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On the Crystallization of 2D Hexagonal Lattices

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Dedicated with admiration to Professor Tom Spencer on occasion of his 60th birthday

Abstract: It is a fundamental problem to understand why solids form crystals at zero temperature and how atomic interaction determines the particular crystal structure that a material selects. In this paper we focus on the zero temperature case and consider a class of atomic potentials $V = V_2 + V_3$, where V_2 is a pair potential of Lennard-Jones type and V_3 is a three-body potential of Stillinger-Weber type. For this class of potentials we prove that the ground state energy per particle converges to a finite value as the number of particles tends to infinity. This value is given by the corresponding value for a optimal hexagonal lattice, optimized with respect to the lattice spacing. Furthermore, under suitable periodic or Dirichlet boundary condition, we show that the minimizers do form a hexagonal lattice.

1. Introduction

One of the major open problems in the study of matter is to understand why solids are crystalline at zero temperatures [12]. Mathematically speaking, the crystallization problem can be stated as follows. Given a set of N atoms interacting through some potential $V(\{y_i\})$ (y_i is the position of the atom i), consider the minimization problem

$$\min_{y_N:\{1,\dots,N\}\to\mathbb{R}^d} V(\{y_i\}).$$

Under some natural assumptions on the potential V, we want to characterize the limiting configuration of the ground state minimizers (if they exist) as the number of particles tends to infinity. When some suitable boundary conditions are imposed, one would like to show that the minimizers form a translated and rotated copy of the perfect crystal lattice. In this natural sense the crystal structure is the preferred phase for solids at the zero temperature.

There are many theoretical results in the one-dimensional case. For rather general molecular models with a wide variety of two-body interaction potentials including the usual Lennard-Jones potential, it can be shown that the ground state is unique and approaches uniform spacing in the infinite-particle limit. We refer the readers to [1,3,8,10–12,15–17] and the references therein for reviews and more extensive references. We remark that there are examples of potentials constructed by Ventevogel [15], Nijboer and Ruijgrok [18] for which energy ground states are not equally spaced. Hamrick and Radin [4] showed that even if a 1D compactly supported two-body potential has periodic ground states, an arbitrary small C^1 perturbation of the potential can have only *aperiodic* ground states. An interesting $1d$ quantum mechanical model, in which the nuclei are treated classically and the electrons are treated quantum mechanically, is studied in [1].

Contrary to the $1d$ case, there are only, a few results in dimension $d \geq 2$. Heitman and Radin [5] considered the following "sticky" potential:

$$V(r) = \begin{cases} +\infty, & 0 \leq r < 1, \\ -1, & r = 1, \\ 0, & r > 1. \end{cases}$$

They proved that the ground states for the sticky potential are necessarily crystalline. Radin [9] also constructed a piecewise-affine potential of the form:

$$V(r) = \begin{cases} +\infty, & 0 \leq r < 1, \\ 24r - 25, & 1 \leq r < \frac{25}{24}, \\ 0, & \frac{25}{24} \leq r < \infty. \end{cases}$$

For this special potential he proved by using geometric arguments that the ground states have uniform bond length and form a triangular lattice in the infinite-particle limit. These potentials are usually called hard-core interactions ($V(r) = +\infty$ if $r \in [0, \rho_0]$ for some $\rho_0 \in [0, 1-\alpha]$). It is natural to ask whether one can extend these results to more realistic potentials. In general this is a rather difficult question due to the lack of mathematical tools and especially the fact that one has to treat short-range and long-distance[1] interactions simultaneously. However recently for a one-parameter family of pair potentials mimicking the behavior of the usual Lennard-Jones potential, Theil [14] proved that the ground state minimizers for this class are given by the usual triangular lattice (more precisely they form a translated, rotated and dilated copy of the triangular lattice). This striking result accords with earlier extensive numerical results on the Lennard-Jones potential (see [19] and references therein). Theil's proof was based on a recently discovered rigidity estimate and a so-called resummation technique. By using these tools he was able to sum the long-distance interactions and extract the main part in terms of a renormalized potential. We follow closely Theil's method in this paper. Specifically we will consider the $2D$ hexagonal lattice (see Fig. 1). In order not to confuse the readers, we first explain a bit the difference between the 2D triangular lattice and the 2D hexagonal lattice.

