\leq 1+3r^2+3r+(r+2)(p_n-6r)-4=-3r^2+(p_n-9)r+2p_n.\end{aligned}$$

Thus, the maximal radius satisfies the following inequality:

$$3r^2-(p_n-9)r+n-2p_n\leq 0.\tag{63}$$

Estimate (61) follows from (63) by solving (63) with respect to r and recalling that $p_n:=\theta_n/2-3$ by Theorem 1.1 and $\theta_n:=2\lceil\alpha_n\rceil$ by (9). □

A direct consequence of (61) is an upper bound on the Hausdorff distance between the sets M_n and $H_{r_{M_n}}$.

Corollary 3.8. *Given a sequence $\{M_n\}$ of minimizers and an associated sequence $\{H_{r_{M_n}}\}$ of maximal hexagons, there holds*

$$d_{\mathcal{H}}(M_n, H_{r_{M_n}}) \leq \mathrm{O}(n^{1/4}), \tag{64}$$

where $d_{\mathcal{H}}$ is the Hausdorff distance.

Proof. Let M_n be a minimizer. We assume with no loss of generality that $n > 6$ so that by Proposition 3.1 the maximal hexagon $H_{r_{M_n}}$ is not degenerate. Then

$$d_{\mathcal{H}}(M_n, H_{r_{M_n}}) \leq \max_{i=0,\cdots,5} \lambda_i.$$

Therefore, by (55) and (62) we obtain that

$$\begin{aligned} d_{\mathcal{H}}(M_n, H_{r_{M_n}}) &\leq p_n - 6\, r_{M_n} \\ &\leq 9 + \sqrt{\lceil \alpha_n \rceil^2 - (\alpha_n)^2 + 75} \\ &= \sqrt{\lceil \alpha_n \rceil^2 - (\alpha_n)^2} + \mathrm{O}(1), \end{aligned}$$

where we used Proposition 3.7 in the second inequality. □

4. Convergence to the Wulff shape

In this section we use the lower bound (61) on the maximal radius r_{M_n} associated to each minimizer M_n of (2) to study the convergence of minimizers to the hexagonal asymptotic shape as the number n of points tends to infinity.

To this end we recall from the introduction that W is the regular hexagon defined as the convex hull of the vectors

$$\left\{ \pm\frac{1}{\sqrt{3}}\boldsymbol{t}_1,\ \pm\frac{1}{\sqrt{3}}\boldsymbol{t}_2,\ \pm\frac{1}{\sqrt{3}}\boldsymbol{t}_3 \right\},$$

where $\mathbf{t_i}$ are defined in Definition 3.2 for $i = 1, 2, 3$. Furthermore, in the following μ will denote the measure

$$\mu := \frac{2}{\sqrt{3}}\chi_W,$$

where χ_W is the characteristic function of W. We recall that by $\|\cdot\|$ we denote the total variation norm and by $\|\cdot\|_{\mathrm{F}}$ the flat norm defined by

$$\|\mu\|_{\mathrm{F}} := \sup\left\{ \int_{\mathbb{R}^2} \varphi\, d\mu : \varphi \text{ is Lipschitz with } \|\varphi\|_{W^{1,\infty}(\mathbb{R}^2)} \leq 1 \right\} \tag{65}$$

for every $\mu \in M_b(\mathbb{R}^2)$.

4.1. **Proof of Theorem 1.2.**
In this subsection we prove Theorem 1.2.

Step 1. We start by considering

$$K_n := \frac{\lceil \alpha_n \rceil}{6n^{3/4}} \sqrt{\lceil \alpha_n \rceil^2 - (\alpha_n)^2}, \tag{66}$$

where $\alpha_n := \sqrt{12n-3}$, see (62). In view of the definition of $H_{r_{M_n}}$ we observe that

