A proof of crystallization in two dimensions

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Abstract

Many materials have a crystalline phase at low temperatures. The simplest example where this fundamental phenomenon can be studied are pair interaction energies of the type $E(\{y\}) = \sum_{1 \le x < x' \le N} V(|y(x) - y(x')|)$ where $y(x) \in \mathbb{R}^2$ is the position of particle x and $V(r) \in \mathbb{R}$ is the pair-interaction energy of two particles which are placed at distance r. Due to the Mermin-Wagner theorem it can't be expected that at finite temperature this system exhibits long-range ordering. We focus on the zero temperature case and show rigorously that under suitable assumptions on the potential V which are compatible with the growth behavior of the Lennard-Jones potential the ground state energy per particle converges to an explicit constant E_*:

$$\lim_{N\to\infty} \frac{1}{N} \min_{y:\{1\ldots N\}\to\mathbb{R}^2} E(\{y\}) = E_*,$$

where $E_* \in \mathbb{R}$ is the minimum of a simple function on $[0, \infty)$. Furthermore, if suitable Dirichlet- or periodic boundary conditions are used, then the minimizers form a triangular lattice. To the best knowledge of the author this is the first result in the literature where periodicity of ground states is established for a physically relevant model which is invariant under the Euclidean symmetry group consisting of rotations and translations.

1. Introduction

The purpose of this paper is to provide a mathematically rigorous analysis for the asymptotic behavior of the ground state energy (minimum energy) of many-particle systems where the interaction is governed by pair-potentials:

$$E(\{y\}) := \frac{1}{2} \sum_{\substack{x,x' \in X_N \\ x \neq x}} V(|y(x) - y(x')|).$$

Here, the finite set X_N indexes the individual particles, $\#X_N = N \in \mathbb{N}$ is the number of particles and $y(x) \in \mathbb{R}^d$ specifies the position of particle x. We will focus on the thermodynamic limit where N tends to infinity. One of the most interesting cases is when V is given by the Lennard-Jones potential $V_{\rm LJ}(r) = r^{-12} - r^{-6}$. Extensive numerical studies in the case $d = 2$ (see [1] and the references therein) suggest that the ground states (energy minimizers) approximate a translated, rotated and dilated copy of the triangular lattice

$$A_2 = \frac{1}{2} \begin{pmatrix} 2 & 1 \\ 0 & \sqrt{3} \end{pmatrix} \mathbb{Z}^2 \subset \mathbb{R}^2$$

and the ground state energy divided by N converges to a constant as $N \to \infty$. In the case $d = 1$ it is know that this is true for rather general (both discrete and continuous) systems, see [2, 3, 5] and the references therein.

The first aim of this paper is to establish sufficient conditions on the potential V such that for $d = 2$ the ground state energy per particle converges to a value that can be found by minimizing over periodic particle configurations; those potentials will be referred to as

$2d$-crystalline. Radin proved in [6] that the class of $2d$-crystalline potentials is not empty by characterizing the set of ground states for a special piecewise-affine potential V_{Radin} which assumes finite and nonzero values in $[1, \frac{25}{24})$ and has its absolute minimum at 1.

We will address the question whether Radin's result persists if the system is generic, i.e. non-integrable in the sense that for finite numbers N the ground states are not translated, rotated and dilated subsets of $\mathcal{A}$ because of the presence of boundary layers or a small number of lattice defects.

It is expected that a more analytical understanding of the underlying mathematical structures will also indicate how to attack the three-dimensional case which cannot be treated with Radin's method since there are several non-equivalent lattices which are natural candidates for the ground state: fcc (face-centered cubic), bcc (body-centered cubic) and hcp (hexagonally close packed) to name only the most classical multi-lattices. The selection of the correct lattice is necessarily based on the contributions of second-nearest neighbor interactions, but the methods developed so far are not capable of dealing with short-range and long-range interactions simultaneously.

We present a new method, based on recently discovered rigidity estimates that covers a natural class of potentials which also allows for power-law behavior at infinity and 0. For the sake of notational simplicity we will assume wlog that the interaction potential is normalized in the sense that $\lim_{r\to\infty} V(r) = 0$ and

$$\min_{r\geq 0} \sum_{\xi\in A_2\setminus\{0\}} V(r|\xi|) = \sum_{\xi\in A_2\setminus\{0\}} V(|\xi|) = -6. \tag{1}$$

Theorem 1.1 (Ground state energy). *There exists a constant $\alpha_0 \in (0, \frac{1}{3})$ such that for each $\alpha \in (0, \alpha_0)$ and every normalized potential $V : [0,\infty) \to [0,\infty]$ which has the properties $V \in C^2(1-\alpha,\infty)$ and*

$$V(r) \geq \frac{1}{\alpha} \text{ for } r \in [0, 1-\alpha], \tag{2}$$

$$V''(r) \geq 1 \text{ for } r \in (1-\alpha, 1+\alpha), \tag{3}$$

$$V(r) \geq -\alpha \text{ for } r \in \left[1+\alpha, \tfrac{4}{3}\right], \tag{4}$$

$$|V''(r)| \leq \alpha r^{-7} \text{ for } r \in \left(\tfrac{4}{3}, \infty\right) \tag{5}$$

the identity

$$\lim_{N\to\infty} \min_{y:X_N\to\mathbb{R}^2} \frac{1}{N} \sum_{\{x,x'\}\subset X_N} V(|y(x)-y(x')|) = -3$$

holds.

Note that the assumptions on V allow both for hard-core interactions ($V(r) = +\infty$ if $r \in [0, \rho_0]$ for some $\rho_0 \in [0, 1-\alpha]$) and soft-core interactions ($V(r) < \infty$ for all $r \in [0,\infty)$). The second aim of this paper is to characterize the actual ground states. This is a delicate problem due to the possible formation of surface layers. Rigorous results can be obtained in simplified situations where suitable boundary conditions are used. In two cases we obtain that the ground states are translated copies of the triangular Bravais lattice A_2. By abuse of notation we identify for $L \in \mathbb{N}$ the quotient space $A_2 \mod LA_2$ with the representatives $A_2 \cap LU$ where $U = \frac{1}{2}\begin{pmatrix} 2 & \sqrt{3} \\ 0 & 1 \end{pmatrix} Q$, and $Q = [0,1) \times [0,1) \subset \mathbb{R}^2$ is the semi-open unit cell.

Theorem 1.2 (Ground states with periodic boundary conditions). *There exists a constant $\alpha_0 \in (0, \frac{1}{3})$ such that for every pair of numbers $\alpha \in (0,\alpha_0)$, $L \in \mathbb{N}$, every potential $V(\cdot)$*

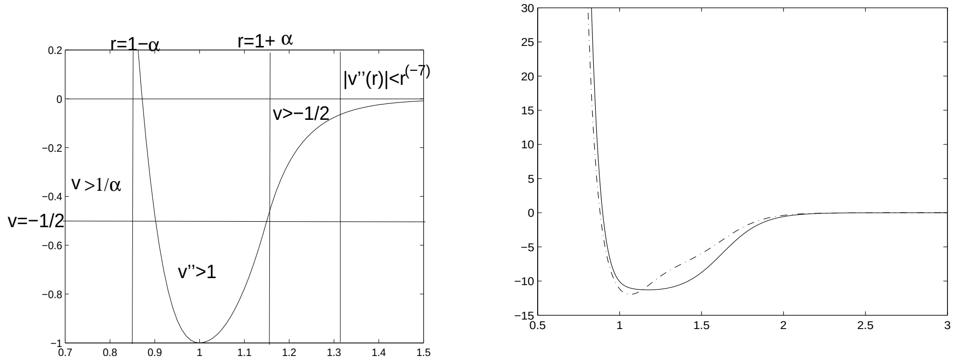


FIGURE 1. Plot of the potential $V(r) = r^{-12} + \tanh(4r - \frac{13}{2}) - 1$ (left) and the associated energies per particle (right) $f(\cdot, \mathbb{Z}^2)$ (dotted line) and $f(\cdot, A_2)$ (solid line).

which satisfies the assumptions of Theorem 1.1 and every ground state $y_{\min} : A_2 \to \mathbb{R}^2$ *of*

$$E_L^{\mathrm{per}}(\{y\}) := \sum_{\substack{x\in A_2\cap L\,U\\ x'\in A_2\setminus\{x\}}} V(|y(x) - y(x')|),$$

subject to

$$y \in Y_L^{\mathrm{per}} := \{y : A_2 \to \mathbb{R}^2 \mid y(x) - y(x') = x - x' \text{ if } x - x' \in LA_2\},$$

there exists a translation vector $\tau \in \mathbb{R}^2$ *such that*

$$\{y_{\min}(x) + \tau \mid x \in A_2\} = A_2.$$

Corollary 1.3 (Stability against compactly supported perturbations)**.** *Let the assumptions of Theorem 1.2 be satisfied and assume that* $\mathcal{A} \subset A_2$ *is an arbitrary but finite set. If the configuration* $y_{\min} : A_2 \to \mathbb{R}^2$ *is a ground state of*

$$E_{\mathcal{A}}(\{y\}) := \sum_{\substack{\{x,x'\}\subset A_2\\ \{x,x'\}\cap\mathcal{A}\neq\emptyset}} V(|y(x) - y(x')|)$$

subject to the constraint

$$y \in Y_{\mathcal{A}}^{\mathrm{Dir}} = \{y : A_2 \to \mathbb{R}^2 \mid y(x) = x \text{ for all } x \in A_2 \setminus \mathcal{A}\},$$

then

$$\{y_{\min}(x) \mid x \in A_2\} = A_2.$$

The normalization (1) does not affect the scope of the results as for general interaction potentials it can be shown without trouble that if the function $V_*(r) = \frac{1}{6}\sum_{\xi\in A_2} V(r|\xi|)$ does not admit a minimizer then the ground state can not be approximated by rotated, dilated and translated copies of subsets of A_2. On the other hand if $r_* \in (0,\infty)$ minimizes V_* and $V_*(r_*) \neq 0$ then we can simply replace $V(r)$ by the rescaled potential $\frac{-1}{V_*(r_*)}V(\frac{r}{r_*})$.

Even in two dimensions for "natural" interaction potentials V the ground states might not converge to a triangular lattice as $N \to \infty$. For example, if $V(r) = r^{-12} + \tanh(4r - \frac{13}{2}) - 1$, then the triangular lattice A_2 leads to a higher energy per particle than the square lattice $\mathbb{Z}^2$, in particular the ground states will not resemble a triangular lattice. This follows from the simple observation that $\min_r f(r, \mathbb{Z}^2) < \min_r f(r, A_2)$ where $f(r, \mathcal{L}) = \sum_{\xi\in\mathcal{L}\setminus\{0\}} V(r|\xi|)$, cf. figure 1.

Notation. The energy per nearest neighbor bond in a homogeneously deformed triangular lattice A_2 is given by the *renormalized potential*

$$V_*(r) := \frac{1}{6} \sum_{\xi \in A_2 \setminus \{0\}} V(r|\xi|).$$

It coincides up to a multiplicative constant with the function $f(r, A_2)$ defined above We will use the shorthand $e(\{x,x'\})$ for $V(|y(x') - y(x')|)$ and $e_*(\{x,x'\})$ for $V_*(|y(x) - y(x')|)$. The letter "C" denotes a generic positive constant which does not depend on α or $\#X_N = N$ as long as $\alpha \in [0, \frac{1}{3}]$. The actual value of C may change from line to line. $B(\eta, r)$ denotes the closed ball centered at $\eta \in \mathbb{R}^2$ with radius r. Subsets of X_N are mostly denoted by calligraphic letters. Throughout the proof we assume that $y_N : X_N \to \mathbb{R}^2$ is a ground state of E and depends on N, i.e. it globally minimizes the energy in the given class of admissible configurations. The main focus of the analysis is to characterize the properties of the state y_N for fixed N, the asymptotic behavior as $N \to \infty$ is only discussed towards the end. For this reason the subscript N is omitted in most cases. Note that the minimization property of y_N is used only in two places: Lemma 2.2 and at the end of the proofs of Theorem 1.2 and Corollary 1.3. The other arguments are only based on the bound (13).

By $\{x, x'\} \subset X_N$ we mean sets with precisely 2 elements.

As the main objective of this paper is to explain the method, which hasn't been used before, we do not make any effort to optimize the constants.

2. Proof of Theorem 1.1

2.1. **Outline.** It is easy to see that

$$\lim_{N\to\infty} \min_{y : X_N \to \mathbb{R}^2} \frac{1}{N} \sum_{\{x,x'\} \subset X_N} e(\{x,x'\}) \leq -3$$

by choosing the trial configuration $y(x) = \Phi(x)$ where $\Phi : \mathbb{N} \to A_2$ is a reasonable bijection which does not create too much surface energy.

To show the much harder direction

$$\lim_{N\to\infty} \min_{y : X_N \to \mathbb{R}^2} \frac{1}{N} \sum_{\{x,x'\} \subset X_N} e(\{x,x'\}) \geq -3 \tag{6}$$

we split the set of all pairs $\mathcal{P} := \{p \subset X \mid \#p = 2\}$ into two parts: short-range and long-range $\mathcal{P} = \mathcal{S}(y_N) \dot{\cup} \mathcal{L}(y_N)$ where

$$\mathcal{S}(y_N) := \{\{x,x'\} \in \mathcal{P} \mid ||y_N(x) - y_N(x')| - 1| \leq \alpha\}$$

is the index set for the short-range interactions and $\mathcal{L}(y_N) := \mathcal{P} \setminus \mathcal{S}(y_N)$ contains the long-range interactions. By construction this splitting is induced by the actual ground state y_N.