Terminology. The 2D triangular lattice (or sometimes called the equilateral triangular lattice) is one of the five 2D Bravais lattices in which each lattice point has 6 nearest neighbors. It has closed packed structure and admits 6-fold symmetries. On the other hand, the hexagonal lattice is a complex lattice where each lattice point has only 3 nearest

[1] In the common mathematical physics literature, potentials which decay no faster than r^{-1} (r is the distance) are called long-range interactions. In this paper long-distance interactions refer to potentials which decay *faster* than r^{-C}, where $C > 1$ is some constant. We thank the anonymous referee for bringing our attention to this point.

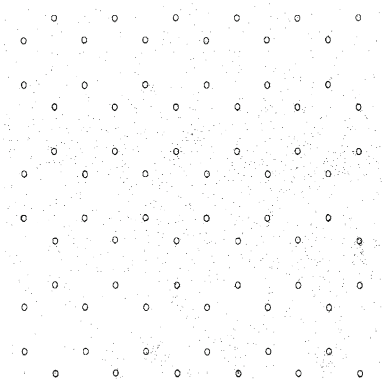

Fig. 1. The hexagonal lattice Hex

neighbors. The hexagonal lattice has an open structure and admits 3-fold symmetries. One realistic example of a hexagonal lattice is the 2D graphite sheet.

We remark that the ground states of Lennard-Jones type potentials which was considered by Theil usually have closed packed structures. To obtain an open structure such as the hexagonal lattice considered here, one can add a suitable 3-body potential to the Lennard-Jones potential so that local bond angles become different from the triangular lattice. Indeed, our main result is, roughly speaking, that for a class of potentials of the form $V = V_2 + V_3$, where V_2 is of Lennard-Jones type and V_3 is the three-body Stillinger-Weber potential (see below), the ground state in the infinite-particle limit is given by the hexagonal lattice. As we shall explain at the end of this introduction, new difficulties arise due to the special nature of the hexagonal lattice.

1.1. Formulation of the main results. Throughout this paper we will use Hex to denote the perfect hexagonal lattice in $\mathbb{R}^2$. To fix notations, we choose a basis such that

$$Hex = \{\xi = ma_1 + na_2 + lb : \ m, n \in \mathbb{Z}, l = 0 \text{ or } 1\},$$

where $a_1 = (\sqrt{3}, 0)$, $a_2 = (\frac{\sqrt{3}}{2}, \frac{3}{2})$, $b = (\sqrt{3}, 1)$. We study the ground state of N particles with interaction potential

$$V(\{y_1, \cdots, y_N\}) = \frac{1}{2}\sum_{i,j} V_2(|y_i - y_j|) + \frac{1}{2}\sum_{i,j,k} V_3(y_i, y_j, y_k).$$

Here V_3 is the 3-body potential. We choose the so-called Stillinger-Weber potential with bond angle θ_{jik} centered at y_i (see Fig. 2):

$$V_3(y_i, y_j, y_k) = \beta f_{a,b}(|y_i - y_j|) f_{a,b}(|y_i - y_k|)(\cos\theta_{jik} + 1/2)^2. \tag{1.1}$$

Note that $V_3(y_i, y_j, y_k) = V_3(y_i, y_k, y_j)$. Due to this symmetry the factor $1/2$ is needed in the sum over (i, j, k). The cut-off function $f_{a,b}(\cdot)$ is defined as follows:

$$f_{a,b}(r) = \begin{cases} \exp\{b/(r-a)\}, & 0 < r < a; \\ 0, & r \geq a. \end{cases}$$