$$\begin{aligned}
|M_n \setminus H_{r_{M_n}}| &= n - (1 + 3\,(r_{M_n})^2 + 3\,r_{M_n}) \\
&\leq n \,-\, 1 \,-\, 3\Big(\frac{\lceil \alpha_n \rceil}{6} - 2 - \frac{1}{6}\sqrt{\lceil \alpha_n \rceil^2 - (\alpha_n)^2 + 33}\Big)^2 \\
&\qquad\qquad - 3\Big(\frac{\lceil \alpha_n \rceil}{6} - 2 - \frac{1}{6}\sqrt{\lceil \alpha_n \rceil^2 - (\alpha_n)^2 + 33}\Big) \\
&= n - \frac{\lceil \alpha_n \rceil^2}{12} + \frac{\lceil \alpha_n \rceil}{6}\sqrt{\lceil \alpha_n \rceil^2 - (\alpha_n)^2} + \mathrm{o}(n^{3/4}) \\
&= \frac{\lceil \alpha_n \rceil}{6}\sqrt{\lceil \alpha_n \rceil^2 - (\alpha_n)^2} + \mathrm{o}(n^{3/4}) \qquad (67)
\end{aligned}$$

where we used Proposition 3.7 in the inequality. Therefore, by (66) and (67) we obtain the estimate

$$|M_n \setminus H_{r_{M_n}}| \leq K_n n^{3/4} + \mathrm{o}(n^{3/4}). \qquad (68)$$

Furthermore, since

$$\left\| \mu_{M_n} - \mu_{H_{r_{M_n}}} \right\| = \frac{\left| M_n \triangle H_{r_{M_n}} \right|}{n}$$

and $H_{r_{M_n}} \subset M_n$, by (68) we also obtain that

$$\left\| \mu_{M_n} - \mu_{H_{r_{M_n}}} \right\| \leq K_n n^{-1/4} + \mathrm{o}(n^{-1/4}). \qquad (69)$$

We now define

$$d_n := 1 + 3\,r_{M_n} + 3\,(r_{M_n})^2$$

and consider the empirical measure $\mu_{D_{d_n}}$ associated to the daisy D_{d_n}. For every point $x_i \in D_{d_n}$ we denote by Z_i the Voronoi cell in $\mathcal{L}_t$ related to x_i, that is the regular hexagon centered in x_i with side $1/\sqrt{3}$ and edges orthogonal to the three lattice directions. Furthermore, let $Z_i^n := \{x/\sqrt{n} \,:\, x \in Z_i\}$. We observe that

$$\left\| \frac{x_i}{\sqrt{n}} - x \right\|_{L^\infty(Z_i^n)} \leq \frac{2}{\sqrt{3n}}, \qquad (70)$$

and

$$\mathcal{L}^2\left(\left(\bigcup_{i=1}^{d_n} Z_i^n \right) \Delta W \right) \leq \mathrm{O}(n^{-1/2}). \qquad (71)$$

For every $\varphi \in W^{1,\infty}(\mathbb{R}^2)$ we obtain that

$$
\begin{aligned}
\Big|\int_{\mathbb{R}^2}\varphi\,d\mu_{D_n}-\int_{\mathbb{R}^2}\varphi\,d\mu\Big| &= \Big|\frac{1}{n}\sum_{i=1}^{d_n}\varphi\Big(\frac{x_i}{\sqrt{n}}\Big)-\frac{2}{\sqrt{3}}\int_W\varphi\,dx\Big|\\
&= \frac{2}{\sqrt{3}}\Big|\sum_{i=1}^{d_n}\varphi\Big(\frac{x_i}{\sqrt{n}}\Big)\mathcal{L}^2(Z_i^n)-\int_W\varphi\,dx\Big|\\
&\le \frac{2}{\sqrt{3}}\Big|\sum_{i=1}^{d_n}\int_{Z_i^n}\Big(\varphi\Big(\frac{x_i}{\sqrt{n}}\Big)-\varphi(x)\Big)\,dx\Big| + \frac{2}{\sqrt{3}}\|\varphi\|_{L^\infty(\mathbb{R}^2)}\mathcal{L}^2\left(\left(\bigcup_{i=1}^{d_n}Z_i^n\right)\Delta W\right)\\
&\le \frac{2}{\sqrt{3}}\|\nabla\varphi\|_{L^\infty(\mathbb{R}^2;\mathbb{R}^2)}\sum_{i=1}^{d_n}\int_{Z_i^n}\Big|\frac{x_i}{\sqrt{n}}-x\Big|\,dx + \frac{2}{\sqrt{3}}\|\varphi\|_{L^\infty(\mathbb{R}^2)}\mathcal{L}^2\left(\left(\bigcup_{i=1}^{d_n}Z_i^n\right)\Delta W\right)\\
&\le \frac{4}{3\sqrt{n}}\|\nabla\varphi\|_{L^\infty(\mathbb{R}^2;\mathbb{R}^2)}\mathcal{L}^2\left(\bigcup_{i=1}^{d_n}Z_i^n\right) + \frac{2}{\sqrt{3}}\|\varphi\|_{L^\infty(\mathbb{R}^2)}\mathcal{L}^2\left(\left(\bigcup_{i=1}^{d_n}Z_i^n\right)\Delta W\right)\\
&\le \frac{4}{3\sqrt{n}}\|\nabla\varphi\|_{L^\infty(\mathbb{R}^2;\mathbb{R}^2)}\frac{\mathcal{L}^2(\hat{H}_{r_{M_n}+1})}{n} + \frac{2}{\sqrt{3}}\|\varphi\|_{L^\infty(\mathbb{R}^2)}\mathcal{L}^2\left(\left(\bigcup_{i=1}^{d_n}Z_i^n\right)\Delta W\right)\\
&\le \|\varphi\|_{W^{1,\infty}(\mathbb{R}^2)}\mathrm{O}(n^{-1/2})
\end{aligned}
\tag{72}
$$