For each $x \in X$ we define the discrete neighborhood

$$\mathcal{N}(x) := \{x' \in X \mid \{x,x'\} \in \mathcal{S}(y_N)\} \cup \{x\},$$

again this set depends on y_N although the dependency is not shown. The defects $\partial X(y_N) := \{x \in X_N \mid \#\mathcal{N}(x) \neq 7\}$ are those particles whose neighborhood cannot be mapped bijectively onto $A_2 \cap B(0,1)$.

Based on simple, combinatorial considerations we will later (Proposition 2.3) establish the estimate

$$\#\mathcal{S}(y_N) \leq 3N - \tfrac{1}{2}\#\partial X(y_N) \tag{7}$$

which shows that the set of short-range interactions grows like N, not N^2. The splitting $\mathcal{P} = \mathcal{S}(y_N)\dot{\cup}\mathcal{L}(y_N)$ is adequate if we can show that the following inequality holds

$$\sum_{p\in\mathcal{P}} e(p) \geq \sum_{p\in\mathcal{S}(y_N)} e_*(p). \tag{8}$$

The claim (6) follows immediately from (7) together with (8). Inequality (8) links the energy of an arbitrary configuration to the renormalized potential V_* which provides the energy per bond of a homogeneously dilated triangular lattice. The crucial point is that the left-hand side of (8) is a complicated sum with $\frac{1}{2}N(N-1)$ terms whereas the right-hand side contains at most $3N$ terms.

We will actually prove a slightly more complicated version of (8), namely

$$\sum_{p\in\mathcal{P}} e(p) \geq -\#\mathcal{S}(y_N) + \frac{1}{C}\sum_{\{x,x\}\in\mathcal{S}(y_N)} \left(|y_N(x) - y_N(x')| - 1\right)^2 + \tfrac{1}{4}\#\partial X(y_N), \tag{9}$$

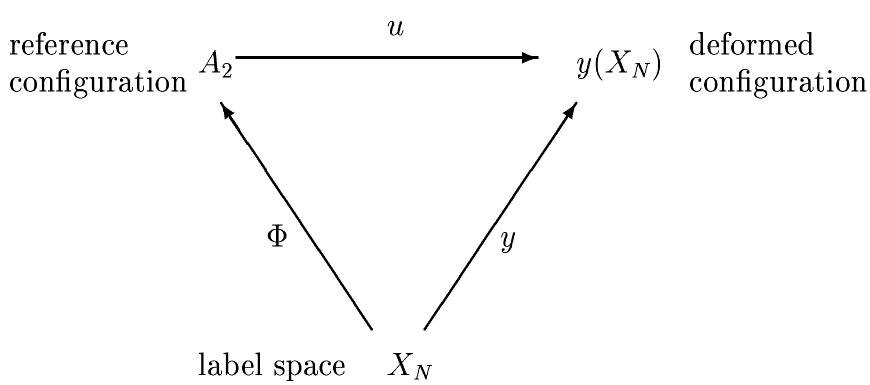
where $C > 0$ is independent of V, α and N. In order to establish the validity of (9) we will demonstrate that away from the defect set $\partial X(y_N)$ there are big patches which can be identified with simply connected subsets of A_2. The statement of the theorem follows since the definition of V_*, (7) and (9) imply (6).

The estimates quantify the errors caused by neglecting two different types of energy contributions:

I) omitted individual bonds and
II) distortion of the bonds.

Errors of type I will be absorbed into the term which is proportional to $\#\partial X(y_N)$ in the right hand side of (9). Errors of type II require a more subtle handling. Using the geometric rigidity bounds from Proposition 4.1 they will be absorbed into the sum over $\mathcal{S}(y_N)$ in the right hand side of (9).

This approach requires us to work with three different spaces and three different maps between these spaces.



2.2. **Combinatorial considerations.** We collect several estimates of the interaction potential V and the renormalized potential V_* which are required later.

Lemma 2.1. *There exists $\alpha_0 > 0$ such that for all $\alpha \in (0, \alpha_0)$ and all V satisfying (1)-(5)*

$$\min_{r\in[1-\alpha,1+\alpha]} V_*''(r) \geq \frac{1}{2}, \tag{10}$$

$$V(r) \geq -2 \text{ for all } r \geq 0, \tag{11}$$

$$|V(r)| \leq \alpha r^{-5} \text{ for all } r \geq \tfrac{4}{3} \tag{12}$$

holds.

Proof. The claim follows directly from assumptions (3), (5) and the definition of V_*. □

The growth and decay estimates for the potential V result in a lower bound for the distance between particles in the ground state.

Lemma 2.2 (Minimum distance). *There exists a number $\alpha_0 \in (0, \frac{1}{3})$ such that for each $\alpha \in (0, \alpha_0)$ and each V satisfying (1)- (5) all ground states $y_N : X_N \to \mathbb{R}^2$ of $E(\cdot)$ satisfy the estimate*

$$\min_{x\neq x'} |y(x) - y(x')| > 1 - \alpha, \tag{13}$$

i.e. the minimum distance between the particle positions is at least $1 - \alpha$.

Proof. Define $M := \max_{\eta\in\mathbb{R}^2} \#(y(X) \cap B(\eta, \frac{1}{2}(1-\alpha)))$. The result is proven if we can show that $M = 1$. We can assume wlog that the maximum is achieved for $\eta = 0$. Set $B_M = B(0, \frac{1}{2}(1-\alpha))$ and $\mathcal{A} = y^{-1}(B_M)$. By assumption (2) we have $\sum_{p\subset\mathcal{A},\, p\in\mathcal{P}} e(p) \geq \frac{1}{2\alpha}M(M-1)$. As we could move the positions $y(\mathcal{A})$ to infinity in such a way that the mutual distances diverge, we obtain the estimate

$$\sum_{\substack{x\in\mathcal{A}\\ x'\in X\setminus\mathcal{A}}} e(\{x,x'\}) \leq -\tfrac{1}{2\alpha}M(M-1). \tag{14}$$

Let now $n(k) := \#y^{-1}((k+1)B_M \setminus kB_M)$. As $\alpha \in [0, \frac{1}{3}]$ the decay estimate (12) provides for each $k \geq 9$ the following lower bound on the interaction energy between the particles indexed by $\mathcal{A}$ and those particles whose positions are contained in $(k+1)B_M \setminus kB_M$:

$$\sum_{\substack{x\in\mathcal{A}\\ y(x')\in(k+1)B_M\setminus kB_M}} e(\{x,x'\}) \geq -n(k)M\alpha((1-\alpha)\tfrac{k-1}{2})^{-5}. \tag{15}$$

Similarly, for $k \in \{2, \ldots, 8\}$ the lower bound (11) yields the estimate

$$\sum_{\substack{x\in\mathcal{A}\\ y(x')\in(k+1)B_M\setminus kB_M}} e(\{x,x'\}) \geq -2n(k)M. \tag{16}$$

There exists a universal constant $C > 0$ such that the ring with outer radius r and thickness $\min\{\frac{1}{2}, r\}$ can be covered with Cr translated copies of $B(0, \frac{1}{3})$, this implies that $n(k) \leq CMk$. It follows from (14) together with estimates (15) and (16) that

$$-CM^2\left(\sum_{k=2}^{8} 2k + \alpha\sum_{k=9}^{\infty}((1-\alpha)\tfrac{k-1}{2})^{-5}\right) \leq -\tfrac{1}{2\alpha}M(M-1). \tag{17}$$

As both sums can be bounded by a constant which does not depend on α as long as $\alpha \in [0, \frac{1}{3}]$, C does not depend on α or M, and M is a positive integer, inequality (17) can only hold with sufficiently small α if $M = 1$. This proves the claim. □

Proposition 2.3. *There exists $\alpha_0 > 0$ such that for all $\alpha \in (0, \alpha_0)$ and all configurations $y : X \to \mathbb{R}^2$ which satisfy (13) estimate (7) holds. Furthermore,*

$$\#\mathcal{N}(x) \leq 7 \text{ for all } x \in X. \tag{18}$$

Proof. The proof that (13) implies (18) follows from elementary geometric considerations. We only show that (18) implies (7). Let $n(x) = \#\mathcal{N}(x) - 1$ be the number of neighboring pairs which contain x, then

$$\begin{aligned}\#\mathcal{S} =& \frac{1}{2}\sum_{x\in X} n(x) = \frac{1}{2}\sum_{x\in X\setminus\partial X} n(x) + \frac{1}{2}\sum_{x\in\partial X} n(x) \overset{(18)}{\leq} 3(\#X - \#\partial X) + \tfrac{5}{2}\#\partial X \\ =& 3\#X - \tfrac{1}{2}\#\partial X,\end{aligned}$$

which proves (7). □

2.3. **Reference configurations and equilateral simplices.** The proof is organized around the concept of "equilateral simplices". An equilateral simplex T is a subset of X with three elements such that there exists a neighborhood $\omega_T \supset T$ and a "continuous" imbedding $\Phi_T : \omega_T \to A_2$ such that $\Phi_T(T) \subset A_2$ is an equilateral simplex with side length λ in the usual sense, cf. Definition 2.6. The ratio of the actual bond lengths $|y(x) - y(x')|$ for $\{x, x'\} \subset T$ and the reference lengths λ is used to account for changes of length and volume. This idea allows us to realize the central step in the proof where the energy contribution of long-range interactions is approximated by renormalized short range interaction energies up to an error which can be controlled. More precisely, instead of summing the individual pair interaction energies in an uncontrolled way we add the energies of equilateral simplices. The interaction energy of each equilateral simplex can be approximated by its volume. Using the additivity of the volume form we can construct an approximation of the interaction energy of equilateral simplices with side length λ by modifying the interaction energy of the simplices with side length 1.

Definition 2.4 (Discrete imbeddings)**.** *Let $y : X \to \mathbb{R}^2$ satisfy (13), $\omega \subset X \setminus \partial X(y)$ and $\Phi : \omega \to A_2$ be a discrete map. Φ is called y-continuous if*

$$|\Phi(x) - \Phi(x')| \leq 1 \text{ for all } \{x, x'\} \in \mathcal{S}(y) \text{ such that } \{x, x'\} \subset \omega. \tag{19}$$

A discrete y-continuous map Φ is called orientation preserving with respect to the configuration y if

$$\det(y(x_2) - y(x_1), y(x_3) - y(x_1)) \cdot \det(\Phi(x_2) - \Phi(x_1), \Phi(x_3) - \Phi(x_1)) \geq 0 \tag{20}$$

holds for all $\{x_1, x_2, x_3\} \subset \omega$ such that $\{x_1, x_2\}, \{x_1, x_3\}, \{x_2, x_3\} \in \mathcal{S}(y)$.

A y-continuous map Φ which is also injective is called discrete imbedding.

Throughout the paper "discrete imbedding" means "discrete orientation preserving imbedding".

Remark 2.5. *In fact discrete imbeddings satisfy the stronger relation*

$$|\Phi(x) - \Phi(x')| = 1 \text{ if and only if } \{x, x'\} \in \mathcal{S}(y),$$

provided that $\{x, x'\} \subset \omega$. This follows from the definition and the obvious fact that for each $\eta \in A_2$ we have that $\#\{\eta' \in A_2 \mid |\eta - \eta'| \in (0, 1]\} = 6$.

We say that $\mathcal{A} \subset A_2$ is a sub-lattice if $\mathcal{A} + \eta - \eta' = \mathcal{A}$ for all $\{\eta, \eta'\} \subset \mathcal{A}$. For a sub-lattice $\mathcal{A}$ the lattice parameter is given by $\lambda = \min\{|\eta - \eta'| \; |\eta, \eta' \in \mathcal{A}, \eta \neq \eta'\}$. A sub-lattice $\mathcal{A}$ is D_6-invariant if $\gamma\mathcal{A} = \mathcal{A}$ for all $\gamma \in D_6$, the maximal subgroup of $O(2)$ which leaves A_2 invariant.

For each $\lambda \in \mathbb{R}$ we define $m(\lambda) \in \mathbb{N}$ to be the number of different D_6-invariant sublattices of A_2 with lattice parameter λ divided by λ^2 e.g. $m(1) = 1$, $m(\sqrt{7}) = 2$. The variable $m(\lambda)$ is introduced for bookkeeping purposes only, it appears in intermediate expressions but is never evaluated or estimated explicitly. A simple geometric consideration shows that

$$m(\lambda) = \tfrac{1}{6}\#(A_2 \cap \{|\eta| = \lambda\}) = \tfrac{1}{6}\# \left\{ k \in \mathbb{Z}^2 \;\middle|\; k \cdot \left(\begin{smallmatrix} 2 & 1 \\ 1 & 2 \end{smallmatrix}\right) k = 2\lambda^2 \right\}. \tag{21}$$

The countable set $\Lambda = \{\lambda > 0 \mid m(\lambda) \neq 0\}$ is the set of distances. With this definition we obtain an equivalent formula for the renormalized potential:

$$V_*(s) = \sum_{\lambda \in \Lambda} m(\lambda) V(\lambda s). \tag{22}$$

Definition 2.6 (Equilateral simplices)**.** *Let $T \subset X$ such that $\#T = 3$ and $\lambda \in \Lambda$. We say that T is an equilateral simplex with side length λ for the configuration y satisfying (13) and write shortly $T \in \mathcal{T}_\lambda(y)$ if either*
$\lambda = 1$ and $p \in \mathcal{S}$ for all $p \subset T$ such that $p \in \mathcal{P}$,
or
if $\lambda > 1$, $B(z, 20\lambda) \cap y(\partial X) = \emptyset$ and there exists a patch $\omega_T \subset X \setminus \partial X$ with $T \subset \omega_T$ and a discrete imbedding $\Phi_T : \omega_T \to \mathcal{A} \subset A_2$ with the properties

$$|\Phi(x) - \Phi(x')| = \lambda \text{ for all } \{x, x'\} \subset T, \tag{23}$$

$$B(z, 5\lambda) \cap A_2 \supset y(\omega_T) \supset B(z, 3\lambda) \cap A_2, \tag{24}$$

where $z = \frac{1}{3} \sum_{x \in T} y(x)$.