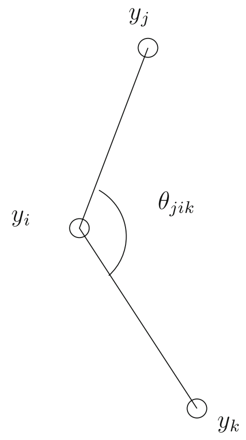

Fig. 2. The bond angle θ_{jik}

Here the parameter a is called the cut-off distance and is usually set to be between the first and second nearest neighbors (of the lattice to be generated). For the 2D Hexagonal lattice, if we take the equilibrium lattice spacing $a_0 = 1$, then it suffices to take $a \in (1, \sqrt{3})$. The form of the cut-off function $f_{a,b}$ is not of particular importance and other functions can be used. The parameters β and b control the strength of the potential. We now state the needed assumptions on the potential V.

Assumption 1.1. Let $0 < \alpha < \frac{1}{12}$ be a parameter and $\gamma > 6$ be a fixed constant. The two-body potential $V_2 = V_2(r; \alpha) : [0, \infty) \to [0, \infty)$ satisfies the following:

(1) $V_2 \in C^2(1 - \alpha, \infty)$
(2) $V_2 > \frac{1}{\alpha}$, for $r \leq 1 - \alpha$,
(3) $V_2'' \geq 1$ for $r \in (1 - \alpha, 1 + \alpha)$,
(4) $V_2(r) \geq -\alpha$ for $r \in [1 + \alpha, \frac{3}{2})$,
(5) $|V_2''(r)| \leq \alpha r^{-\gamma}$ for $r > \frac{3}{2}$,
(6) V_2 is normalized in the sense that $\lim_{r\to\infty} V_2(r) = 0$ and

$$\min_{r\geq 0} \sum_{0\neq\xi\in Hex} V_2(r|\xi|) = \sum_{0\neq\xi\in Hex} V_2(|\xi|) = -3.$$

See Fig. 3 for a schematic drawing of V_2. The three-body potential V_3 is the Stillinger-Weber potential (see (1.1)). We fix a, b and let β be an adjustable parameter. In this sense the total potential $V = V_2 + V_3$ forms a two-parameter (α and β) family of functions.

Our first theorem states that the energy per particle converges to a finite value in the thermodynamic limit.

Theorem 1.2 (Main theorem). *There exist constants* $\alpha_0 \in (0, \frac{1}{12})$, $\beta_0 > 0$ *such that the following holds for any* $0 < \alpha < \alpha_0$, $\beta > \beta_0$, $L \in \mathbb{N}$, *and any potential* V *satisfying Assumption 1.1:*

$$\lim_{N\to\infty} \min_{y:X_N\to\mathbb{R}^2} \frac{1}{N} V(\{y_1, \ldots, y_N\}) = -\frac{3}{2}.$$

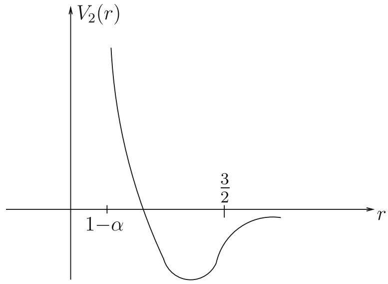

Fig. 3. The potential energy V_2

The value $-3/2$ is the value given by the optimal hexagonal lattice.

The next theorems are on the characterization of the ground states. Due to possible formation of surface layers suitable boundary conditions have to be imposed. The first result concerns the periodic boundary condition.

Theorem 1.3 (Ground states with periodic boundary conditions)**.** *There exist constants* $\alpha_0 > 0$, $\beta_0 > 0$ *such that the following holds for any* $0 < \alpha < \alpha_0$, $\beta > \beta_0$, $L \in \mathbb{N}$, *and any potential* V *satisfying Assumption 1.1: For any ground state* $y_{min} : Hex \to \mathbb{R}^2$ *of*

$$E_L^{per}(\{y\}) := \sum_{\substack{x \in Hex \cap Q_L \\ x' \in Hex \setminus \{x\}}} V_2(|y(x) - y(x')|) + \sum_{\substack{x_1 \in Hex \cap Q_L \\ x_2 \in Hex \setminus \{x_1\} \\ x_3 \in Hex \setminus \{x_1, x_2\}}} V_3(y(x_1), y(x_2), y(x_3)),$$

subject to the boundary condition:

$$y \in Y_L^{per} := \left\{ y : Hex \to \mathbb{R}^2 | y(x) - y(x') = x - x' \text{ if } x - x' \in LHex \right\},$$

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

$$\{y_{min}(x) + \tau | x \in Hex\} = Hex.$$

The following corollary establishes that the hexagonal lattice as the ground state of our potential is stable in the sense of compact perturbations. One can also regard this as a Dirichlet boundary value problem.