where we used (70) and (71) in the third and the last inequality, respectively.

By combining (69) with (72) we obtain that

$$
\mu_{M_n'} \rightharpoonup^* \mu \quad \text{weakly* in } M_b(\mathbb{R}^2), \tag{73}
$$

and

$$
\big\|\mu_{M_n'}-\mu\big\|_{\mathrm{F}} \le K_n n^{-1/4} + \mathrm{o}(n^{-1/4}), \tag{74}
$$

where $M_n' := M_n - q_n$, with $q_n \in \mathcal{L}_t$ such that $H_{r_{M_n}} = D_{1+3r_{M_n}+3r_{M_n}^2} + q_n$.

Step 2. Assertions (12)–(14) directly follow from (68), (69), and (74) since by (62) and (66) a direct computation shows that

$$
\begin{aligned}
K_n &= \frac{\lceil\alpha_n\rceil}{6n^{3/4}}\sqrt{\lceil\alpha_n\rceil^2-(\alpha_n)^2}\\
&= \frac{2}{3^{1/4}}\sqrt{\lceil\sqrt{12n-3}\,\rceil-\sqrt{12n-3}}+\mathrm{o}(1)\\
&= K_t\sqrt{\lceil\sqrt{12n-3}\,\rceil-\sqrt{12n-3}}+\mathrm{o}(1)
\end{aligned}
\tag{75}
$$

□

We notice here that Theorem 1.2 implies in particular the convergence (up to traslations) of the empirical measures associated with the minimizers to the measure μ not only with respect to the weak∗-converge of measures, but also with respect to the flat norm (see (65)).

We remark that an alternative approach to the one adopted in Theorem 1.2 is that of defining a unique n-configurational Wulff-shape W_n for all the minimizer with n atoms. For example we could define

$$
W_n := \hat{W}_n \cap \mathcal{L}_t,
$$

where $\hat{W}_n$ is the hexagon with side $p_n/6$ and center $x_{\tau(1)}$. We remark that the $\mathrm{O}(n^{1/4})$ estimate on the Hausdorff distance and the $\mathrm{O}(n^{3/4})$-law still hold true by replacing the maximal hexagon $H_{r_{M_n}}$ with W_n.

More precisely, by Proposition 3.7 we have that

$$d_{\mathcal{H}}(W_n, H_{r_{M_n}}) \leq \left|\frac{p_n}{6} - r\right| \leq \sqrt{\lceil\alpha_n\rceil^2 - (\alpha_n)^2} + \mathrm{O}(1) \tag{76}$$

and that

$$\begin{aligned} |W_n \setminus H_{r_{M_n}}| &\leq \left|3\Big(\Big\lfloor\frac{p_n}{6}\Big\rfloor\Big)^2 + 3\Big(\Big\lfloor\frac{p_n}{6}\Big\rfloor\Big) - 3\,(r_{M_n})^2 - 3\,r_{M_n}\right| \\ &= 3\Big(\Big\lfloor\frac{p_n}{6}\Big\rfloor + r_{M_n} + 1\Big)\left|\Big\lfloor\frac{p_n}{6}\Big\rfloor - r_{M_n}\right| \\ &\leq \frac{p_n}{6}\sqrt{\lceil\alpha_n\rceil^2 - (\alpha_n)^2} + \mathrm{o}(n^{3/4}) \\ &= \frac{\lceil\alpha_n\rceil}{6}\sqrt{\lceil\alpha_n\rceil^2 - (\alpha_n)^2} + \mathrm{o}(n^{3/4}) \end{aligned} \tag{77}$$