The definition is motivated by the following lemma which provides for each equilateral simplex $T \in \mathcal{T}_\lambda(y)$ a quantitative link between λ and the side length of a deformed simplex $y(T) \subset \mathbb{R}^2$.

Lemma 2.7. *There exists a pair of constants $\alpha_0, K > 0$ such that for all $\alpha \in (0, \alpha_0)$, if $\lambda \in \Lambda$, the configuration y satisfies (13) and $T \in \mathcal{T}_\lambda(y)$, then for all $\{x, x'\} \subset T$ the estimate*

$$\left| \tfrac{1}{\lambda} |y(x) - y(x')| - 1 \right| \leq K\alpha \tag{25}$$

holds.

Proof. See appendix. □

Definition 2.6 is brought to life by Proposition 2.8 which asserts that for any pair $x, x' \in X$ with the property that $y(\partial X) \cap B(\frac{1}{2}(y(x) + y(x')), 28|y(x) - y(x')|) = \emptyset$ we can find an equilateral simplex T which contains x and x'. In other words, the absence of defects provides enough rigidity so that we can embed defect-free regions into the triangular lattice A_2.

Proposition 2.8. *There exists a number $\alpha_0 > 0$ such that for all $\alpha \in (0, \alpha_0)$, all configurations y satisfying (13) and all pairs $\{x_1, x_2\} \subset X$ the set*

$$\mathcal{T}(x_1, x_2) = \{T \in \cup_{\lambda \in \Lambda \setminus \{1\}} \mathcal{T}_\lambda(y) \mid \{x_1, x_2\} \subset T\}$$

satisfies the following assertions.

1. *$\#\mathcal{T}(x_1, x_2) \leq 2$ and there exists a unique number $\lambda \in \Lambda$ such that $T(x_1, x_2) \subset \mathcal{T}_\lambda(y)$.*
2. *If $B \cap y(\partial X) = \emptyset$, where $B = B(\frac{1}{2}(y(x_1) + y(x_2)), 28|y(x_1) - y(x_2)|)$, then $\#\mathcal{T}(x_1, x_2) = 2$.*

(3) *Conversely, if* $\#\mathcal{T}(x_1, x_2) \le 1$, *then* $y(\partial X) \cap B \neq \emptyset$.

Proof. See appendix. □

The central motivation for the introduction of the scaling parameter λ is that it provides us a natural method to pass information about the deformation on large scales to small scales. In particular, the area covered by the big deformed simplices can be computed up to a surface error by summing the area of the small simplices that lie within the big simplices.

Proposition 2.9. *There exists a pair of constants* $C, \alpha_0 > 0$ *such that for every* $\alpha \in (0, \alpha_0)$, *all configurations* $y : X \to \mathbb{R}^2$ *satisfying (13) and every* $\lambda \in \Lambda$ *the following estimates are true.*

$$0 \le \#\mathcal{T}_1 - \tfrac{1}{m(\lambda)}\#\mathcal{T}_\lambda(y) \le C\lambda^2\#\partial X, \tag{26}$$

$$0 \le \sum_{S\in\mathcal{T}_1} \mathrm{meas}(\mathrm{conv}(y(S))) - \frac{1}{\lambda^2 m(\lambda)} \sum_{T\in\mathcal{T}_\lambda(y)} \mathrm{meas}(\mathrm{conv}(y(T))) \le C\lambda^2\#\partial X, \tag{27}$$

$$\#\{T \in \mathcal{T}_\lambda(y) \mid \omega_T \supset \{x\}\} \le C\lambda^2 m(\lambda) \text{ for all } x \in X. \tag{28}$$

Proof. See appendix. □

The strength of this result is based on the fact that just one mild assumption on the minimum inter-particle distance of arbitrary N-particle configurations implies that interesting large-scale geometric objects such as equilateral simplices enjoy the natural scaling estimates up to errors which are bounded by the number of defects, a purely local concept.

We use the notion of equilateral simplices to define a further splitting of the set of short range interactions $\mathcal{S}(y)$ and long-range interactions $\mathcal{L}(y)$. For $j = 0, 1, 2$ let

$$\begin{aligned}\mathcal{S}_j(y) :=& \{p \in \mathcal{S}(y) \mid \text{there exists precisely } j \text{ simplices } T \in \mathcal{T}_1 \text{ such that } p \subset T\},\\ \mathcal{L}_j(y) :=& \{p \in \mathcal{L}(y) \mid \text{there exists } \lambda \in \Lambda \setminus \{1\} \text{ and precisely } j \text{ simplices } T \in \mathcal{T}_\lambda(y)\\ & \text{such that } p \subset T\}.\end{aligned}$$

Proposition 2.8.1 implies that $\mathcal{P} = \bigcup_{j=0}^2 (\mathcal{S}_j(y) \cup \mathcal{L}_j(y))$. The partitioning of the set of pairs induces a partitioning of the energy

$$\begin{aligned}\sum_{p\in\mathcal{P}} e(p) =& \frac{1}{2}\sum_{\lambda\in\Lambda}\sum_{T\in\mathcal{T}_\lambda}\sum_{p\subset T, \#p=2} e(p) + \sum_{p\in\mathcal{S}_0} e(p) + \frac{1}{2}\sum_{p\in\mathcal{S}_1} e(p) + \sum_{p\in\mathcal{L}_0} e(p) + \frac{1}{2}\sum_{p\in\mathcal{L}_1} e(p)\\ =& I_1 + I_2 + I_3 + I_4 + I_5.\end{aligned} \tag{29}$$

It will be demonstrated in the following section that I_1, I_2, I_3 carry the dominating part of the energy and the terms I_4, I_5 can be estimated by small surface terms.

2.4. **Resummation.** This section contains the centerpiece of the proof where the analytical and combinatorial estimates are combined to establish (9). An important step in our analysis consists in creating a link between long range interactions and the volume of big deformed simplices (Lemma 2.10). The difference between the interaction energy of a deformed simplex and the interaction energy of a rigid simplex can be approximated by the difference between the volumes. The error can be controlled by the quadratic distortion of the simplex.

The crucial point is that the volume is robust enough to provide information regardless of the structure of possible singularities such as defects or dislocations (Proposition 2.9).

Lemma 2.10. *There exists two constants $C, \alpha_0 > 0$ such that for all $\alpha \in (0,\alpha_0)$, $f \in C^2([0,\infty))$, $\lambda \in (0,\infty)$ and all $Y = \{y_0, y_1, y_2\} \subset \mathbb{R}^2$ with the property, $\left|\frac{1}{\lambda}|y_i - y_j| - 1\right| \leq \alpha$ for $i \neq j$, the inequality*

$$\begin{aligned} &\left|\tfrac{2\sqrt{3}}{\lambda} f'(\lambda)\left(\mathrm{meas}(\mathrm{conv}(Y)) - \tfrac{\sqrt{3}}{4}\lambda^2\right) + 3f(\lambda) - \tfrac{1}{2}\sum_{i\neq j} f(|y_i - y_j|)\right| \\ \leq\ & C\left(\tfrac{1}{\lambda}|f'(\lambda)| + \|f''\|_{L^\infty((1-\alpha)\lambda,(1+\alpha)\lambda)}\right)\sum_{i\neq j}(|y_i - y_j| - \lambda)^2 \end{aligned} \tag{30}$$

holds.

Proof. Let $i \neq j$ and set $\delta_{ij} = \frac{1}{\lambda}|y_i - y_j| - 1$. Heron's formula, which gives the area of a triangle in terms of it side lengths, yields

$$\begin{aligned} \mathrm{meas}(\mathrm{conv}(Y)) =& \tfrac{\sqrt{3}}{4}\lambda^2\left(1 + \tfrac{2}{3}\textstyle\sum_{i\neq j}\delta_{ij} + O\left(\sum_{i\neq j}\delta_{ij}^2\right)\right)^{\frac{1}{2}} \\ =& \tfrac{\sqrt{3}}{4}\lambda^2 + \tfrac{1}{4\sqrt{3}}\lambda^2\textstyle\sum_{i\neq j}\delta_{ij} + O\left(\lambda^2\sum_{i\neq j}\delta_{ij}^2\right), \end{aligned}$$

where the O-constant is bounded by a universal number as long as $\alpha \in (0,1)$. By Taylor's theorem $|f(|y_i - y_j|) - f(\lambda) - \lambda f'(\lambda)\delta_{ij}| \leq \frac{\lambda^2}{2}\|f''\|_{L^\infty((1-\alpha)\lambda,\infty)}\delta_{ij}^2$. Plugging these two estimates into the left hand side of (30) yields the claim. □

We extract the leading energy contribution of the long-range interactions. By Lemma 2.10 and decay estimate (5) we obtain for every $\lambda \in \Lambda \setminus \{1\}$ and $T \in \mathcal{T}_\lambda(y)$

$$\begin{aligned} \sum_{p\subset T, \#p=2} e(p) \geq& 3V(\lambda) + \tfrac{2\sqrt{3}}{\lambda}V'(\lambda)\left(\mathrm{meas}(\mathrm{conv}(y(T))) - \tfrac{\sqrt{3}}{4}\lambda^2\right) \\ &- C\alpha\lambda^{-7}\sum_{\{x,x'\}\subset T}\left(|y(x) - y(x')| - \lambda\right)^2. \end{aligned} \tag{31}$$

Now we are in the position to carry out the most important step of the proof and localize the long-range interactions. Proposition 2.9 implies that

$$\begin{aligned} &\sum_{T\in\mathcal{T}_\lambda}\left[3V(\lambda) + \tfrac{2\sqrt{3}}{\lambda}V'(\lambda)\left(\mathrm{meas}(\mathrm{conv}(y(T))) - \tfrac{\sqrt{3}}{4}\lambda^2\right)\right] \\ \geq& m(\lambda)\sum_{S\in\mathcal{T}_1}\left[3V(\lambda) + 2\sqrt{3}\lambda V'(\lambda)\left(\mathrm{meas}(\mathrm{conv}(y(S))) - \tfrac{\sqrt{3}}{4}\right)\right] - C\alpha\lambda^{-3}m(\lambda)\#\partial X \end{aligned} \tag{32}$$

Another application of Lemma 2.10 transforms the main term in (32) back into a pair sum

$$\begin{aligned} &3V(\lambda) + \tfrac{2\sqrt{3}}{\lambda}V'(\lambda)\left(\mathrm{meas}(\mathrm{conv}(\lambda y(S))) - \tfrac{\sqrt{3}}{4}\lambda^2\right) \\ \geq& \sum_{\{x,x'\}\subset S} V\left(\lambda\,|y(x) - y(x')|\right) - C\alpha\lambda^{-5}\sum_{\{x,x'\}\subset S}\left(|y(x) - y(x')| - 1\right)^2, \end{aligned} \tag{33}$$

where $S \in \mathcal{T}_1(y)$ is arbitary. For each simplex $T \in \mathcal{T}_\lambda(y)$ we choose $x \in T$ arbitrary and set $\Omega = B(z, 20\lambda)$ and $\Omega' = B(z, 3\lambda)$, where $z = \frac{1}{3}\sum_{x\in T} y(x)$. By Definition 2.6 and estimate (25) for $\alpha \in (0, \frac{1}{2K})$ the inclusion $y^{-1}(\Omega') \subset \omega_T$ holds and there exists a constant $M \in \mathbb{N} \cap [\lambda, 2\lambda]$ and a translation vector $\tau \in A_2$ such that

$$\Phi_T(y(T)) \subset \tau + \mathrm{conv}\left\{\binom{0}{0}, M\binom{1}{0}, \tfrac{M}{2}\binom{2}{\sqrt{3}}\right\} \cap A_2 \subset \Phi_T(\omega_T)$$

holds. The L^2-rigidity estimate provided by Proposition 4.3 applied to $u(\xi) := y(\Phi^{-1}(\xi))$ gives a bound on the distortion of the big simplex T in terms of the distortion of the smaller simplices $S \in \mathcal{T}_1(y)$:

$$\sum_{\{x,x'\}\subset T} (|y(x)-y(x')|-\lambda)^2 \le C\log(\lambda) \sum_{\substack{\{x,x'\}\in\mathcal{S}\\ \{x,x'\}\subset\omega_T}} (|y(x)-y(x')|-1)^2.$$

We use this inequality to localize the error term in (31).

$$\begin{aligned}\lambda^{-7}\sum_{T\in\mathcal{T}_\lambda}\sum_{\{x,x'\}\subset T} (|y(x)-y(x')|-\lambda)^2 \le& C\lambda^{-7}\log(\lambda)\sum_{T\in\mathcal{T}_\lambda}\sum_{\substack{\{x,x'\}\in\mathcal{S}\\ \{x,x'\}\subset\omega_T}} (|y(x)-y(x')|-1)^2\\ \le& C\lambda^{-5}\log(\lambda)m(\lambda)\sum_{\{x,x'\}\in\mathcal{S}} (|y(x)-y(x')|-1)^2. \qquad (34)\end{aligned}$$