Corollary 1.4 (Stability against compactly supported perturbations) *Let the assumptions of Theorem 1.2 be satisfied and assume that* $\mathcal{A} \subset Hex$ *is an arbitrary but finite set. If* $y_{min} : Hex \to \mathbb{R}^2$ *is a ground state of the minimization problem*

$$E_{\mathcal{A}}(\{y\}) = \sum_{\substack{\{x, x'\} \subset Hex \\ \{x, x'\} \cap \mathcal{A} \neq \emptyset}} V_2(|y(x) - y(x')|) + \sum_{\substack{\{x_1, x_2, x_3\} \subset Hex \\ \{x_1, x_2, x_3\} \cap \mathcal{A} \neq \emptyset}} V_3(y(x_1), y(x_2), y(x_3)),$$

subject to the Dirichlet constraint:

$$y \in Y_{\mathcal{A}}^{Dir} = \left\{ y : Hex \to \mathbb{R}^2 | y(x) = x \text{ for all } x \in Hex \setminus \mathcal{A} \right\},$$

then we have

$$\{y_{min}(x) | x \in Hex\} = Hex.$$

1.2. Outline of the proof. By constructing suitable trial configurations (e.g. use a N-atom subset of the perfect hexagonal lattice Hex which does not create too much surface energy), it is not difficult to prove the upper bound

$$\limsup_{N\to\infty} \min_{y:X_N\to\mathbb{R}^2} \frac{1}{N} V(\{y_1,\ldots,y_N\}) \le -\frac{3}{2}.$$

Therefore the bulk of the analysis is devoted to proving the lower bound. This consists of several steps.

Step 1. Characterization of the local structure of the ground states. In this step, by carefully adjusting the strength of the two-body and three-body potential, one can show that for ground states particles are well-separated and have uniform bond angle locally. This leads further to the notion of regular and defected atoms (see Definition 3.3), the splitting of good and bad pairs (see (4.8), (4.9)). The neighborhood of regular atoms can be mapped into the perfect Hex lattice 1-1 and onto locally through a discrete imbedding. The contribution of the good pairs and bad pairs will be estimated separately in the following steps.

Step 2. Resummation of the two-body potential energy V_2.[2] In this step one sums up the contribution of all pairs to V_2 in an orderly fashion which we now describe. The main contribution is from good pairs. The bad pairs will be treated as remainder terms. For any good pair, one can show that it belongs uniquely to the side edge of two deformed hexagons (see Definition 4.1) sharing a common edge. Therefore the total contribution of the good pairs can be summed at the level of deformed hexagons. For deformed hexagons, by using the volume form which is additive, one can then Taylor expand and sum up the linear part of the two-body energy, giving rise to the renormalized potential energy V_* (see (4.2)). The quadratic error term from the Taylor expansion along with the contribution of the bad pairs are the error terms which will be treated in Step 3.

Step 3. Estimate and resummation of the error terms. The error terms from Step 2 consist of 4 types.

(1) Contribution due to bad pairs. This will be estimated as surface terms (see Lemma 6.1).
(2) Contribution due to quadratic variations of good pairs which are not nearest neighbors. This can be re-summed using our two-scale distortion estimate (Proposition 10.6) which will be bounded by quadratic variations of nearest and second nearest neighbors.
(3) Contribution due to quadratic variations of second nearest neighbors. This term arises due to the simple fact that the area of a hexagon is not uniquely determined by its side lengths, or more precisely, one has to further specify the internal angles or chord lengths. We use the three-body angular potential together with the quadratic variation of nearest neighbors to take care of this term (see Lemma 6.4).
(4) Contribution due to quadratic variation of nearest neighbors. We deal with this term by using the uniform convexity assumption on the renormalized potential energy (see (4.3)), and also the combinatorial Lemma 3.5.