for every minimizer M_n. Therefore, we obtain that

$$d_{\mathcal{H}}(M_n', W_n) \leq \mathrm{O}(n^{1/4})$$

by (64) and (76), and

$$|M_n' \triangle W_n| \leq \mathrm{O}(n^{3/4}) \tag{78}$$

by (68) and (78), with $M_n' := M_n - q_n$ where $q_n \in \mathcal{L}_t$ are chosen in such a way that

$$H_{r_{M_n}} = D_{1+3r_{M_n}+3r_{M_n}^2} + q_n.$$

Furthermore, from (78) it follows that

$$\left\|\mu_{M_n'} - \mu_{W_n}\right\| = \frac{|M_n' \triangle W_n|}{n} \leq \mathrm{O}(n^{-1/4}).$$

4.2. **Proof of Theorem 1.3.** In this subsection we prove that the estimates (12)–(14) are sharp.

Step 1. In this step we show that there exists a sequence of minimizers $\overline{M}_n$ such that, denoting by $H_{r_{\overline{M}_n}}$ their maximal hexagons,

$$|\overline{M}_n \setminus H_{r_{\overline{M}_n}}| = K_n n^{3/4} + \mathrm{o}(n^{3/4}).$$

We will explicitly construct the minimizers $\overline{M}_n$. To this end we denote by $\hat{H}_{r_n}$ the closure of the regular hexagon in $\mathbb{R}^2$ with center in $x_{\tau(1)}$ and side r_n defined by

$$r_n := \left\lceil \frac{\lceil\alpha_n\rceil}{6} - \frac{1}{6}\sqrt{\lceil\alpha_n\rceil^2 - (\alpha_n)^2}\right\rceil,$$

and we introduce $H_{r_n} := \hat{H}_{r_n} \cap \mathcal{L}_t$. Furthermore, we define

$$h_n := \frac{p_n}{2} - 3r_n$$

and we consider the region

$$\hat{A}_n := \{x + h_n \boldsymbol{t}_2 \ : \ x \in \hat{H}_{r_n}\} \setminus \hat{H}_{r_n}$$

that consists of two parallelograms of height h_n constructed on two consecutive sides of H_{r_n} (see Figure 6).

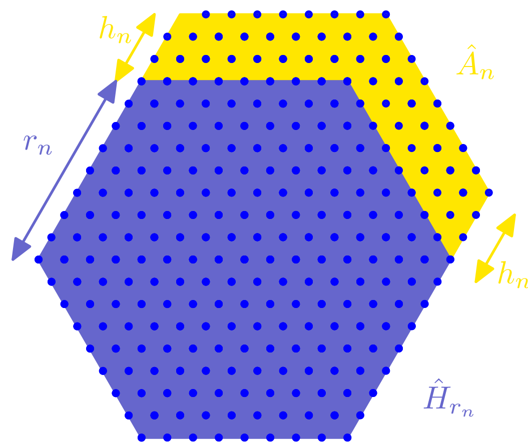

FIGURE 6. The form of a minimizer $\overline{M}_n$ constructed in the proof of Theorem 1.3 is shown. The configuration $\overline{M}_n$ is contained in the union of the hexagon $\hat{H}_{r_n}$ drawn in the darkest color (blue) and the region $\hat{A}_n$ constructed on two of its sides drawn in the lightest color (yellow).

Let $c := |(\hat{H}_{r_n} \cup \hat{A}_n) \cap \mathcal{L}_t|$. We denote by C_c the configuration defined by

$$C_c := \left(\hat{H}_{r_n} \cup \hat{A}_n\right) \cap \mathcal{L}_t$$

and we observe that, by construction, the perimeter of C_c satisfies

$$P(C_c) = p_n. \tag{79}$$

We subdivide the remaining proof of the claim into two substeps.