The final inequality above is a consequence from (28). The error terms terms which appear in (32), (33) and (34) can be bounded uniformly

$$\sum_{\lambda\in\Lambda\setminus\{1\}} \left((1+\log(\lambda))\,\lambda^{-5}+\lambda^{-3}\right)m(\lambda) \le C \sum_{k\in\mathbb{Z}^2\setminus\{0\}} \left(k\cdot\begin{pmatrix}2&1\\1&2\end{pmatrix}k\right)^{-\frac{3}{2}} < \infty. \qquad (35)$$

After these considerations we can estimate the big sum $\sum\limits_{\lambda\in\Lambda\setminus\{1\}}\sum\limits_{T\in\mathcal{T}_\lambda}\sum\limits_{p\subset T,\#p=2} e(p)$ by a much simpler sum which contains only nearest-neighbor terms.

$$\begin{aligned}&\tfrac{1}{2}\sum_{\lambda\in\Lambda\setminus\{1\}}\sum_{T\in\mathcal{T}_\lambda}\sum_{p\subset T,\#p=2} e(p)\\ \ge&\tfrac{1}{2}\sum_{\lambda\in\Lambda\setminus\{1\}}\sum_{S\in\mathcal{T}_1}\sum_{\{x,x'\}\subset S} V(\lambda|y(x)-y(x')|)m(\lambda)\\ &-C\alpha\sum_{\lambda\in\Lambda\setminus\{1\}}\left((1+\log(\lambda))\lambda^{-5}\sum_{\{x,x'\}\in\mathcal{S}}(|y(x)-y(x')|-1)^2+\lambda^{-3}\#\partial X\right)m(\lambda)\\ \overset{(35)}{\ge}&\tfrac{1}{2}\sum_{\lambda\in\Lambda\setminus\{1\}}\sum_{\{x,x'\}\in\mathcal{S}} V(\lambda|y(x)-y(x')|)m(\lambda) \qquad (36)\\ &-C\alpha\left(\sum_{S\in\mathcal{T}_1}\sum_{\{x,x'\}\subset S}(|y(x)-y(x')|-1)^2+\#\partial X\right)\end{aligned}$$

Now we interchange the sum over λ and the sum over S in (36), use formula (22) and obtain the estimate

$$\begin{aligned}&\frac{1}{2}\sum_{\lambda\in\Lambda\setminus\{1\}}\sum_{T\in\mathcal{T}_\lambda}\sum_{p\subset T,\#p=2} e(p) \qquad (37)\\ \ge&\frac{1}{2}\sum_{S\in\mathcal{T}_1}\sum_{\{x,x'\}\subset S}\left[e_*(\{x,x'\})-e(\{x,x'\})-C\alpha(|y(x)-y(x')|-1)^2\right]-C\alpha\#\partial X\end{aligned}$$

The lower bound on the minimum distance (13) implies that $\#(\mathcal{S}_0(y)+\mathcal{S}_1(y)) \le C\#\partial X$. Inequality (12) gives for each $p\in\mathcal{S}(y)$ the estimates

$$|e_*(p)-e(p)| \le \frac{1}{6}\sum_{\xi\in A_2,|\xi|>1} \alpha((1-\alpha)|\xi|)^{-5} \le C\alpha$$

and

$$\sum_{p\in\mathcal{S}_0\cup\mathcal{S}_1} |e(p)-e_*(p)| \le C\alpha\#\partial X. \tag{38}$$

Consequentially (37) can be improved to

$$\begin{aligned}&\frac{1}{2}\sum_{\lambda\in\Lambda\setminus\{1\}}\sum_{T\in\mathcal{T}_\lambda}\sum_{p\subset T,\#p=2} e(p)\\ &\ge \sum_{\{x,x'\}\in\mathcal{S}}\left[e_*(\{x,x'\})-e(\{x,x'\})-C\alpha(|y(x)-y(x')|-1)^2\right]-C\alpha\#\partial X.\end{aligned}$$

The only difference between (37) and the above inequality is that the right hand side of the latter inequality contains all nearest-neighbor interactions whereas the former only those which belong to equilateral simplices with side length 1. We end up with the estimate

$$\begin{aligned}I_1+I_2+I_3 &\ge \sum_{\{x,x'\}\in\mathcal{S}}\left[e_*(\{x,x'\})-C\alpha(|y(x)-y(x')|-1)^2\right]-C\alpha\#\partial X\\ &\ge -3\#\mathcal{S}+\frac{1}{C}\sum_{p\in\mathcal{S}}(e_*(p)+1)-C\alpha\#\partial X. \end{aligned}\tag{39}$$

The last inequality follows from (7) together with assumptions (1) and (10) if α is sufficiently small. It remains to show that the sum I_4+I_5 can be estimated by a small surface term. For every $d\in[0,\infty)$ there are at most

$$n(d) := Cd^3\#\partial X \tag{40}$$

index pairs $\{x,x'\}\subset X$ such that $||y(x)-y(x')|-d|\le\frac{1}{2}$ and $\{x,x'\}\in\mathcal{L}_0$. To see this we first apply Proposition 2.8.3 and obtain that for each index pair $\{x,x'\}\in\mathcal{L}_0$ there exist $x_b\in\partial X$ such that $y(x)\in B(y(x_b),28|y(x)-y(x')|)$. The lower bound on the minimum distance between particles (13) implies that for every $x_b\in\partial X$ there are at most Cd^2 labels $x\in X$ such that $y(x)\in B(y(x_b),28|y(x)-y(x')|)$ and Cd labels $x'\in X$ such that $||y(x)-y(x')|-d|\le\frac{1}{2}$. This proves (40).

By (4) and (5) this implies that

(41)

$$I_4+I_5=\sum_{p\in\mathcal{L}_0\cup\mathcal{L}_1} e(p)\ge -\left(n(\tfrac{4}{3})\alpha+\sum_{d=2}^{\infty} n(d+\tfrac{1}{3})\|V\|_{L^\infty\left(\frac{1}{3}+d,\infty\right)}\right)\#\partial X\ge -C\alpha\#\partial X.$$

Adding (39) and (41) gives the desired inequality (9). The proof of Theorem 1.1 is finished.

3. Proof of Theorem 1.2

In contrast to the situation of Theorem 1.1 the number of particles is now infinite, with the consequence that there are configurations $y(X)$ such that $\partial X=\emptyset$. This is not possible if the number of particles is finite. Infinite energies are avoided by working with special boundary conditions. The usage of the term "boundary conditions" which is typically connected with partial differential equations is slightly non-standard in this context. It simply refers to the fact that we are considering kinematically constrained settings and that the constraints have a natural spatial structure.

The idea is to show that a suitable version of the main estimate (9) holds in both cases. We will use this estimate in connection with the competitor $y(x)\equiv x$ to demonstrate that minimizers $y_{\min}$ are rigid, i.e. $\partial X=\emptyset$ and $|y_{\min}(x)-y_{\min}(x')|=1$ if $\{x,x'\}\in\mathcal{S}$ which means that all the nearest neighbors have precisely distance 1 from each other.

It can be shown with elementary methods that every nonempty set $\Omega \subset \mathbb{R}^2$ with the properties

$$\min_{\substack{y,y'\in\Omega\\ y\neq y'}} |y-y'| \geq 1 \text{ and} \tag{42}$$

$$\#\{y' \in \Omega \mid |y-y'| \leq 1\} = 7 \text{ for all } y \in \Omega \tag{43}$$

is countable and there exists a rotation $R \in SO(2)$ and a translation $\tau \in \mathbb{R}^2$ such that

$$R\Omega + \tau = A_2.$$

Let $L \in \mathbb{N}$; a set $X \subset A_2$ is L-periodic if $X + LA_2 = X$. We introduce the equivalence relation $\sim$ on the set of subset ω an L-periodic set X: $\omega \sim \omega'$ if there is a vector $\tau \in LA_2$ such that $\omega' = \omega + \tau$. We say that a map $y : X \to \mathbb{R}^2$ is L-periodic if $y(x+\tau) = y(x) + \tau$ for all $x \in X$ and all $\tau \in LA_2$. For a L-periodic map the defects ∂X, neighbors $\mathcal{S}$ and the equilateral simplices $\mathcal{T}_\lambda$ are periodic sets and we can define the natural quotient sets $\widetilde{X} := X/\sim$, $\widetilde{\partial X} := \partial X/\sim$, $\widetilde{\mathcal{S}} := \mathcal{S}/\sim$, $\widetilde{\mathcal{P}} := \mathcal{P}/\sim$, $\widetilde{\mathcal{T}}_\lambda := \mathcal{T}_\lambda/\sim$.

The proof of Theorem 1.1 is hinged on the lower bound on the inter-particle distance (13). The proof of (13) is based on a construction where those particles that are too close to each other are moved to infinity and thereby effecively removed from the system without increasing the energy.

As the definition of E_L^{per} doesn't allow removal of particles we have to relax the minimization problem slightly in order to rescue (13). This is achieved by removing L-periodic subsets from A_2: If $X \subset A_2$ is L-periodic we set

$$E_L^{\text{per}}(X, \{y\}) := \sum_{\{p \subset X \mid \#p=2\}/\sim} e(p).$$

Clearly $E_L^{\text{per}}(X, \cdot) = E_L^{\text{per}}(\cdot)$ (defined in Theorem 1.2) if $X = A_2$. Furthermore, since there are only 2^{L^2} possible L-periodic sets X, a minimizer $(X_{\min}, y_{\min})$ of E_L^{per} exists. Due to the more complicated mechanism of particle-removal we have to establish a new version of Lemma 2.2.

Lemma 3.1. *There exists $\alpha_0 \in (0, \frac{1}{2})$ such that for all $\alpha \in (0, \alpha_0)$, $L \in \mathbb{N}$ and all minimizers $(X_{\min}, y_{\min})$ of $E_L^{\text{per}}(\cdot, \cdot)$ the minimum distance between the particles satisfies estimate (13).*

Proof. It can be assumed wlog that $L \geq 4$ as the cases $L' \in \{1, 2, 3\}$ are covered by $L = 4L'$. Let M and $\mathcal{A}$ be defined as in the proof of Lemma 2.2. In the periodic situation we have to take the interaction between the particles in $\mathcal{A}$ and the mirror images into account. The decay estimate (5) implies that

$$\sum_{x\in\mathcal{A}} \sum_{x' \in (\mathcal{A}+LA_2)\setminus\mathcal{A}} e(\{x, x'\}) \geq -CM^2\alpha,$$

where $C = \sum_{\xi \in LA_2\setminus\{0\}} (|\xi| - 2)^{-5}$. We replace (14) by the estimate

$$\sum_{x\in\mathcal{A}} \sum_{x' \in X\setminus(\mathcal{A}+LA_2)} e(\{x, x'\}) \leq -\tfrac{1}{2\alpha} M(M-1) + CM^2\alpha.$$

and (17) by

$$-CM^2 \left(\sum_{k=2}^{8} 2k + \alpha \sum_{k=9}^{\infty} ((1-\alpha)\tfrac{k-1}{2})^{-5} \right) \leq -\tfrac{1}{2\alpha} M(M-1) + CM^2\alpha.$$

Repeating the reasoning at the end of the proof of Lemma 2.2 we obtain that $M = 1$ if α is sufficiently small, the only difference is that one additional term on the right-hand side is created by periodicity. $\square$

We claim now that for configurations X, y which satisfy the bound (13) a suitably adapted version of (9) holds:

$$E_L^{\mathrm{per}}(X, \{y\}) \geq \frac{1}{C} \sum_{\{x,x'\} \in \widetilde{\mathcal{S}}} (e_*(\{x, x'\}) - 1) + \tfrac{1}{4}\#\widetilde{\partial X} - 3\#\widetilde{X}. \tag{44}$$

The proof of Theorem 1.1 can be adapted to the periodic setting by simply replacing the sets X, ∂X, $\mathcal{S}$, $\mathcal{T}_\lambda$ with the corresponding quotient sets $\widetilde{X}$, $\widetilde{\partial X}$, $\widetilde{\mathcal{S}}$, $\widetilde{\mathcal{T}}_\lambda$ and the elements of those quotient sets by representatives.

As the identity map $y(x) \equiv x$ is L-periodic for every $L \in \mathbb{N}$ and therefore an admissible competitor we obtain that $E_L^{\mathrm{per}}(X_{\min}, \{y_{\min}\}) + 3L^2 \leq 0$ and together with (44)

$$0 \geq \frac{1}{C} \sum_{\{x,x'\} \in \widetilde{\mathcal{S}}} (e_*(\{x, x'\}) + 1) + \tfrac{1}{4}\#\widetilde{\partial X}_{\min} + 3(L^2 - \#\widetilde{X}_{\min}).$$

Since $\#\widetilde{X} \leq L^2$ this estimate shows that $\#\widetilde{X}_{\min} = L^2$, $\partial\widetilde{X}_{\min} = \emptyset$, and $|y_{\min}(x) - y_{\min}(x')| = 1$ for all $\{x, x'\} \in \mathcal{S}$.

Hence, the set $\Omega = \{y_{\min}(x) \mid x \in A_2\}$ satisfies (42) and (43) and consequentially $R\Omega + \tau = A_2$ for a rotation $R \in SO(2)$ and a translation $\tau \in \mathbb{R}^2$. By the periodicity of $y_{\min}$ we can choose $R = \mathrm{Id}$, this is precisely the claim and the proof of Theorem 1.2 is finished.

