Crystalline and Isoperimetric Square Configurations

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We present crystallization results for planar atomic interactions governed by two- and three-body terms with the resulting periodicity being that of the square lattice. The emergence of a (square) Wulff shape for ground states is established by showing the optimality of ground-state configurations in terms of a discrete isoperimetric inequality. Furthermore, an $n^{3/4}$ law for the deviation from the asymptotic Wulff shape is established with an explicit constant for the leading term.

1 Introduction

In this paper the fundamental crystallization problem of analytically explaining why particles at low temperature arrange in periodic lattices is considered. We work in the classical framework and refer to the two-dimensional problem in the square lattice. At low temperatures particle interactions are expected to be essentially determined by particle positions. More precisely, if every particle configuration is identified with the set of its particle positions $x_1, \ldots, x_n$ in $\mathbb{R}^2$, the crystallization problem consists in verifying the periodicity of ground-state configurations of a suitable energy $E : \mathbb{R}^{2n} \to \mathbb{R} \cup \{+\infty\}$. The energy E is given by the sum of a two-body and a three-body interaction contribution, E_2 and E_3, respectively.

The literature on two-dimensional crystallization includes [2] as a first result for a two-body sticky interaction energy, inducing triangular lattice periodicity. The result was then extended in [5] to the case of short-ranged soft interactions. The first result accounting for long-range interactions has been instead achieved in [7] where an E_2 term of Lennard-Jones type has been considered. Analogous results are established in [1] for the hexagonal lattice by adding a three-body interaction term that favors triples of bonded particles forming bond angles $2\pi/3$ and $4\pi/3$. Furthermore, the emergence of a macroscopic Wulff shape for the triangular lattice with short-ranged two-body interactions has been recently investigated in [6, 8].

In this paper we summarize the results contained in [3]. We consider a short-range E_2 term and a E_3 term that favors bond angles of $\pi/2$, π, and $3\pi/2$, with a resulting square ordering (see detailed hypotheses on E in Section 2). Let $\beta(n) := \lfloor 2n - 2\sqrt{n} \rfloor$ where $\lfloor\cdot\rfloor$ is the right-continuous integer-part $\lfloor x \rfloor := \max\{z \in \mathbb{Z} : z \leq x\}$. Under the assumptions of Section 2 on the interaction energy, we prove the following main crystallization result.

Theorem 1.1 *Ground states of E are connected subsets of the unit square lattice and their energy is $-\beta(n)$.*

As the energy E favors particle clustering and 'boundary' particles have in general less bonds, ground states can be intuitively expected to have minimal 'perimeter', or maximal 'area'. This intuition is verified in Section 4 by introducing a suitable notion of perimeter and area of configurations, and by showing that ground states are characterized as those configurations which realize equality in a discrete isoperimetric inequality (see Theorem 4.1). Furthermore, the exact quantification of ground-state perimeter achieved in Theorem 4.1 allows us (still under the assumptions of Section 2) to show the emergence of an asymptotic (square) Wulff shape for ground states and to investigate the ground-state deviation from it. In the following, let us denote by $\mu_{\{y_1,\ldots,y_n\}}$ the empirical measure $\frac{1}{n}\sum_i \delta_{y_i/\sqrt{n}}$ of the rescaled configuration $\{y_1/\sqrt{n}, \ldots, y_n/\sqrt{n}\}$.

Theorem 1.2 *Ground states approach the square of side $\lfloor\sqrt{n}\rfloor$ as the particle number n grows. More precisely, if $\{C_n\}$ is a sequence of ground states and μ is the Lebesgue measure restricted to the unit square $[0,1]^2$, then $\{\mu_{C'_n}\}$ weak$*$-converge to μ where each C'_n is a suitable rotation and translation of C_n. Furthermore, every ground state (up to a rotation and a translation) differs from $S_n := \{(i,j) : i,j = 0,\ldots,\lfloor\sqrt{n}\rfloor\}$ by at most $3n^{3/4} + \mathrm{O}(n^{1/2})$ particles.*

We observe that Theorem 1.2 that is established in Section 4 provides an explicit constant for the leading-order term $n^{3/4}$ of the deviation of ground states from the Wulff shape (see also [6]). Moreover, it easily follows from this result (see in particular (14)) that

$$\|\mu_{C'_n} - \mu_{S_n}\| = \frac{\#(C'_n \triangle S_n)}{n} \leq 3n^{-1/4} + \mathrm{O}(n^{-1/2})$$

where $\|\cdot\|$ stands for the total variation norm. We also have that $\|\mu_{C'_n} - \mu\|_F \leq 3n^{-1/4} + \mathrm{O}(n^{-1/2})$ where $\|\cdot\|_F$ denotes the flat norm. These results nicely reflect the inherent multiscale nature of the crystallization phenomenon.