After all these considerations, we are led to the following bound:

$$V \ge -\frac{3}{2}N + (\frac{3}{2} - C\alpha)\#\partial X_N + \sum_{\{x,x'\}\in\mathcal{S}} \frac{\theta}{4}(|y(x) - y(x')| - 1)^2,$$

[2] Since the three-body potential V_3 is short-ranged, no resummation is needed for V_3.

where C, θ are constants. By taking α sufficiently small, we obtain the desired lower bound.

As noted earlier, the arguments presented here are closely modelled on [14], which treated the case of the 2D Lennard-Jones potential having the triangular lattice as the ground state minimizer. The main difficulty in extending this result to the case of the hexagonal lattice is in the resummation step and the estimate of quadratic variations. We overcome these difficulties by performing a two-scale resummation of the two-body potential energy and a two-scale distortion estimate. This yields a lower bound of the two-body potential energy in terms of the sum of the renormalized potential energy, the surface term and the quadratic variations in nearest and second nearest neighbors. Since the three-body potential V_3 is nonnegative, we can use the strength of the angular potential V_3 together with quadratic variations of the nearest neighbors to control the quadratic variations in second nearest neighbors. By using a combinatorial lemma and the uniform convexity of the renormalized potential energy, we are able to obtain the desired lower bound on the total potential energy.

1.3. Notations and organization of the paper. We will use the shorthand $e(\{x, x'\})$ to denote $V(|y(x)-y(x')|)$ and similarly $e_*(\{x, x'\})$ for $V_*(|y(x)-y(x')|)$. $B(\eta, r)$ denotes the closed ball centered at $\eta \in \mathbb{R}^2$ with radius r. The letter $\mathcal{P}$ denotes the set of all possible pairs, i.e. $\mathcal{P} = \left\{\{x, x'\} \subset X_N\right\}$. The letter $\mathcal{S} = (y_N)$ denote the set of short-range range pairs, i.e.

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

We sometimes use the letter C to denote generic constants which does not depend on N or α.

This paper is organized as follows. The local structure theorems are proved in Sect. 2. Sections 3 and 4 introduce discrete imbeddings, deformed hexagons and partition pairs. Section 5 contains the key step of the proof: resummation of the two-body potential energy V_2. Sections 6 and 7 consist of the proof of Theorem 1.2, Theorem 1.3 and Corollary 1.4. Finally more technical estimates are collected in the Appendix.

2. Local Structure Theorems: Minimum Distance and Uniform Bond Angle

Throughout this section we will relax our assumptions on the potential $V = V_2 + V_3$. We shall state the minimal conditions on the potential so that the local structure theorems (see below) hold true.

Definition 2.1. *The three body potential $V_3(y_i, y_j, y_k)$ is said to be short-ranged if for some constant $\kappa > 0$, $V_3(y_i, y_j, y_k) = 0$ whenever all three conditions $|y_i - y_j| > \kappa$, $|y_i - y_k| > \kappa$, $|y_j - y_k| > \kappa$ hold.*

Remark 2.2. The above condition is rather weak. It simply says that the three body potential is only effective on the triples such that one of the mutual distance is less than κ. In fact as we shall see below, Lemma 2.3 remains true even if we only assume that V_3 decays at infinity.

We are now ready to prove a local structure theorem for ground states. It states that the interatomic distance of ground states has a natural lower bound. A similar proposition was proved in [14] for V_2 being of Lennard-Jones type. For the exact Lennard-Jones potential, a more quantitative version with explicit constants can be found in [19]. An interesting upper bound is also proved there.