Proof of Corollary 1.3. Again we salvage the lower bound (13) by enlarging the set of competitors slightly. For $\mathcal{A}' \subset \mathcal{A}$ we set

$$E(\mathcal{A}', \{y\}) = \sum_{\substack{\{x,x'\} \subset X \\ \{x,x'\} \cap \mathcal{A}' \neq \emptyset}} V(|y(x) - y(x')|),$$

where $X = (A_2 \setminus \mathcal{A}) \cup \mathcal{A}'$. As before $E(\mathcal{A}', \cdot) = E_{\mathcal{A}}(\cdot)$ if $\mathcal{A}' = \mathcal{A}$. Let $\mathcal{A}_{\min}, y_{\min}$ be the minimizer of $E(\cdot, \cdot)$. Clearly $y_{\min}$ satisfies the bound (13) since the proof of Lemma 2.2 can be repeated for this case, word by word. We determine the properties of $\mathcal{A}_{\min}, y_{\min}$ by comparing the minimization problem with the periodic situation which has been analyzed earlier.

Let $Y = A_2 \cap \frac{L}{2}\begin{pmatrix} 2 & 1 \\ 0 & \sqrt{3} \end{pmatrix} Q - \frac{L}{4}\binom{3}{\sqrt{3}}$ where $Q = [0, 1) \times [0, 1) \subset \mathbb{R}^2$ is the semi-open unit square and let $X_{\mathrm{per}} := Y + LA_2$ and $y_{\mathrm{per}}(x) := \tau + y_{\min}(x - \tau)$ if $x \in X_{\mathrm{per}}$, $\tau \in LA_2$, $x + \tau \in Y$. Clearly X_{per} is L-periodic and y_{per} is a projection of $y_{\min}$ onto the set of L-periodic maps. Due to the compactness of $\mathcal{A}$ we can assume that $A \subset B(0, C)$ for some number $C > 0$. Let us define the following sets of pairs

$$\begin{aligned} \mathcal{P} &:= \{p \subset A_2 \mid \#p = 2\}, \\ \mathcal{P}_{\min} &:= \{p \in \mathcal{P} \mid p \cap (\mathcal{A} \setminus \mathcal{A}_{\min}) = \emptyset\}, \\ \mathcal{P}_{\mathrm{per}} &:= \{p \in \mathcal{P} \mid p \cap (\mathcal{A} \setminus \mathcal{A}_{\min} + LA_2) = \emptyset\} \end{aligned}$$

which by construction obey the inclusion $\mathcal{P}_{\mathrm{per}} \subset \mathcal{P}_{\min} \subset \mathcal{P}$. We set $e(\{x, x'\}) := V(|y_{\min}(x) - y_{\min}(x')|)$ if $\{x, x'\} \in \mathcal{P}_{\min}$ and $e_{\mathrm{per}}(\{x, x'\}) := V(|y_{\mathrm{per}}(x) - y_{\mathrm{per}}(x')|)$ if

$\{x,x'\} \in \mathcal{P}_{\text{per}}$. By the decay properties of V, for all $\varepsilon > 0$ there exists $L_\varepsilon \in \mathbb{N}$ such that

$$\sum_{\{p \in \mathcal{P}_{\text{per}} \mid p \cap \mathcal{A}_{\min} \neq \emptyset\}} |e_{\text{per}}(p) - e(p)| \leq \varepsilon, \tag{45}$$

$$\sum_{\{p \in \mathcal{P}_{\min} \setminus \mathcal{P}_{\text{per}} \mid p \cap \mathcal{A}_{\min} \neq \emptyset\}} |e(p)| \leq \varepsilon \tag{46}$$

if $L \geq L_\varepsilon$. Let $\mathcal{S}_{\text{per}} := \{\{x,x'\} \in \mathcal{P}_{\text{per}} \mid ||y_{\text{per}}(x) - y_{\text{per}}(x')| - 1| < \alpha\}$ and define the quantity

$$I := \frac{1}{C} \sum_{\{x,x'\} \subset \mathcal{S}_{\text{per}}/\sim} ||y_{\text{per}}(x) - y_{\text{per}}(x')| - 1|^2 + \frac{1}{4}\#\widetilde{\partial X}_{\text{per}} + 3(L^2 - \#Y),$$

the equivalence relation $\sim$ has been defined in the previous section. We will demonstrate now that $I = 0$ by relating the $E_{\mathcal{A}}$ to E_L^{per}. By equation (44)

$$\begin{aligned} I \leq & E_L^{\text{per}}(Y + LA_2, \{y_{\text{per}}\}) + 3L^3 \\ = & \sum_{\{p \in \mathcal{P}_{\text{per}} \mid p \cap \mathcal{A}_{\min} \neq \emptyset\}} e_{\text{per}}(p) + \frac{1}{2} \sum_{\{p \in \mathcal{P}_{\text{per}} \mid p \cap \mathcal{A}_{\min} = \emptyset, p \subset Y\}} e_{\text{per}}(p) + 3L^2. \end{aligned}$$

The last equality is obtained by simply rewriting E_L^{per} in a more explicit way. By definition of $\mathcal{P}_{\text{per}}$ and y_{per} we can replace $\mathcal{A}_{\min}$ by $\mathcal{A}$ and $e_{\text{per}}(\{x,x'\})$ by $e_{\text{r}}(\{x,x'\}) := V(|x-x'|)$ in the second sum without changing the value of the sum. By (45) and (46) we can replace the periodic configuration y_{per} by the original minimum energy configuration $y_{\min}$ and $\mathcal{P}_{\text{per}}$ by $\mathcal{P}_{\min}$ in the first sum without changing its value by more than 2ε, hence

$$I \leq \sum_{\{p \in \mathcal{P}_{\min} \mid p \cap \mathcal{A}_{\min} \neq \emptyset\}} e(p) + \frac{1}{2} \sum_{\{p \in \mathcal{P}_{\text{per}} \mid p \cap \mathcal{A} = \emptyset, p \subset Y\}} e_{\text{r}}(p) + 3L^2 + 2\varepsilon.$$

The first sum is equal to $E_{\mathcal{A}}(\mathcal{A}_{\min}, \{y_{\min}\})$ and can be estimated by $E_{\mathcal{A}}(A_2)$ due to the minimality of $y_{\min}$. Let $Z := Y \cup \mathcal{A}$. By definition of Z we can replace the set Y by Z and $\mathcal{P}_{\text{per}}$ by $\mathcal{P}$ in the second sum without changing it.

$$I \leq \sum_{\{p \in \mathcal{P} \mid p \cap \mathcal{A} \neq \emptyset\}} e_{\text{r}}(p) + \frac{1}{2} \sum_{\{p \in \mathcal{P} \mid p \cap \mathcal{A} = \emptyset, p \subset Z\}} e_{\text{r}}(p) + 3L^2 + 2\varepsilon = E_L^{\text{per}}(A_2) + 3L^2 + 2\varepsilon = 2\varepsilon,$$

where the last two equations follow directly from the definition of E_L^{per}. As ε is arbitrary and $L^2 - \#Y = \#\overline{\mathcal{A} \setminus \mathcal{A}_{\min}}$ for sufficiently large L, where $\overline{U} := (U + B(0,1)) \cap A_2$ if $U \subset A_2$, we obtain that $\mathcal{A}_{\min} = \mathcal{A}$, $\partial X_{\text{per}} = \emptyset$ and $||y_{\text{per}}(x) - y_{\text{per}}(x')| - 1| \leq C\varepsilon$ for all $\{x,x'\} \in \mathcal{S}_{\text{per}}$. Since $y_{\text{per}}(x)$ and $y_{\text{per}}(x')$ are independent of L if L is sufficiently big, this proves that $|y_{\text{per}}(x) - y_{\text{per}}(x')| = 1$ for all $\{x,x'\} \in \mathcal{S}_{\text{per}}$. Hence, the set $\Omega = \{y_{\text{per}}(x) \mid x \in A_2\}$ satisfies (42) and (43) and consequentially $R\Omega + \tau = A_2$ for a rotation $R \in SO(2)$ and a translation $\tau \in \mathbb{R}^2$. By the periodicity of y_{per} we can choose $R = \text{Id}$. Since $y_{\text{per}}(x) = y_{\min}(x)$ for all $x \in Y$ we obtain that $\tau = 0$ and $y_{\min}(x) = x$ for all $x \in A_2$. The proof of Corollary 1.3 is finished.

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4. Appendix

4.1. **Geometric rigidity.** We provide bounds on the global distortion in terms of the local distortion. Both, L^∞ and L^2-estimates, are required.

Proposition 4.1. *There is a universal constant* $\alpha \in (0, \frac{1}{2})$ *such that for every pair of domains* $\Omega' \subset \Omega \subset \mathbb{R}^d$ *with the property* $\inf_{x\in\Omega'} \operatorname{dist}(x, \partial\Omega) \geq \frac{\sqrt{2\alpha}}{1-2\alpha}\operatorname{diam}(\Omega')$ *and all maps* $u \in W^{1,\infty}(\Omega)$ *satisfying* $\|\nabla u - SO(d)\|_{L^\infty(\Omega)} \leq \alpha$ *the estimate*

$$\sup_{\{x,x'\}\subset\Omega'} \left| \frac{|u(x) - u(x')|}{|x - x'|} - 1 \right| \leq \alpha \tag{47}$$

holds.

Under the additional assumption that $u \in C^1$ estimate (47) has been established in [8]. Since C^1 is not dense in the set of Lipschitz functions, we have to construct a more modern version of the proof.

Proof. The idea of the proof is to demonstrate that for two image points $u(x), u(x') \in u(\Omega')$ the geodesic $\beta \subset u(\Omega')$, which connects those two points, is in fact a straight line.

For each pair $x \neq x' \in \mathbb{R}^d$ we denote by

$$S_\alpha(x, x') \subset \mathbb{R}^d = \left\{ \xi \in \mathbb{R}^d \mid |\xi - x| + |\xi - x'| \leq \tfrac{1+2\alpha}{1-2\alpha}|x - x'| \right\}$$

the ellipsoid of revolution with foci x and x' and eccentricity $\frac{1+2\alpha}{1-2\alpha}$.

We will now show that the claim is true for all $S_\alpha(x, x') \subset \Omega$. To this end we construct a path $\gamma \in C([0, 1], \Omega)$ which minimizes the arc-length

$$I_u(\gamma) = \limsup_{\Delta\to 0} \left\{ \sum_{k=1}^{K} |u(\gamma(t_k)) - u(\gamma(t_{k-1}))| \;\middle|\; 0 = t_0 < \ldots < t_K = 1,\ \max_{k\in\{1\ldots K\}} t_k - t_{k-1} < \Delta \right\}$$

of the image $t \to u(\gamma(t))$ subject to the boundary condition $\gamma(0) = x$, $\gamma(1) = x'$. Since u is only Lipschitz but not necessarily C^1, the functional $I_u(\cdot)$ is in general neither continuous in $L^\infty(0, 1)$ or similar function spaces nor convex, therefore existence of minimizers can't be established by a naive application of the direct method.

To overcome this difficulty we use the following trick. As the path $t \to u((1-t)x + tx')$ is an admissible competitor, $(1 + \alpha)|x - x'|$ is an upper bound for $\inf_\alpha I_u(\gamma)$. Let $\mathcal{C} \subset W^{1,\infty}([0, 1], u(\Omega))$ be the set of paths β for which there exists a path $\gamma \in W^{1,\infty}([0, 1], \Omega)$ such that $\beta = u \circ \gamma$ and the boundary condition $\gamma(0) = x$, $\gamma(1) = x'$ is satisfied. We can assume without loss of generality that β passes through $u(\Omega)$ with constant speed, i.e. $\frac{\mathrm{d}}{\mathrm{d}t}|\frac{\mathrm{d}\beta}{\mathrm{d}t}| = 0$. Clearly $I_u(\gamma) = \int_0^1 |\dot{\beta}| \,\mathrm{d}t =: J(\beta)$.

We show now that the Lipschitz constant of γ is controlled by the Lipschitz constant of β. First we establish that u is locally injective, i.e. for any $t \in [0, 1]$ there exists a pair of open sets $O \subset \Omega$, $U \subset u(\Omega)$ such that $\gamma(t) \in O$, $u(\gamma(t)) \in U$ and $u : O \to U$ is injective. Thanks to Kohn's rigidity estimate [4, (1.5.ii)] we can find a universal constant $C > 0$ with the property that for all x, x' with $B(x, |x - x'|) \subset \Omega$ there exists a matrix $R \in SO(d)$ such that

$$|u(x) - u(x') - R(x - x')| \leq C|x - x'|\alpha, \tag{48}$$

which implies injectivity of u as long as $C\alpha < 1$.

Since $\det(\nabla u) \geq \frac{1}{2}$ the map u is quasi-regular i.e. there exists a constant $K > 0$ with the property that $|\nabla u|^d \leq K \det(\nabla u)$ almost everywhere. By Reshetnyak's theorem ([7, Theorem I.4.1]) u is discrete and open, and by injectivity $u : O \to U$ is a homoemorphism. Now $|\dot{\gamma}(t)| = \left|(\nabla u|_U(\beta(t)))^{-1} \dot{\beta}(t)\right| \leq \frac{1+\alpha}{1-\alpha}|x - x'|$. Hence γ is Lipschitz continuous with Lipschitz constant $\frac{1+\alpha}{1-\alpha}|x - x'|$.

Let now $(\beta_n)_{n\in\mathbb{N}} \subset \mathcal{C}$ be a minimizing sequence of $J(\cdot)$ which converges in the weak-* topology of $W^{1,\infty}$ to β. The convexity of $J(\cdot)$ implies that $\liminf_{n\to\infty} J(\beta_n) \geq J(\beta)$. The global Lipschitz bound $\|\dot{\beta}_n\|_{L^\infty} \leq (1+\alpha)|x-x'|$ implies that $\lim_{n\to\infty} \|\beta_n - \beta\|_{C([0,1])} = 0$, hence $\beta \in C([0,1], \overline{u(\Omega)})$. Similarly we obtain that there exists $\gamma_n, \gamma \in C\left([0,1], \overline{\Omega}\right)$ such that $\beta_n = u \circ \gamma_n$ and $\lim_{n\to\infty} \|\gamma_n - \gamma\|_{C([0,1])} = 0$. Clearly $\beta = u \circ \gamma$ and γ satisfies the boundary conditions $\gamma(0) = x$, $\gamma(1) = x'$. This shows that γ is a minimizer of $I_u(\cdot)$.