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2 Notation and Assumptions on the Interaction Energy

We denote a *configuration* of n particles by $C_n := \{x_1, \cdots, x_n\} \in \mathbb{R}^{2n}$, the distance between two of its particles, x_i and x_j, by ℓ_{ij}, and the counterclockwise-oriented angle between the two segments $x_i - x_j$ and $x_k - x_j$ by θ_{ijk}. The *energy* of a configuration C_n is defined by

$$E(C_n) := E_2(C_n) + E_3(C_n) = \frac{1}{2}\sum_{i\neq j} v_2(\ell_{ij}) + \frac{1}{2}\sum_{(i,j,k)\in\mathcal{A}} v_3(\theta_{ijk}) \tag{1}$$

where the functions $v_2 : [0,\infty) \to [-1,\infty]$ and $v_3 : [0, 2\pi] \to [0,\infty)$ are the two-body and the three-body interaction potentials. We choose a strongly-repulsive, short-ranged two-body potential satisfying the following assumptions

$$v_2(\ell) = +\infty \quad \text{if } \ell < 1, \quad v_2(\ell) = -1 \quad \text{if } \ell = 1, \quad v_2(\ell) = v(\ell) \quad \text{if } 1 < \ell < \ell^*, \quad v_2(\ell) = 0 \quad \text{if } \ell \geq \ell^*, \tag{2}$$

where v is any function taking values in $(-1, 0)$ and $\ell^* \in (1, \sqrt{2})$ is given. On the other hand, let $\sigma \in (0, \pi/8)$ and define

$$I_1 := \left[\frac{\pi}{2} - \sigma, \frac{\pi}{2} + \sigma\right], \quad I_2 := [\pi - \sigma, \pi + \sigma], \quad I_3 := \left[\frac{3\pi}{2} - \sigma, \frac{3\pi}{2} + \sigma\right], \quad I := I_1 \cup I_2 \cup I_3. \tag{3}$$

Let $\theta_{\min} := 2\arcsin(1/(2\sqrt{2})) \approx 0.23\,\pi$. The three-body potential v_3 vanishes only at $\pi/2$, π, and $3\pi/2$, it is symmetric with respect to π, convex in I_1, and satisfies the following non-degeneracy and symmetry conditions:

$$v_3(\theta) > 8 \quad \text{if } \theta \in (\theta_{\min}, 2\pi/5], \quad v_3(\theta) > 4 \quad \text{if } \theta \notin I, \quad v_3(\theta) = v_3(\theta + \pi/2) = v_3(\theta + \pi) \quad \text{if } \theta \in I_1, \tag{4a}$$

$$\text{and} \quad v'_{3,-}\left(\frac{\pi}{2}\right) := \lim_{t\nearrow 0} \frac{1}{t} v_3(t + \pi/2) < -\frac{2}{\pi}. \tag{4b}$$

We say that two particles x_i and x_j are *bonded* or that there is an (*active*) *bond* between x_i and x_j, if $1 \leq \ell_{ij} < \ell^*$, in this case $v_2(\ell_{ij})$ is negative. The set $\mathcal{A}$ in (1) is defined as the set of all triples (i, j, k) for which the angle θ_{ijk} separates two active bonds. The angle θ_{ijk} is said to be a (*active*) *bond angle* if $(i, j, k) \in \mathcal{A}$. We observe that the hard-interaction assumption $v_2 = \infty$ on $[0, 1)$ can be relaxed by asking v_2 to be very large in a right neighborhood of 0 (see [1, 3, 4]). The *bond graph* of a configuration C_n is the graph consisting of all its vertices and active bonds. We note that the simple cycles of a bond graph are polygons, and that, since $v_2(\ell)$ vanishes for $\ell \geq \sqrt{2}$, every bond graph is a planar graph. Moreover, from (2) it follows that the minimal angle between two active bonds is $\theta_{\min}$ for all finite-energy configurations.