Lemma 2.3 (*Minimum distance*). *Assume that for some constants $C_1 > 0$, $\kappa > 2$, the two-body potential V_2 satisfies*

$$V_2(r) \begin{cases} \geq \frac{1}{\alpha}, & \text{if } 0 < r < 1-\alpha \\ \geq -\frac{C_1}{r^\kappa}, & \text{if } r \geq 1-\alpha. \end{cases}$$

and V_2 decays at the infinity:

$$\lim_{r\to\infty} V_2(r) = 0.$$

Assume that the three-body potential V_3 is short-ranged and nonnegative. Then there exists a constant $\alpha_0 = \alpha_0(C_1, \kappa) \in (0, \frac{1}{3})$ such that if $0 < \alpha < \alpha_0$, then any ground state $y_N : X_N \to \mathbb{R}^2$ of $V = V_2 + V_3$ satisfies

$$\min_{x\neq x'} |y(x) - y(x')| > 1 - \alpha. \tag{2.1}$$

Remark 2.4. Since by assumption V_3 is nonnegative and V_2 can be arbitrarily large near $r = 0$ (by adjusting the parameter α), it is not surprising that V_2 alone controls the minimum interatomic distance of the ground state.

Proof. Define $M := \max_{\eta\in\mathbb{R}^2} \# \left(y(X_N) \cap B(\eta, \frac{1}{2}(1-\alpha))\right)$. It suffices to show $M = 1$. WLOG assume the maximum is achieved at $\eta = 0$ and set $B_M = B(0, \frac{1}{2}(1-\alpha))$, $\mathcal{A} = y^{-1}(B_M)$. The set $\mathcal{A}$ contains particles whose mutual distance is at least $1-\alpha$. Since by assumption $V_2(r) \geq \frac{1}{\alpha}$ for $r \leq 1-\alpha$, we have

$$\sum_{p\subset\mathcal{A}} e(p) \geq \frac{1}{2\alpha} M(M-1).$$

Denote by $V_3(\mathcal{A})$ the total three-body potential generated by triples of atoms in $\mathcal{A}$, then since $\#\mathcal{A} = M$, we have by assumption

$$V_3(\mathcal{A}) \geq 0.$$

Denote by $V_3(\mathcal{A}, X_N\backslash\mathcal{A})$ the total three-body potential generated by triples of atoms $\{x_1, x_2, x_3\}$ such that $\{x_1, x_2, x_3\} \cap \mathcal{A} \neq \emptyset$, $\{x_1, x_2, x_3\} \cap (X_N\backslash\mathcal{A}) \neq \emptyset$. By assumption we have also

$$V_3(\mathcal{A}, X_N\backslash\mathcal{A}) \geq 0.$$

Now if we move the positions $y(\mathcal{A})$ to infinity in such a way that the mutual distances diverge, then since $\lim_{r\to\infty} V_2(r) = 0$ and V_3 is short-ranged, we have

$$\begin{aligned}\sum_{\substack{x\in\mathcal{A}\\ x'\in X_N\backslash\mathcal{A}}} e(\{x, x'\}) &\leq -\frac{1}{2\alpha} M(M-1) - V_3(\mathcal{A}) - V_3(\mathcal{A}, X_N\backslash\mathcal{A}) \\ &\leq -\frac{1}{2\alpha} M(M-1). \end{aligned} \tag{2.2}$$

The next step is to estimate the LHS of the above inequality. Let $n(k) = \#y^{-1}((k+1)B_M \backslash kB_M)$. For $k \geq 3$, if $x \in \mathcal{A}$ and $y(x') \in (k+1)B_M \backslash kB_M$, then $|y(x) - y(x')| \geq \frac{(k-1)}{2}(1-\alpha) \geq 1-\alpha$, this yields

$$\sum_{\substack{x\in\mathcal{A} \\ y(x')\in(k+1)B_M\backslash kB_M}} e(\{x, x'\}) \geq -n(k)\cdot M \cdot \frac{C_1}{\left(\frac{k-1}{2}(1-\alpha)\right)^{\kappa}}. \tag{2.3}$$