Substep 1.1. We claim that for every n big enough there exists a minimizer $\overline{M}_n$ such that

$$H_{r_n} \subseteq \overline{M}_n \subseteq C_c$$

and $|C_c \setminus \overline{M}_n| \leq 2r_n - 1$.

We begin by observing that

$$\begin{aligned} c := |C_c| &= |H_{r_n}| + (2r_n + 1)h_n \\ &= 1 + 3r_n^2 + 3r_n + \left(r_n + \frac{1}{2}\right)(p_n - 6r_n) \\ &= -3r_n^2 + p_n r_n + 1 + \frac{p_n}{2}. \end{aligned} \tag{80}$$

Then, a direct computation shows that

$$3s^2 - p_n s - 1 - \frac{p_n}{2} \geq 0 \tag{81}$$

for every $s \in \left[\frac{\lceil \alpha_n \rceil}{6} - 3 - \frac{1}{6}\sqrt{\lceil \alpha_n \rceil^2 + 3}, \frac{\lceil \alpha_n \rceil}{6} - 3 + \frac{1}{6}\sqrt{\lceil \alpha_n \rceil^2 + 3}\right]$, and, for n big enough,

$$3s^2 + (2 - p_n)s - 2 - \frac{p_n}{2} + n \geq 0 \tag{82}$$

for every $s \in \mathbb{R}$. In particular, (81) and (82) hold for $s = r_n$ and for n sufficiently large, yielding

$$0 \le c - n \le 2r_n - 1. \tag{83}$$

We now observe that by the definition of C_c it is possible to remove up to $2r_n - 1$ points from $C_c \setminus H_{r_n}$ without changing the perimeter of the configuration. In view of (83) we construct $\overline{M}_n$ by removing in such a way $c - n$ points from C_c. It follows from (79) that $P(\overline{M}_n) = p_n$ and hence, the claim holds true.

Substep 1.2. Let $\overline{M}_n$ be the sequence of ground states constructed in the previous substep. In view of (83), and of the definition of α_n and p_n, there holds

$$\begin{aligned} |C_n \setminus H_{r_n}| &= (2r_n + 1)h_n \\ &= -6(r_n)^2 - 3r_n + p_n r_n + 1 + \frac{p_n}{2} \\ &= \frac{\lceil \alpha_n \rceil}{6}\sqrt{\lceil \alpha_n \rceil^2 - (\alpha_n)^2} + \mathrm{o}(n^{3/4}). \end{aligned} \tag{84}$$

Moreover, by the definition of $\overline{M}_n$ we have that

$$|C_n \setminus \overline{M}_n| \le 2r_n - 1 = \mathrm{O}(n^{1/2}) = \mathrm{o}(n^{3/4}). \tag{85}$$

The thesis follows from combining (84) and (85) since H_{r_n} is by construction the maximal hexagon of $\overline{M}_n$.

Step 2. In this last step we remark that

$$\limsup_{n\to+\infty} K_n = K_t \limsup_{n\to+\infty} \sqrt{\lceil \sqrt{12n-3}\, \rceil - \sqrt{12n-3}} \le K_t,$$

and that for those $n_j \in \mathbb{N}$ of the form $n_j = 2 + 3j + 3j^2$ there holds

$$K_{n_j} \to \frac{2}{3^{1/4}} =: K_t \tag{86}$$

as $j \to +\infty$.

In fact, we have that

$$\begin{aligned} \sqrt{12n_j - 3} &= \sqrt{12(1 + 3j + 3j^2) + 9} \\ &= (6j+3)\sqrt{1 + \frac{12}{(6j+3)^2}} \\ &= 6j + 3 + \frac{12}{(6j+3)\left[1 + \sqrt{1 + \frac{12}{(6j+3)^2}}\,\right]}, \end{aligned}$$

which in turn yields

$$\lceil \sqrt{12n-3}\, \rceil - \sqrt{12n-3} = 1 - \frac{12}{(6j+3)\left[1 + \sqrt{1 + \frac{12}{(6j+3)^2}}\,\right]} \to 1$$

as $j \to +\infty$. □

It is remarkable that the leading terms in the estimates (68), (69), and (74) established in Step 1 of Theorem 1.2 are optimal for every $n \in \mathbb{N}$ as it follows from Step 1 of the proof of Theorem 1.3.