We say that aconfiguration is *square* if it is a (rotated and translated) subset of the *square lattice* $\mathbb{Z}^2$ (notice that the energy is invariant under rotations and translations). Furthermore, a configuration is *connected* if every particle is connected to every other by a simple path in the bond graph, and it is *regular* if every particle in it has at most four bonds, every bond angle is in I, and every simple cycle of its bond graph has at least four edges. Straightforward comparison arguments (competitors being constructed by simply moving a single particle) show that grounds states are regular, and that $E(C_n) \geq -b(C_n)$ (with equality corresponding to square configurations C_n) where $b(C_n)$ denotes the number of bonds in the bond graph of C_n.

Moreover, a connected configuration with $n \geq 4$ particles is said to be *closed* if it has no acyclic bonds, i.e., every bond is an edge of a simple cycle. Given a closed configuration C_n, we identify its *boundary polygon* consisting of (at least four) vertices and containing all the other particles in its interior region, and we denote it by $\mathcal{B}(C_n)$. In addition, let $d(C_n)$ be the number of *boundary particles*, i.e. the particles of the boundary polygon, and C_n^{bulk} be the *bulk configuration* consisting of the remaining $n - d(C_n)$ *interior vertices*. The *bulk energy* of C_n is then defined by $E^{\text{bulk}}(C_n) := E(C_n^{\text{bulk}})$ and the *boundary energy* by $E^{\text{bnd}}(C_n) := E(C_n) - E^{\text{bulk}}(C_n) = E(C_n) - E(C_n^{\text{bulk}})$. The set of all bonds and the set of all bond angles which are deactivated in C_n by removing boundary particles are denoted, respectively, by $\Gamma(C_n)$ and by $\Theta(C_n)$. Since $v_2 \geq -1$, we obtain that the elementary inequality

$$E^{\text{bnd}}(C_n) \geq -\#\Gamma(C_n) + \sum_{\theta_i \in \Theta(C_n)} v_3(\theta_i), \tag{5}$$

which reduces to $E^{\text{bnd}}(C_n) = -\#\Gamma(C_n)$ in case of a square configuration C_n.

3 The Square Crystallization Result

In this section we establish Theorem 1.1. We begin by constructing a ground-state candidate with $n \in \mathbb{N}$ particles that we denote by D_n. If $n = m^2$ for some $m \in \mathbb{N}$, we let D_n be the $m \times m$ square in $\mathbb{Z}^2$, while if $n = m^2 + k$ for some $1 \leq k < 2m + 1$, we obtain D_n by progressively adding the k particles to D_{m^2} at specific sites of $\mathbb{Z}^2$. In fact, we add the first particle right above the upper left corner of the $m \times m$ square, and then, if necessary, we clockwisely add particles in such a way that each new particle is bonded to the previouse one and, whenever possible, to the original $m \times m$ square. Notice that

$b(D_n)$ may be computed by recursion: $b(D_1) = 0$, $b(D_{n+1}) - b(D_n) = 1$ if $n = m^2$ or $n = m^2 + m$ for some $m \in \mathbb{N}$, or $b(D_{n+1}) - b(D_n) = 2$ otherwise. It is not difficult to show that $\beta(n) := \lfloor 2n - 2\sqrt{n} \rfloor$ solves the recursion (see [3, Proposition 4.1]), so that indeed $E(D_n) = -\beta(n)$.

We now observe that $\#\Gamma(C_n)$ can be estimated in terms of $d(C_n)$ for a regular and closed configuration C_n. Let us denote by φ_i, for $i = 1, \cdots, \varepsilon d$, the internal angles of $\mathcal{B}(C_n)$ that are in I_1, by ψ_i, $i = 1, \cdots, \eta d$, the ones in I_2 and by ξ_i, $i = 1, \cdots, \nu d$, the ones in I_3. Here, ε, η, and ν are the ratios of the internal angles of $\mathcal{B}(C_n)$ that belong to I_1, I_2, and I_3 respectively. Since $\sigma < \pi/8$ in (3), given a boundary vertex x and the corresponding internal angle θ of $\mathcal{B}(C_n)$, we infer that if θ is in I_1, then x needs to be two-bonded, because otherwise there would be a bond angle at x smaller than $5\pi/16$ and so not in I. By a similar argument, if $\theta \in I_2$, then x is at most three-bonded, and if θ is in I_3, then x has at most four bonds. It follows that

$$\#\Gamma(C_n) \leq (1 + \eta + 2\nu)\, d(C_n) = (\varepsilon + 2\eta + 3\nu)\, d(C_n). \tag{6}$$