On the other hand, for $k = 1, 2$, $x \in \mathcal{A}$ and $y(x') \in (k+1)B_M \backslash kB_M$, it is possible that $|y(x) - y(x')| \leq 1-\alpha$ for some pairs x, x'. In this case since $V_2(r) \geq 0$ for $r \leq 1-\alpha$, we simply neglect these pairs and count those for which $|y(x) - y(x')| \geq 1-\alpha$. Thus we obtain the estimate for $k = 1, 2$,

$$\sum_{\substack{x\in\mathcal{A} \\ y(x')\in(k+1)B_M\backslash kB_M}} e(\{x, x'\}) \geq -n(k)\cdot M \cdot \frac{C_1}{(1-\alpha)^{\kappa}}. \tag{2.4}$$

Adding (2.3) and (2.4), we obtain

$$\sum_{\substack{x\in\mathcal{A} \\ x'\in X_N\backslash\mathcal{A}}} e(\{x, x'\}) \geq -MC_1\left(\frac{4}{1-\alpha}\right)^{\kappa}\sum_{k=1}^{\infty}\frac{n(k)}{k^{\kappa}}. \tag{2.5}$$

To estimate $n(k)$, observe that for each k, the thickness of the ring $(k+1)B_M \backslash kB_M$ is $(1-\alpha)/2 < 1/2$. There exists a universal constant $C > 0$ such that the ring is covered by $C \cdot k$ translated copies of $B(0, 1/3)$; this gives $n(k) \leq CMk$. By (2.2) and (2.5), we have

$$-M^2CC_1\left(\frac{4}{1-\alpha}\right)^{\kappa}\sum_{k=1}^{\infty}\frac{1}{k^{\kappa-1}} \leq -\frac{1}{2\alpha}M(M-1). \tag{2.6}$$

Now if we take α_0 such that

$$CC_1 6^{\kappa}\sum_{k=1}^{\infty}\frac{1}{k^{\kappa-1}} = \frac{1}{4\alpha_0},$$

then clearly for $\alpha < \alpha_0$, the above inequality only has the solution $M = 1$. The lemma is proved. □

The next lemma states that if the three-body potential V_3 is sufficiently strong, then any ground state of $V = V_2 + V_3$ has uniform bond angle. The term bond angle is understood in the natural sense. To make things precise we introduce the following definition.

Definition 2.5 (*Bond and Bond angle*)**.** *Two atoms x, x' are said to be α-bonded (w.r.t. the configuration $y : X_N \to \mathbb{R}^2$) if $1-\alpha \leq |y(x) - y(x')| \leq 1+\alpha$. For any triple x_0, x_1, x_2, assume x_1, x_0 is α-bonded and x_2, x_0 is α-bonded. Then the bond angle of $\{x_0, x_1, x_2\}$ with center at x_0 is defined as the unique angle $\theta \in [0, \pi]$ such that $\cos\theta = \frac{(y(x_1)-y(x_0))\cdot(y(x_2)-y(x_0))}{|y(x_1)-y(x_0)|\cdot|y(x_2)-y(x_0)|}$. Sometimes we write θ as $\theta_{x_1x_0x_2}$.*

To control local bond angles, it is necessary to consider the explicit form of V_3. We shall prove the following lemma for V_3 being of the Stillinger-Weber type (1.1). Similar lemmas can be proven for other potentials with necessary modifications.

Lemma 2.6 (*Uniform bond angle*). *Assume V_2 satisfies the hypothesis in Lemma 2.3 with the parameter $\alpha < \alpha_0$. Let V_3 be the Stillinger-Weber potential* (1.1) *with the cut-off distance $1 < a < \sqrt{3}$ and β being the adjustable parameter. Assume $\alpha_0 < a - 1$. Then there exist constants $\beta_0 = \beta_0(C_1, \kappa, a, b) > 0$, $C_3 = C_3(C_1, \kappa, a, b) > 0$, such that if $\beta > \beta_0$, the following holds for any ground state of $V = V_2 + V_3$:*