We use the minimality of γ in order localize the path. Let $t \in [0,1]$, then

(49)
$$|x-\gamma(t)| + |x'-\gamma(t)| \leq \int_0^1 |\dot{\gamma}| \,\mathrm{d}s \leq \frac{1}{1-\alpha} \int_0^1 |\nabla u(\gamma)\dot{\gamma}| \,\mathrm{d}s = \tfrac{1}{1-\alpha} I_u(\gamma) \leq \tfrac{1+\alpha}{1-\alpha}|x-x'|.$$

Hence $\gamma(t) \in S_\alpha(x,x')$ for all $t \in [0,1]$.

The inclusions $S_\alpha \subset \Omega$ and $\partial u(\Omega) \subset u(\partial\Omega)$ (due to the openness of u) imply that the minimal path β is contained in the open set $u(\Omega)$ and consequentially the Euler-Lagrange equation $\beta'' = 0$ is satisfied. In particular, β is a straight line segment that connects $u(x)$ and $u(x')$. Inequality (49) shows that

$$|u(x) - u(x')| \geq (1-\alpha)|x-x'|.$$

□

The following lemma links gradient estimates for continuous interpolations to the distortion of simplices.

Lemma 4.2. *There exist two universal constants $K, \alpha_0 > 0$ such that for each pair of triples $y_i, \eta_i \in \mathbb{R}^2$, $i = 0,1,2$ with the properties*

$$\det(y_1 - y_0, y_2 - y_0)\det(\eta_1 - \eta_0, \eta_2 - \eta_0) \geq 0,$$
$$||y_i - y_j| - 1| \leq \alpha_0 \text{ and } |\eta_i - \eta_j| = 1 \text{ if } i \neq j$$

the inequalities

$$\min_{R\in SO(2)} |F-R|^2 \leq K \max_{i\neq j} ||y_i - y_j| - 1|^2, \tag{50}$$

$$\min_{R\in SO(2)} |F^{-1}-R|^2 \leq K \max_{i\neq j} ||y_i - y_j| - 1|^2, \tag{51}$$

hold, where $|M| := \sqrt{\mathrm{trace}(M^TM)}$ for a 2×2-matrix M. The matrix $F \in \mathbb{R}^{2\times 2}$ is the gradient of the unique affine map $u : \mathrm{conv}\{\eta_0, \eta_1, \eta_2\} \to \mathbb{R}^2$ which satisfies $u(\eta_i) = y_i$ for $i = 0,1,2$.

Proof. We define the matrix $Y_0 = \frac{1}{2}\left(\begin{smallmatrix} 2 & 1 \\ 0 & \sqrt{3}\end{smallmatrix}\right)$ and the vectors $v_1 = \left(\begin{smallmatrix} 1 \\ 0\end{smallmatrix}\right)$, $v_2 = \left(\begin{smallmatrix} 0 \\ 1\end{smallmatrix}\right)$, $v_3 = \left(\begin{smallmatrix} 1 \\ -1\end{smallmatrix}\right)$. As reflections, rotations and translations of η_i and y_i leave (50) invariant, we can assume that $\eta_i = Y_0 v_i$ and $F\eta_i$ give the sides of the triangles $\{\eta_i\}$ and $\{y_i\}$, respectively. We choose $C > 0$, such that for all $M \in GL(2)$ the following implication holds:

$$\max_{i=1,2,3} ||M\,\eta_i| - 1| < 1 \Rightarrow \min_{R\in SO(2)} |M - R| \leq C.$$

Since $|x^2 - 1| \leq 3|x-1|$ for $0 \leq x \leq 2$, it suffices to prove

$$l := \min_{R\in SO(2)} |F-R| \leq C\,m$$

with $m := \max_{i=1,2,3} ||F\eta_i|^2 - 1|$. It is known that $l = \left|\sqrt{F^TF} - \mathrm{Id}\right|$. For the right-hand side we get $m \geq |\eta_i \cdot (F^TF - \mathrm{Id})\eta_i|$ since $|\eta_i| = 1$. We set $G := F^TF - \mathrm{Id}$ and conclude $m \geq |\eta_3 \cdot G\eta_3| \geq 2|\eta_2 \cdot G\eta_1| - |\eta_1 \cdot G\eta_1| - |\eta_2 \cdot G\eta_2|$, i.e. $\frac{3}{2}m \geq |\eta_2 \cdot G\eta_1|$.

This shows that $|GY_0v_1| = |G\eta_1| \leq Cm$. Similarly $|GY_0v_2| \leq Cm$ and we get $|GY_0| \leq Cm$, hence $|G| \leq Cm$. For $H := \left(\sqrt{F^TF} + \mathrm{Id}\right)^{-1}$, we obtain $|H| \leq 2$ and thus

$$l = |G\,H| \leq 2|G|\,|H| \leq C\,m.$$

This proves (50).

To establish (51) let $R \in SO(2)$, $S \in \mathbb{R}^{2\times 2}_{\mathrm{sym}}$ be the polar decomposition of F, i.e. $F = RS$ and set $H := S - \mathrm{Id}$. The previously derived estimate $|G| \leq Cm$ implies that $|2H + H^2| \leq Cm$ and consequentially $|H| \leq Cm$ by positivity of H^2. Since $F^{-1} = (\mathrm{Id} - H + H^2 - \ldots)R^T$ this implies (51). ☐

We apply the previous lemma to bound the distortion of large equilateral simplices by the distortions of the small simplices inside.

Proposition 4.3. *Let $M \in \mathbb{N}\setminus\{0,1\}$ and $\Omega = \mathrm{conv}\{\binom{0}{0}, M\binom{1}{0}, \frac{M}{2}\binom{2}{\sqrt{3}}\} \subset \mathbb{R}^2$ be a dilated unit simplex. There exist a universal constant $C > 0$ such that for all $u : \Omega \cap A_2 \to \mathbb{R}^2$ the estimate*

$$\min_{\substack{\tau\in\mathbb{R}^2\\ R\in SO(2)}} \max_{x\in\partial\Omega\cap A_2} |u(x) - \tau - Rx|^2 \leq C\log(M) \sum_{\substack{x,x'\in\Omega\cap A_2\\ |x-x'|=1}} \big||u(x) - u(x')| - 1\big|^2 \tag{52}$$

holds.

Proof. We extend u to a continuous map in $W^{1,\infty}(\Omega)$ by interpolation. By Lemma 4.2 for each triple $\{x_1, x_2, x_3\} \subset A_2$ with the property $|x_i - x_j| = 1$ if $i \neq j$ and each $x \in \mathrm{int}(\mathrm{conv}\{x_1, x_2, x_3\})$ we have that

$$\mathrm{dist}(\nabla u(x), SO(2)) \leq K \sum_{i\neq j} \big||u(x_i) - u(x_j)| - 1\big|^2.$$

A theorem by Müller, Friesecke and James in [9] states that there is a universal constant C which does not depend on u such that for each u we can find a rotation matrix $R \in SO(2)$ with the property

$$\int_\Omega |\nabla u - R|^2 \leq C \int_\Omega \mathrm{dist}(\nabla u, SO(d))^2. \tag{53}$$

Let $L = 3M$ and $\gamma : [0, L] \to \partial\Omega$ be a path which follows $\partial\Omega$ at unit speed, i.e. $\gamma(0) = \gamma(L) = 0$, $|\frac{\mathrm{d}}{\mathrm{d}t}\gamma| = 1$ and $\partial\Omega = \{y(s) \mid s \in [0, L]\}$. For $l \in [0, L] \cap \mathbb{Z}$ let $x_l = \gamma(l) \in A_2$ and $\tau = \frac{1}{L}\sum_{l=1}^{L} u(x_l)$. Define for $s \in [0, L]$ the function $v(s) := u(\gamma(s)) - \tau - R\gamma(s)$. By the standard trace theorem

$$\|v\|^2_{H^{\frac{1}{2}}([0,L])} \leq C \int_\Omega |\nabla u - R|^2, \tag{54}$$

where $\|v\|^2_{H^{\frac{1}{2}}([0,L])} = \sum_{k\in\mathbb{Z}} |k||\widehat{v}(k)|^2$ and

$$\widehat{v}(k) = \frac{1}{L}\int_0^L v(s)e^{2\pi i k\frac{s}{L}}\,\mathrm{d}s \tag{55}$$

is the k-th Fourier coefficient of v. We use the convention that $[r] = \max\{s \in \mathbb{Z} \mid s \leq r\}$ but only within this proof. For each $k \in \{[\frac{1-L}{2}], \ldots, [\frac{L-1}{2}]\} \subset \mathbb{Z}$ we define the k-th discrete Fourier coefficient of v by

$$\check{v}(k) = \frac{1}{L}\sum_{l=0}^{L-1} v(l)e^{2\pi i k\frac{l}{L}}$$

such that

$$v(l)=\sum_{k=[\frac{1-L}{2}]}^{[\frac{L-1}{2}]}\check{v}(k)e^{-2\pi ik\frac{l}{L}}. \tag{56}$$

It will be demonstrated that the inequality

$$|\check{v}(k)|\leq\tfrac{\pi^2}{2}|\widehat{v}(k)| \tag{57}$$

holds. The case $k=0$ is trivial since by definition $\widehat{v}(0)=\check{v}(0)=0$. After integrating the right hand side in (55) twice by parts one obtains that for $k\in\{[\frac{1-L}{2}]\ldots[\frac{L-1}{2}]\}\setminus\{0\}$

$$\begin{aligned}|\widehat{v}(k)|&=\frac{L}{4\pi^2k^2}\left|\sum_{l=0}^{L-1}(v(l+1)-2v(l)-v(l-1))e^{2\pi ik\frac{l}{L}}\right|\\&=\tfrac{1}{(2\pi\frac{k}{L})^2}\left|2(1-\cos(2\pi\tfrac{k}{L}))\check{v}(k)\right|\geq\tfrac{4}{\pi^2}|\check{v}(k)|,\end{aligned}$$

this implies that

$$\sum_{k\in\{[\frac{1-L}{2}]\ldots[\frac{L-1}{2}]\}}|\check{v}(k)|^2|k|\leq(\tfrac{\pi}{2})^4\|v\|^2_{H^{\frac{1}{2}}([0,L])}. \tag{58}$$

Clearly $\|v\|_{L^\infty([0,L])}=\max_{l\in\{0\ldots L\}}|v(l)|\leq\sum_{k\in\{[\frac{1-L}{2}]\ldots[\frac{L-1}{2}]\}\setminus\{0\}}|\check{v}(k)|$ by the discrete reconstruction formula (56). Putting the previous estimate, (57) and (58) together implies that

$$\begin{aligned}\|v\|^2_{L^\infty([0,L])}&\leq\left(\sum_{k\in\{[\frac{1-L}{2}]\ldots[\frac{L-1}{2}]\}\setminus\{0\}}|\check{v}(k)|\right)^2\\&\leq\sum_{k\in\{[\frac{1-L}{2}]\ldots[\frac{L-1}{2}]\}\setminus\{0\}}\frac{1}{|k|}\sum_{k\in\{[\frac{1-L}{2}]\ldots[\frac{L-1}{2}]\}}|k||\check{v}(k)|^2\leq C\log(L)\|u\|^2_{H^{\frac{1}{2}}(\partial\Omega)}.\end{aligned}$$

Together with (54) and (53) this implies (52). □

4.2. **Proof of Proposition 2.8.** The assertions in Proposition 2.8 are concerned with the question whether certain subsets $\omega\subset X$ can be imbedded into A_2 such that the neighborhood relation which is encoded by the set of edges $\mathcal{S}$ is preserved. For the proof we require an existence and uniqueness theorem of such imbeddings Φ (Proposition 4.8). The proof of Proposition 4.8 is constructive: For each path γ which connects two points $x_1,x_2\in X$ the imbedding $\Phi|_\gamma$ solves a certain 'ordinary' second order difference equation (59) which depends on γ. The construction of the difference equation is particularly simple in two dimensions due to the possibility to identify $\mathbb{R}^2$ with $\mathbb{C}$.

The imbedding Φ is independent of the path γ provided that all paths are equivalent, i.e. they can be homotoped into each other. The equivalence of paths is a nontrivial consequence of the defect-freeness of ω.

Definition 4.4. *A map $\gamma:[0,K]\cap\mathbb{N}\to X$ is a discrete path of length K if $\{\gamma(k),\gamma(k+1)\}\in\mathcal{S}$ for all $k\in\{0\ldots K-1\}$. A path γ is closed if $\gamma(K)=\gamma(0)$. A closed path is simple if $\gamma|_{\{0\ldots K-1\}}$ is injective.*

Let $\gamma\subset X\setminus\partial X$ be a closed, simple path. The set $\Omega(\gamma)\subset\mathbb{R}^2$ is the unique bounded domain which has the property $\partial\Omega(\gamma)=\cup_k[y(\gamma(k)),y(\gamma(k+1))]$ whose existence is guaranteed by Jordan's curve theorem. We say that γ is positively oriented if γ passes through $\partial\Omega(\gamma)$ in the positive sense.