Proof of Theorem 1.1. *Step 1 (boundary energy estimate).* We here establish that $E^{\mathrm{bnd}}(C_n) \geq -2d(C_n) + 4$ holds for a regular and closed configuration C_n, and that the inequality is strict in case of a nonsquare configuration C_n with a square C_n^{bulk}. For simplicity we often omit the dependence on C_n in the formulas.

Since the sum of the internal angles of a polygon with d sides is $\pi(d-2)$, we first observe that

$$\varepsilon d\varphi + \eta d\psi + \nu d\xi = \pi(d-2), \quad \text{where} \quad \varphi := \frac{1}{\varepsilon d}\sum_{i=1}^{\varepsilon d}\varphi_i, \quad \psi := \frac{1}{\eta d}\sum_{i=1}^{\eta d}\psi_i, \quad \xi := \frac{1}{\nu d}\sum_{i=1}^{\nu d}\xi_i. \tag{7}$$

By (4a) and the convexity of v_3 in I_1 we have $v_3(\psi_i) \geq 2v_3(\psi_i/2)$ for $i = 1, \cdots, \eta d$ and $v_3(\xi_i) \geq 3v_3(\xi_i/3)$ for $i = 1, \cdots, \nu d$. Still the convexity of v_3 in I, together with (5), (14) and (7), entails

$$E^{\mathrm{bnd}} \geq -\varepsilon d - 2\eta d - 3\nu d + \sum_{i=1}^{\varepsilon d} v_3(\varphi_i) + 2\sum_{i=1}^{\eta d} v_3\left(\frac{\psi_i}{2}\right) + 3\sum_{i=1}^{\nu d} v_3\left(\frac{\xi_i}{3}\right) \geq -\delta d + \delta d v_3(\alpha(\delta)), \tag{8}$$

where $\delta := \varepsilon + 2\eta + 3\nu$ and $\alpha(\delta) := \pi(d-2)/(\delta d)$. By looking at (8), we immediately have that $E^{\mathrm{bnd}}(C_n) \geq -2d(C_n) + 4$ if $\delta \leq \delta^* := 2 - 4/d$, otherwise, the same follows from the crucial hypothesis (4b) since (4b) implies

$$v_3(\alpha(\delta)) \geq v_3\left(\frac{\pi}{2}\right) + v'_{3,-}\left(\frac{\pi}{2}\right)\left(\alpha(\delta) - \frac{\pi}{2}\right) > -\frac{2}{\pi}\left(\alpha(\delta) - \frac{\pi}{2}\right) = \frac{\delta d - 2d + 4}{\delta d}. \tag{9}$$

We now verify that if a bond in Γ has not length 1 or a bond angle of Θ is not in $\{\pi/2, \pi, 3\pi/2\}$, then $E^{\mathrm{bnd}} > -2d + 4$. Notice that (8) has to hold with equality in order to have $E^{\mathrm{bnd}} = -2d + 4$. However, recalling (5), (8) is strict if the length of a bond in Γ is not 1 or if an angle in Θ which is adjacent to an interior vertex differs from $\pi/2$, π, or $3\pi/2$. Otherwise, equality in (8) implies that $\sum_{\theta_i \in \Theta} v_3(\theta_i) = \delta d v_3(\alpha(\delta))$, but this relation, taking the strict inequality in (9) into account, readily entails $\delta = \delta^*$, thus $\alpha(\delta) = \pi/2$, and this shows that all the other angles of Θ are in $\{\pi/2, \pi, 3\pi/2\}$ as well.