Finally, we notice that the bounded quantities K_n defined in (66) are 0 for every $n \in \mathbb{N}$ that can be written as $n = 1 + 3k + 3k^2$ for some $k \in \mathbb{N}$. This reflects the fact that for those n the daisy D_n is the unique minimizer, whose maximal hexagon $H_{r_{D_n}}$ is the daisy itself. Therefore, Theorem 1.3 also entails that, by adding a point to every EIP (2) with $n = 1 + 3i + 3i^2$ for some $i \in \mathbb{N}$, we pass not only from a problem characterized by uniqueness of solutions to a problem with nonuniqueness, but also from a situation of zero deviation of the minimizer from its maximal hexagon to the situation in which minimizers include one that attains the maximal deviation.

Acknowledgements

The authors were supported by CNR-ISPS grant *VarEvol* and by the Austrian Science Fund (FWF) project P 27052-N25. This work has been funded by the Vienna Science and Technology Fund (WWTF) through project MA14-009. Partial support by the Wolfgang Pauli Institute under the thematic project *Crystals, Polymers, Materials* is also acknowledged. E.D. and P.P. thank the Center for Nonlinear Analysis (NSF Grant No. DMS-0635983), where part of this research was carried out. E.D. was partially funded by the National Science Foundation (NSF) under Grant No. DMS- 0905778. and under the PIRE Grant No. OISE-0967140. E.D. is a member of the INDAM-GNAMPA Project 2015 *Critical phenomena in the mechanics of materials: a variational approach.*

References

[1] Y. Au Yeung, G. Friesecke, B. Schmidt. Minimizing atomic configurations of short range pair potentials in two dimensions: crystallization in the Wulff-shape, *Calc. Var. Partial Differential Equations*, **44** (2012), 81–100.

[2] S.L. Bezrukov. Edge isoperimetric problems on graphs, in: Graph theory and combinatorial biology (Balatonlelle, 1996). *Bolyai Soc. Math. Stud.*, **7** (1999), 157–197.

[3] X. Blanc, M. Lewin. The crystallization conjecture: a review, to appear on *EMS Surv. Math. Sci* (2015).

[4] E. Davoli, P. Piovano, U. Stefanelli. Wulff shape emergence in graphene, in preparation (2015).

[5] L.H. Harper, *Global methods for combinatorial isoperimetric problems.* Cambridge Studies in Advanced Mathematics, 90. Cambridge University Press, Cambridge, 2004.

[6] R. Heitmann, C. Radin. Ground states for sticky disks, *J. Stat. Phys.*, **22** (1980), 3:281–287.

[7] E. Mainini, U. Stefanelli. Crystallization in carbon nanostructures, *Comm. Math. Phys.*, **328** (2014), 2:545–571.

[8] E. Mainini, P. Piovano, U. Stefanelli. Finite crystallization in the square lattice. *Nonlinearity*, **27** (2014), 717–737.

[9] E. Mainini, P. Piovano, U. Stefanelli. Crystalline and isoperimetric square configurations, *Proc. Appl. Math. Mech.*, **14** (2014), 1045–1048.

[10] C. Radin. The ground state for soft disks, *J. Stat. Phys.*, **26** (1981), 2:365–373.

[11] B. Schmidt. Ground states of the 2D sticky disc model: fine properties and $N^{3/4}$ law for the deviation from the asymptotic Wulff-shape. *J. Stat. Phys.*, **153** (2013), 727–738.

[12] N.G. Trillos, D. Slepcev. Continuum Limit of Total Variation on Point Clouds. *Arch. Rational Mech. Anal.*, Digital Object Identifier (DOI) 10.1007/s00205-015-0929-z.

(Elisa Davoli) Faculty of Mathematics, University of Vienna, Oskar-Morgenstern-Platz 1, A-1090 Vienna, Austria

E-mail address: elisa.davoli@univie.ac.at

(Paolo Piovano) Faculty of Mathematics, University of Vienna, Oskar-Morgenstern-Platz 1, A-1090 Vienna, Austria

E-mail address: paolo.piovano@univie.ac.at

(Ulisse Stefanelli) Faculty of Mathematics, University of Vienna, Oskar-Morgenstern-Platz 1, A-1090 Vienna, Austria

E-mail address: ulisse.stefanelli@univie.ac.at