The matrix $Q_\gamma(k) \in SO(2)$ is the unique rotation matrix which satisfies the equation

$$Q\phi(\gamma(k-1)) + \phi(\gamma(k+1)) = 0, \tag{59}$$

where $\phi : \mathcal{N}(\gamma(k)) \to A_2$ is a an arbitrary discrete imbedding such that $\phi(\gamma(k)) = 0$.

The Burgers vector associated to simple closed path γ and a direction $v \in A_2$ is defined by

$$b(\gamma, v) = \sum_{k=0}^{K-1} \prod_{i=0}^{k} Q_\gamma(i) v,$$

where $Q_\gamma(0) = \mathrm{Id}$ and $\gamma_K = \gamma_0$

Since $SO(2)$ is an Abelian group the Burgers vector b is well-defined without further stipulation concerning the order in which the matrices are multiplied.

Remark 4.5. *It is obvious from the definition that closed paths γ with length smaller or equal than two satisfy $\mathrm{vol}(\Omega(\gamma)) = b(\gamma, v) = 0$. On the other hand, if γ is an arbitrary closed and simple path with $\mathrm{vol}(\Omega(\gamma)) = 0$, then the length of γ is smaller or equal to two.*

The Burgers vector measures the defectiveness of a configuration. It depends on the chosen coordinate frame (characterized by v in the two-dimensional situation). If all possible Burgers vectors are 0 then the configuration is a deformed subset of the lattice A_2; a precise version of this connection is given in the statement and the proof of Proposition 4.8.

On the other hand, because of Lemma 4.7 the matrix Q is independent of the choice of ϕ.

The map ϕ can be reconstructed from (59) by treating $\gamma(k+1)$ as unknown.

Lemma 4.6. *Let $\gamma \subset X \setminus \mathcal{N}(\partial X)$ be a simple closed path which is longer than 2 and $v \in A_2$ be a direction. There exists a pair of simple closed, positively oriented paths $\mu_i \subset X$ and a pair of directions v_i, $i = 1, 2$ such that*

1. $y(\mu_1) \cup y(\mu_2) \subset \Omega(\gamma)$,
2. $\mathrm{vol}(\Omega(\mu_1)) + \mathrm{vol}(\Omega(\mu_2)) < \mathrm{vol}(\Omega(\gamma)) - \frac{1}{4}$,
3. $\sum_{k_1} \prod_{i_1=0}^{k_1} Q_{\mu_1}(i_1) v_1 + \sum_{k_2} \prod_{i_2=0}^{k_2} Q_{\mu_2}(i_2) v_2 = \sum_k \prod_{i=0}^{k} Q_\gamma(i) v$.

We require a lemma which provides elementary geometric assertions. Since there is no multi-scale aspect present in the proof it is omitted.

Lemma 4.7. *There exists $\alpha_0 > 0$ such that for all $\alpha \in (0, \alpha_0)$ the following assertion is true. Let $x \in X \setminus \mathcal{N}(\partial X)$ and $x' \in \mathcal{N}(x) \setminus \{x\}$. For each pair $\xi, \xi' \in A_2$ such that $|\xi - \xi'| = 1$ there exists a unique discrete imbedding $\phi : \mathcal{N}(x) \to A_2$ such that $\phi(x) = \xi$ and $\phi(x') = \xi'$. In particular, $\mathrm{conv}(y(\mathcal{N}(x))) \cap y(X) = y(\mathcal{N}(x))$.*

Proof of Lemma 4.6. Let $\phi : \mathcal{N}(\gamma(0)) \to A_2$ be a discrete imbedding such that $\phi(\gamma(0)) = 0$. Let $\widetilde{x} := \phi^{-1}(R_{\frac{\pi}{3}} \phi(\gamma(1))$, where the matrix $R_\zeta \in SO(2)$ is given by $\left(\begin{smallmatrix} \cos\zeta & -\sin\zeta \\ \sin\zeta & \cos\zeta \end{smallmatrix}\right)$.

Case I: $\widetilde{x} \notin \gamma$. Define

$$\mu_1(k) = \begin{cases} \gamma(0) & \text{if } k = 0, \\ \widetilde{x} & \text{if } k = 1, \\ \gamma(k-1) & \text{if } k \in \{2 \ldots K+1\}, \end{cases}$$

$\mu_2 = (\gamma(0))$ and $v_1 = v_2 = R_{\frac{\pi}{3}} v$. Since γ is simple, closed and positively oriented $y(\widetilde{x}) \in \Omega(\gamma)$ and in particular assertion (1) is true. Furthermore, $\mathrm{vol}(\mathrm{conv}\{y(\gamma(0)), y(\gamma(1)), y(\widetilde{x})\}) > \frac{1}{4}$ if α_0 is sufficiently small, therefore assertion (2) holds. The definition of μ_1 yields that $Q_{\mu_1}(1) = R_{-\frac{\pi}{3}}$, $Q_{\mu_1}(2) = R_{\frac{\pi}{3}} Q_\gamma(1)$. Since $R_{\frac{\pi}{3}} + R_{-\frac{\pi}{3}} = \mathrm{Id}$ a simple calculation shows that also assertion (3) holds.

Case II: $\widetilde{x} \in \gamma$. Let $K_1 := \gamma^{-1}(\widetilde{x})$ and define

$$\mu_1(k) = \begin{cases} \widetilde{x} & \text{if } k = 0, \\ \gamma(k) & \text{if } k \in \{1 \ldots K_1 - 1\}, \end{cases} \quad \mu_2(k) = \begin{cases} \gamma(0) & \text{if } k = 0, \\ \gamma(k + K_1) & \text{if } x \in \{1 \ldots K - K_1\}, \end{cases}$$

$v_1 = R_{-\frac{\pi}{3}} v$ and $v_2 = R_{\frac{\pi}{3}} v$. Like in the previous case assertions (1)-(3) can be checked by inspection. □

The following result states that in the absence of singularities it is possible to define a discrete reference configuration, i.e. for a simply connected and defect free subset $\omega \subset X$ we can find an discrete imbedding $\Phi : \omega \to A_2$.

Proposition 4.8 (Existence of a reference configuration). *There exist constants $\alpha_0, K > 0$ such that for all $\alpha \in (0, \alpha_0)$ and all domains $\Omega' \subset \Omega \subset \mathbb{R}^2$ with the properties $\operatorname{dist}(\Omega', \partial\Omega) \geq 3\operatorname{diam}(\Omega') + 2$, Ω is convex and $\Omega \cap y(\partial X) = \emptyset$ there exists a discrete imbedding $\Phi : \omega \to A_2$, where $\omega = y^{-1}(\Omega')$. Furthermore, the following assertions are true.*

(1) *Φ is unique up to rotation and translation, i.e. for each discrete imbedding Φ' : $\omega \to A_2$, there exists a rotation matrix $R \in SO(2)$ such that*

$$\Phi'(x) - \Phi'(x') = R(\Phi(x) - \Phi(x')) \quad \text{for all } x, x' \in \omega. \tag{60}$$

(2) *Φ satisfies the rigidity estimate*

$$\sup_{\{x,x'\} \subset \omega} \left| \frac{|\Phi(x) - \Phi(x')|}{|y(x) - y(x')|} - 1 \right| \leq K\alpha. \tag{61}$$

(3) *Φ is surjective in the sense that if $B(y(x), r) \subset \Omega'$ for some $x \in X$ and $r > 0$, then*

$$\Phi(\omega) \supset B(\Phi(x), \tfrac{1}{2}r) \cap A_2. \tag{62}$$

Proof. The proof is a bit lengthy but conceptually very obvious. We define the map Φ by summing along paths and show that the values $\Phi(x)$ are independent of the choice of the path. This is achieved by proving that in defect-free patches the closed paths can be deformed to a point.

Let $\Omega_2 = \{\eta \in \Omega \mid \operatorname{dist}(\eta, \partial\Omega) \geq 2\}$. We first demonstrate that for almost every $\eta \in \Omega_2$ there exists a small simplex $T \in \mathcal{T}_1$ such that $\eta \in \operatorname{int}(\operatorname{conv}(y(T)))$. It can be assumed wlog that there exists $x_0 \in y^{-1}(\Omega_2)$, otherwise the assertion is trivial. Let

$$\lambda = \{s \in [0,1] \mid (1-s)y(x_0) + s\eta \in \cup_{T \in \mathcal{T}_1} \operatorname{conv}(y(T))\}.$$

We will show now that λ is both closed and open relatively to the closed unit interval $[0,1] \subset \mathbb{R}$. λ is closed as it arises as a finite intersection of closed sets. Let $s_0 \in \partial\lambda \cap (0,1)$. By construction there exists $T_0 \in \mathcal{T}_1$ such that $y(T_0) \subset \Omega$ and $\xi = (1-s_0)y(x_0) + s_0\eta \in \partial\operatorname{conv}(y(T_0))$. Consequentially we can find $\sigma \in [0,1]$ and $x_1, x_2 \in T_0$ such that $\xi = \sigma y(x_1) + (1-\sigma)y(x_2)$. The measure of set of those points $\eta \in \mathbb{R}^2$ with the property that $\sigma = 0$ or $\sigma = 1$ is zero, therefore we can neglect the extreme cases and assume that $\sigma \in (0,1)$. By Lemma 4.7 there exists $\varepsilon > 0$ such that for all $s \in (s_0 - \varepsilon, s_0 + \varepsilon)$ we have that $(1-s)y(x_0) + s\eta \in \cup_{T \in \mathcal{T}_1} \operatorname{conv}(y(T))$, which is a contradiction to the assumption that $s_0 \in \partial\lambda \cap (0,1)$. Since λ is nonempty this implies that $\lambda = [0,1]$ and in particular

$$\Omega_2 \subset \bigcup_{T \in \mathcal{T}_1} \operatorname{conv}(y(T)). \tag{63}$$

Fix $x_1 \in y^{-1}(\Omega_2)$. We construct a path which connects x_0 and x_1. Let S be the line segment $[y(x_0), y(x_1)]$. We can assume that S intersects all edges transversally, i.e. $y(x_1) - y(x_0)$ is not a multiple of $y(x') - y(x'')$ for any $\{x', x''\} \in \mathcal{S} \setminus \{x_0, x_1\}$, otherwise, we remove the degeneracies by modifying y slightly. By the preceding consideration for almost every point $s \in S$ there exists a unique simplex $T_s \in \mathcal{T}_1$ such that $s \in \mathrm{conv}(T_s)$. We enumerate the simplices T_s in the order they intersect S; this yields a finite sequence $(T_k)_{k \in 0 \ldots K} \in \mathcal{T}_1$ with the property that $x_0 \in T_0$, $x_1 \in T_K$ and $\#(T_{k-1} \cap T_k) = 2$ for all $k = 1 \ldots K$. The connecting path γ is constructed by walking along the edges of the simplices T_k. It can be assumed wlog that γ is injective, otherwise we have to remove the loops. To construct Φ we first fix a direction $v \in A_2$ such that $|v| = 1$. Let γ be a path of length K which connects x_0 and x_1, i.e. $\gamma(0) = x_0$ and $\gamma(K) = x_1$. We define now

$$\Phi(x) := \sum_{k=0}^{K-1} \prod_{i=0}^{k} Q_\gamma(i) v, \tag{64}$$

where $Q_\gamma(i)$ is defined by (59), and demonstrate that Φ is a discrete imbedding.

It can be seen without difficulty that continuity (19) and orientation preservation (20) follow directly from the construction of Φ if for each x the value $\Phi(x_1)$ does not depend on the choice of the path γ in (64). Indeed, let $x, x' \in y^{-1}(\Omega)$ be neighbors. We choose an arbitrary path γ which connects x_0 with x_1 and set $\gamma' = (\gamma, x')$. Recall now Remark 4.5, with this particular choice of γ' we obtain

$$\Phi(x') - \Phi(x) = \phi(x'') \text{ for all } x'' \in \mathcal{N}(x), \tag{65}$$

where ϕ is the unique discrete imbedding $\mathcal{N}(x) \to A_2$ such that $\phi(x) = 0$ and $\phi(x') = \Phi(x') - \Phi(x)$. Since ϕ is a discrete imbedding equation (65) proves that Φ is continuous in the discrete sense.

Similarly we obtain orientation-preservation. Let $\{x_1, x_2, x_3\} \subset y^{-1}(\Omega_2)$ such that $\{x_1, x_2\}$, $\{x_1, x_3\}$, $\{x_2, x_3\} \in \mathcal{S}$. Since in particular $\{x_1, x_2, x_3\} \subset \mathcal{N}(x_1)$ and the previously constructed discrete imbedding ϕ satisfies by construction inequality (20) so does Φ by equation (65).

In order to show that the value $\Phi(x)$ does not depend on the path γ we assume that γ' is a different path which connects x to x_0. The path $\overline{\gamma}'$ is obtained by reversing the order of γ. Let $\gamma'' = (\gamma, \overline{\gamma}')$ be a closed path which starts and ends at x_0. It can be assumed wlog that γ'' is simple, otherwise we split it up into a collection of simple paths. We want to show that the Burgers vector of γ'' is zero. To this end we construct a sequence of paths $\gamma_{m,l} \subset X$ and directions $v_{l,m} \in A_2$, $l \in \{1 \ldots L\}$, $m \in \{1 \ldots l\}$ such that

$$y(\gamma_{l,m}) \subset \Omega(\gamma''),$$

$$\sum_{m=1}^{l} b(\gamma_{l,m}, v_{l,m}) = b(\gamma'', v), \tag{66}$$

$$\mathrm{vol}(\Omega(\gamma_{L,m})) = 0 \text{ for all } m \in \{1 \ldots L\}. \tag{67}$$

Equations (66), (67) together with Remark 4.5 show that $b(\gamma'', v) = 0$.