Step 2 (induction on bond graph layers). In this step we follow the classical induction argument introduced by Radin in [5] that has been recently revisited in [3, 4]. We refer the reader to [3, 4] for more details. We begin by observing that the statement of the Theorem is trivial for $n \leq 4$, and we then proceed by induction. We prove that if the assertion holds for a ground state C_m with $m < n$, then it holds also for C_n. By contradiction we suppose that C_n is not square and we observe that a contradiction may be easily reached for a configuration C_n that it is not closed by considering subconfigurations and by using elementary properties of the function $\beta(n)$ (see [3]). Instead, for a closed configuration C_n that is not square, we argue as follows. Either C_n^{bulk} is not square itself and hence, by induction we have that $E^{\mathrm{bulk}} > -\beta(n-d)$, or C_n^{bulk} is square and so from *Step 1* it follows that $E^{\mathrm{bnd}} > -2d + 4$. Therefore, by *Step 1*, in both cases we obtain that

$$E = E^{\mathrm{bulk}} + E^{\mathrm{bnd}} > -\lfloor 2(n-d) - 2\sqrt{n-d}\, \rfloor - 2d + 4\,. \tag{10}$$

Finally, by combining (10) with the Euler formula for planar graphs we have that $E > -\beta(n)$ holds (see [3]), and this contradicts the fact that C_n is a ground state. □

4 Isoperimetric Inequality and Convergence to the Wulff Shape

Let us define the area A and the perimeter P of a regular configuration C_n by $A(C_n) := \mathcal{L}^2(F(C_n))$ and $P(C_n) := \mathcal{H}^1(\partial F(C_n)) + 2\mathcal{H}^1(G(C_n))$, respectively, where $F(C_n) \subset \mathbb{R}^2$ is the closure of the union of the regions enclosed by the simple cycles of C_n that consists of only 4 bonds, $G(C_n) \subset \mathbb{R}^2$ is the union of all bonds which are not included in $F(C_n)$, and $\mathcal{H}^1$ denotes the one-dimensional Hausdorff measure. For square configurations, we easily see that $E(C_n) = -2A(C_n) - \frac{1}{2}P(C_n)$.

We characterize ground states as solutions of a discrete isoperimetric problem. In the following, $\lceil x \rceil := \min\{z \in \mathbb{Z} : x \leq z\}$.

Theorem 4.1 *Every connected square configuration C_n with $n > 1$ satisfies*

$$\sqrt{A(C_n)} \leq k_n P(C_n) \qquad \text{where} \qquad k_n := \frac{\sqrt{n - \lceil 2\sqrt{n}-1 \rceil}}{2\lceil 2\sqrt{n}-1\rceil - 2}\,. \tag{11}$$

Moreover, ground states correspond to those configurations for which (11) *holds with the equality, and, equivalently, to those configurations that attain the maximum area, i.e.* $n - \lceil 2\sqrt{n} - 1\rceil$*, and the minimum perimeter, i.e.* $2\lceil 2\sqrt{n} - 1\rceil - 2$.

Proof. *Step 1.* We begin by establishing that (11) holds for a particular class of configurations called *quasirectangles* and denoted by $R_n^{r,c,e}$ where the triplet (r, c, e) is assumed to be in $\mathcal{T}_n := \{(r, c, e) \in \mathbb{N}^3 \mid r \leq c,\ 1 \leq e \leq c,\ rc + e = n\}$. A quasirectangle $R_n^{r,c,e}$ is a square configuration obtained by adding a connected line of e extra particles to the $(r \times c)$-rectangle (consisting of r aligned rows each with c particles) in such a way that each extra particle is bonded to one and only one particle of the rectangle. Let us define k_n by

$$k_n := \max_{(r,c,e)\in\mathcal{T}_n} \frac{\sqrt{A\left(R_n^{r,c,e}\right)}}{P\left(R_n^{r,c,e}\right)} = \max\left\{ \frac{\sqrt{n-(r+c)}}{2(r+c)-2} \;\middle|\; r, c \in \mathbb{N} \text{ and } n - \max\{r, c\} \leq rc < n \right\} \tag{12}$$