We set $\gamma_{1,1} = \gamma$, $v_{1,1} = v$ and determine $\gamma_{l,m}$, $v_{l,m}$ for $l > 1$ inductively. If $\mathrm{vol}(\Omega(\gamma_{l,m})) = 0$ for all $m \in \{1 \ldots l\}$ we set $L = l$ and are done. Otherwise there exists $m_* \in \{1 \ldots l\}$ such that $\mathrm{vol}(\Omega(\gamma_{l,m_*})) > 0$ and consequentially the length of γ_{l,m_*} is bigger than 2. We apply Lemma 4.6 to γ_{l,m_*} and set

$$\gamma_{l+1,m} = \begin{cases} \gamma_{l,m} & \text{if } m \in \{1 \ldots m_* - 1\}, \\ \mu_1 \text{ if} & \text{if } m = m_*, \\ \mu_2 \text{ if} & \text{if } m = m_* + 1, \\ \gamma_{l,m-1} & \text{if } m \in \{m_* + 2 \ldots l\}, \end{cases}$$

and $v_{l+1,m}$ analogous. Since both $y(\mu_1)$ and $y(\mu_2)$ are contained in $\Omega(\gamma'')$ all the paths $\gamma_{l,m}$ which are longer than 2 satisfy the assumptions of Lemma 4.6. By construction the total volume $\sum_{m=1}^{l} \mathrm{vol}(\Omega(\gamma_{l,m}))$ decreases by at least $\frac{1}{4}$ in each step, hence this procedure terminates after at most $4\mathrm{vol}(\Omega(\gamma''))$ steps.

We show now that Φ is unique in the sense of (60). If Φ' is another discrete imbedding it can be seen by exactly the same considerations that the value $\Phi'(x)$ is completely determined by $\Phi'(x_0)$ and $\Phi'(\Phi^{-1}(v))$. By Lemma 4.7 ϕ_0 and ϕ_0' differ only by a translation and a rotation.

The proof of estimates (61) and (62) is based on geometric rigidity. By Lemma 4.7 we can define for all $\eta \in \cup_{T\in\mathcal{T}_1}\mathrm{int}(\mathrm{conv}(y(T)))$ the affine map u by interpolation between the values $u(y(x)) = \Phi(x)$ for $x \in T$. By (63) the definition of u can be extended continuously to Ω_2. Clearly $u \in W^{1,\infty}(\Omega_2)$ and by Lemma 4.2 $\|\nabla u - SO(2)\|_{L^\infty(\Omega_2)} \le K\alpha$. Proposition 4.1 gives the bound

$$\sup_{\{\eta,\eta'\}\subset\Omega'} \left|\tfrac{|u(\eta)-u(\eta')|}{|\eta-\eta'|} - 1\right| \le K\alpha,$$

and in particular (61). Surjectivity (62) follows from the estimate above together with the invariance of domain theorem. □

Proof of Lemma 2.7. Let $z = \frac{1}{3}\sum_{x\in T} y(x)$, $\Omega = B(z, 20\lambda)$ and $\Omega' = B(\eta, 3\lambda)$. Proposition 4.8 implies that there exists a discrete imbedding $\Phi : y^{-1}(\Omega') \to A_2$ which

(1) coincides with Φ_T up to rotation and translation and
(2) satisfies (61).

This proves the claim. □

Proof of Proposition 2.8. (1) If $|y(x_1) - y(x_2)| \le 1 + \alpha$, then by Lemma 2.7 $T \notin \cup_{\lambda\in\Lambda\setminus\{1\}}\mathcal{T}_\lambda$.

Assume from now on that $|y(x_1) - y(x_2)| \ge 1 + \alpha$. Let $T_1, T_2 \in \cup_{\lambda\in\Lambda}\mathcal{T}_\lambda$ such that $T_1 \ne T_2$, and let for $i \in \{1,2\}$ λ_i, ω_i and Φ_i denote the associated side-lengths, domains and discrete imbeddings. We will demonstrate first that $\lambda_1 = \lambda_2$. Assume wlog that $\lambda_1 \le \lambda_2$ and let $z = \frac{1}{2}(y(x_1) + y(x_2))$. Lemma 2.7 implies that $|y(x_1) - y(x_2)| \le \frac{4}{3}\lambda_1$, $\lambda_2 \le 2\lambda_1$ and $\max_{i=1,2} |z - \frac{1}{3}\sum_{x\in T_i} y(x)| \le \lambda_2$. Let $\Omega = B(\eta, 14\lambda_1)$ and $\Omega' = B(\eta, 2\lambda_1)$. The assumptions imply that $\omega := y^{-1}(\Omega) \subset \omega_1 \cap \omega_2$ and $\{x_1, x_2\} \subset \omega$. By Proposition 4.8 there exists a discrete imbedding $\Phi : y^{-1}(\Omega') \to A_2$ and matrices $Q_1, Q_2 \in SO(2)$ such that

$$\Phi(x') - \Phi(x_1) = Q_1(\Phi_1(x') - \Phi_1(x_1)) = Q_2(\Phi_2(x') - \Phi_2(x_1))$$

for all $x' \in \omega$. The choice $x' = x_2$ establishes that $\lambda_1 = \lambda_2$. Let now $T_3 \in \mathcal{T}_\lambda$ such that $\{x, x'\} \subset T_3$. It will be demonstrated that T_3 necessarily either coincides with T_1 or with T_2.

By the same argumentation used above we can assume that $\Phi_3(x) = \Phi(x)$ for all $x \in \omega$. Let $\{x_3\} = T_3 \setminus \{x_1, x_2\}$. The lattice point $\eta = \Phi(x_3) \in A_2$ solves the equation

$$|\eta - \Phi(x_1)| = |\eta - \Phi(x_2)| = \lambda. \tag{68}$$

Proposition 4.8 entails that $A_2 \cap B(\Phi(x_1), \lambda) \subset \Phi(y^{-1}(B(y(x_1), \frac{4}{3}\lambda)))$ and consequentially $\eta \in \Phi(\omega)$. In two dimensions (68) has at most two solutions which are exhausted by $\eta \in \Phi((T_1 \cup T_2) \setminus \{x_1, x_2\})$, therefore T_3 necessarily either agrees with T_1 or with T_2.

(2) For $\lambda = 1$ the claim follows from Lemma 4.7. If $\lambda > 1$ let $\Omega = B(z, 28|y(x_1) - y(x_2)|)$ and $\Omega' = B(z, 5|y(x_1) - y(x_2)|)$, where $z = \frac{1}{2}(y(x_1) + y(x_2))$. Proposition 4.8 implies that there exists a discrete imbedding $\Phi : y^{-1}(\Omega') \to A_2$ such that $B(\Phi(x_1), \lambda) \cap A_2 \subset \Phi(\omega)$, where $\lambda = |\Phi(x_1) - \Phi(x_2)|$. Let $\eta_\pm = \Phi(x_1) + Q_\pm(\Phi(x_2) - \Phi(x_1))$ where $Q_\pm$ is the rotation by $\frac{2\pi}{3}$ in the clockwise (+) and counter-clockwise (-) direction. Since A_2 is invariant under $Q_\pm$ we obtain that $\eta_\pm \in A_2$. By (62) $\eta_\pm \in \Phi(y^{-1}(\Omega))$ hence there are two preimages $x_\pm = X$. Set now $T_\pm = \{x_1, x_2, x_\pm\}$, $\omega_\pm = y^{-1}(\Omega)$. By construction both simplices $T_\pm$ satisfy (23). Estimate (61) implies that $|\frac{1}{3}\sum_{x \in T_\pm} y(x) - y(x_1)| \leq \lambda$, hence the inclusion (24) is satisfied.

(3) This claim follows directly from Proposition 2.8.2.

□

Proof of Proposition 2.9. We first establish estimate (26). Let for each $x \in X$ and $\lambda \in \Lambda$

$$s(x, \lambda) = \#\{T \in \mathcal{T}_\lambda \mid x \in T\}$$

be the number of simplices with side length λ which have x as a corner. We start with the identity

$$\sum_{x \in X} s(x, \lambda) = 3\#\mathcal{T}_\lambda, \tag{69}$$

which expresses the trivial fact that the sum the of number of books read by each member of a group can also be computed by adding the number of readers of each book. We will demonstrate that for each $x \in X$

$$s(x, \lambda) \leq m(\lambda) s(x, 1). \tag{70}$$

This claim is trivial if $s(x, \lambda) = 0$. Let $\mathcal{T}(x, \lambda) = \{T \in \mathcal{T}_\lambda \mid x \in T\}$ and set $\Omega = B(y(x), 28\lambda)$, $\Omega' = B(y(x), 4\lambda)$ and $\omega = y^{-1}(\Omega')$. The definition of T entails that $\Omega \cap y(\partial X) = \emptyset$, hence the prerequisites of Proposition 4.8 are satisfied and we can construct a discrete imbedding $\Phi : \omega \to A_2$. In particular, we obtain that $s(x, 1) = 6$. For any other simplex $T' \in \mathcal{T}(x, \lambda)$ we set $\{x_1, x_2\} = T' \setminus \{x\}$. Lemma 2.7 implies that $T' \subset \omega$ and by uniqueness of Φ we can find a rotation matrix $R \in SO(2)$ such that $\Phi_{T'}(x_1) - \Phi_{T'}(x_2) = R(\Phi(x_1) - \Phi(x_2))$. This implies that $|\Phi(x_1) - \Phi(x_2)| = \lambda$. The number of pairs $\{\eta_1, \eta_2\} \subset A_2$ which satisfies the equations $|\eta_1 - \Phi(x)| = |\eta_2 - \Phi(x)| = |\eta_1 - \eta_2|$ can be expressed as $\#(\{|\eta - \Phi(x)| = \lambda\} \cap A_2)$, together with formula (21) this implies that $s(x, \lambda) \leq 6m(\lambda)$ which yields the bound (70).

For the other direction we apply again Proposition 2.8.2 and deduce that for each $x \in X$ with the property that $s(x, \lambda) < 6m(\lambda)$ there exists $x_b \in \partial X$ such that $y(x_b) \in B(y(x), 28\lambda)$. Since the minimum distance between particles is bounded from below by $\frac{1}{2}$ (Lemma 2.2) we have the bound

$$\#y^{-1}(B(y(x_b), 28\lambda)) \leq C\lambda^2. \tag{71}$$

By (18) and (70) we obtain that the number of simplices in $\mathcal{T}_\lambda$ which have at least one corner lying in $B(y(x_b), 28\lambda)$ is bounded by $C\lambda^2 m(\lambda)$.

To prove (27) we associate to each $T \in \mathcal{T}_\lambda$ and $S \in \mathcal{T}_1$ the geometry factor

$$\mu(S, T) = \frac{\text{meas}\,(\text{conv}(y(S)) \cap \text{conv}(y(T)))}{\text{meas}(\text{conv}(y(S)))} \in [0, 1], \quad n(S, \lambda) = \sum_{T \in \mathcal{T}_\lambda} \mu(S, T) \in [0, \lambda^2 m(\lambda)].$$

If $\text{dist}(y(S), y(\partial X)) > 2\lambda$ we can define $\omega = y^{-1}(B(y(x), 4\lambda))$ as before and obtain the existence of a discrete imbedding $\Phi : \omega \to A_2$ by applying Proposition 4.8. There are precisely $6m(\lambda)$ different sets $\{\eta_1, \eta_2, \eta_3\} \subset A_2$ such that $\eta_1 = \Phi(x)$, $|\eta_i - \eta_j| = \lambda$ for $i \neq j$. This implies that

$$n(S, \lambda) \leq m(\lambda)\lambda^2 \tag{72}$$

with equality if $\mathrm{dist}(y(S), y(\partial X)) > 20\lambda$. This shows that for each $\lambda \in \Lambda$

$$\begin{aligned}\sum_{T\in\mathcal{T}_\lambda} \mathrm{meas}(\mathrm{conv}(y(T))) &\overset{Lemma\ 2.7}{=} \sum_{T\in\mathcal{T}_\lambda}\sum_{S\in\mathcal{T}_1} \mathrm{meas}(\mathrm{conv}(y(S)) \cap \mathrm{conv}(y(T))) \\ &= \sum_{S\in\mathcal{T}_1}\sum_{T\in\mathcal{T}_\lambda} \mu(S,T)\mathrm{meas}(\mathrm{conv}(y(S))) = \sum_{S\in\mathcal{T}_1} n(S,\lambda)\mathrm{meas}(\mathrm{conv}(y(S))) \\ &\leq m(\lambda)\lambda^2 \sum_{S\in\mathcal{T}_1} \mathrm{meas}(\mathrm{conv}(y(S)))\end{aligned}$$

by (72). For the opposite direction we use that $n(S, \lambda) = m(\lambda)\lambda^2$ if $\mathrm{dist}(y(S), y(\partial X)) > 2\lambda$ and obtain that

$$\begin{aligned}&\geq \lambda^2 m(\lambda)\Bigg(\sum_{S\in\mathcal{T}_1} \mathrm{meas}(\mathrm{conv}(y(S))) - \sum_{\substack{S\in\mathcal{T}_1 \\ \mathrm{dist}(y(S),y(\partial X))\leq 28\lambda}} \mathrm{meas}(\mathrm{conv}(y(S)))\Bigg) \\ &\geq \lambda^2 m(\lambda)\left(\sum_{S\in\mathcal{T}_1} \mathrm{meas}(\mathrm{conv}(y(S))) - C\lambda^2 \#\partial X\right).\end{aligned}$$

The last inequality is due to the fact that for each $x \in \partial X$ there are at most $C\lambda^2$ simplices with side length 1 within a disk of radius λ^2.

Proof of (28). This follows directly from (70) and (71). □

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