where the second equality follows from the fact that $A(R_n^{r,c,e}) = (r-1)(c-1)+e-1 = n-(r+c)$ and $P(R_n^{r,c,e}) = 2(r+c)-2$. Thus, k_n is realized at the minimum admissible value of $r+c$ that can be analytically computed to be equal to $\ell_n := \lceil 2\sqrt{n}-1\rceil$. Observe that the configuration D_n introduced in Section 3 is a quasirectangle that realized the maximum in (12) since the sum of its rows and columns is exactly ℓ_n. Therefore, we have that $\sqrt{A(D_n)} = k_n P(D_n)$, and from the same reasoning it follows also that the maximum area and the minimum perimeter among quasirectangles are realized by $A(D_n) = n - \ell_n$ and $P(D_n) = 2\ell_n - 2$, respectively. Inequality (11) is now a direct consequence of the fact that we can always rearrange the particles of a connected square configuration C_n in a quasirectangle without increasing its perimeter and decreasing its area, see [3, Lemma 7.3]. Therefore, it follows also that $A(D_n)$ maximizes the area and $P(D_n)$ minimizes the perimeter among all connected square configurations.

Step 2. We now prove the second statement. Every connected square configuration C_n that satisfies $\sqrt{A(C_n)} = k_n P(C_n)$ is a ground state since by the elementary relation $E(C_n) = -2A(C_n) - \frac{1}{2}P(C_n)$ we have that

$$E(D_n) \leq E(C_n) = -2A(C_n) - \frac{P(C_n)}{2} = -2k_n^2 P^2(C_n) - \frac{P(C_n)}{2} \leq -2k_n^2 P^2(D_n) - \frac{P(D_n)}{2} = E(D_n),$$

where we used the fact that D_n is a ground state that minimizes the perimeter as established in *Step 1*.

Moreover, from an analogous argument it follows that $P(G_n) = P(D_n)$ and that $A(G_n) = A(D_n)$ for every ground state G_n. Since we have seen in *Step 1* that $\sqrt{A(D_n)} = k_n P(D_n)$, the proof is concluded. □

Proof of Theorem 1.2. Let C_n be a ground state and $R(C_n)$ be the minimal $(\ell_1 - 1) \times (\ell_2 - 1)$-rectangle (with $\ell_1 \geq \ell_2$ and sides parallel to the two directions of its unit square lattice of reference, say $\mathcal{L}$) that contains C_n. Since every ground state C_n is connected in the directions of the square lattice, by Theorem 4.1 we obtain that $\ell_1 + \ell_2 = \frac{1}{2}P(C_n) + 2 = 2\lceil\sqrt{n}-1\rceil + 1 = \ell_n + 1$. By solving the maximum problem $\ell_1 - \ell_2 := \max\{a - b \ :\ a, b \in \mathbb{N},\ ab \geq n,\ a + b = \ell_n + 1\}$ we observe that

$$\ell_1 - \ell_2 = 2\left\lfloor \frac{\lceil 2\sqrt{n}\rceil + \sqrt{(\lceil 2\sqrt{n}\rceil)^2 - 4n}}{2} \right\rfloor - \lceil 2\sqrt{n}-1\rceil - 1 \leq 2\left\lfloor \frac{\sqrt{(\lceil 2\sqrt{n}\rceil)^2-4n}}{2}\right\rfloor \leq 2n^{1/4} + 1. \tag{13}$$

and hence, we have $\sqrt{n} \leq \ell_1 \leq \sqrt{n}+n^{1/4}+1$ and $\sqrt{n}-n^{1/4}-1 \leq \ell_2 \leq \sqrt{n}$. Therefore, we obtain that $d(R'_n, S_n) \leq n^{1/4}+2$ where d denotes the Hausdorff distance and R'_n is a suitable rotation and translation of $R_n := \overline{R(C_n)} \cap \mathcal{L}$. Let us now define C'_n as the analogous rotation and translation of C_n. Since we have that

$$\begin{aligned} \#(C'_n \triangle S_n) &\leq \#(R'_n \setminus S_n) + \#(S_n \setminus R'_n) + \#((R'_n \cap S_n) \setminus C'_n) \\ &\leq 2\#(R'_n \setminus S_n) + \#(S_n \setminus R'_n) \leq (2\ell_2 + \lfloor\sqrt{n}\rfloor + 1)d(R'_n, S_n) \leq (3\sqrt{n} + 1)(n^{1/4} + 2), \end{aligned} \tag{14}$$

the assertion follows. □

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