If $\{x_0, x_1, x_2\}$ is such that x_0, x_1 is α-bonded and x_0, x_2 is α-bonded, then the bond angle θ satisfies

$$\left|\theta - \frac{2\pi}{3}\right| \le \frac{C_3}{\sqrt{\beta}}.$$

Proof. Let $\{x_0, x_1, x_2\}$ be such that both x_0, x_1 and x_0, x_2 are α-bonded. Let $V_2(x_0, X_N\backslash x_0)$ and $V_3(x_0, X_N\backslash x_0)$ denote the contribution to the total two-body or three-body potential due to x_0. If we move $y(x_0)$ to infinity (this corresponds to removing the particle x_0 from the system), then by the minimizing property of the ground state, we have

$$V_2(x_0, X_N\backslash x_0) + V_3(x_0, X_N\backslash x_0) \le 0. \tag{2.7}$$

To estimate $V_3(x_0, X_N\backslash x_0)$, note that V_3 is always positive, therefore $V_3(x_0, X_N\backslash x_0) \ge V_3(y(x_0), y(x_1), y(x_2))$. Since $\alpha_0 < a - 1$, by the definition of the Stillinger-Weber potential (1.1) we have

$$V_3(y(x_0), y(x_1), y(x_2)) \ge \beta \cdot e^{\frac{2\gamma}{1+\alpha_0-\alpha}} (\cos\theta + \frac{1}{2})^2. \tag{2.8}$$

On the other hand, the term $V_2(x_0, X_N\backslash x_0)$ can be estimated by the same method as in Lemma 2.3 (see (2.5)):

$$V_2(x_0, X_N\backslash x_0) \ge -CC_1 \cdot 6^\beta \sum_{k=1}^{\infty} \frac{1}{k^{\beta-1}}. \tag{2.9}$$

From (2.7), (2.8), (2.9), we have

$$(\cos\theta + \frac{1}{2})^2 \le \frac{C_2}{\beta},$$

where C_2 is some constant depending on (C_1, κ, a, b). Since by definition $0 \le \theta \le \pi$, this gives us for $\beta > \beta_0$ with β_0 sufficiently large:

$$|\theta - \frac{2\pi}{3}| \le \frac{C_3}{\sqrt{\beta}}.$$

The lemma is proved. □

Corollary 2.7 (*Minimum distance and uniform bond angle*). *There exist positive numbers $\alpha_0, \beta_0, C > 0$, such that if $0 < \alpha < \alpha_0$ and $\beta > \beta_0$, then any ground state $y_N : X_N \to \mathbb{R}^2$ of $V(\cdot)$ satisfies the following:*

(1) (*Minimum distance property*)

$$\min_{x \neq x'} \left| y(x) - y(x') \right| > 1 - \alpha. \tag{2.10}$$

(2) (*Uniform bond angle*). *If* $\{x_0, x_1, x_2\}$ *are such that*

$$|y(x_0) - y(x_i)| \leq 1 + \alpha \qquad \textit{for } i = 1, 2,$$

then the bond angle $\theta_{x_1 x_0 x_2}$ *satisfies*

$$\left| \cos\theta_{x_1 x_0 x_2} + 1/2 \right| \leq \frac{C}{\sqrt{\beta}}. \tag{2.11}$$

Proof. This follows directly from Lemmas 2.3 and 2.6. □

3. Discrete Imbeddings and a Combinatorial Lemma

Throughout this section and the next sections we will be using the following assumption.

Assumption 3.1. Let $y : X_N \to \mathbb{R}^2$ satisfy:

(1) Minimum distance property:

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

(2) Uniform bond angle property: if $|y(x_i) - y(x_0)| \leq 1 + \alpha$, $i = 1, 2$, then

$$\left| \theta_{x_1 x_0 x_2} - \frac{2\pi}{3} \right| \leq \frac{C}{\sqrt{\beta}}.$$

Here C is a constant and α, β will be adjustable parameters.

Definition 3.2 (*Neighboring atoms*)**.** *Two atoms* $x \neq x' \in X_N$ *are said to be in neighborhood if* $|y(x) - y(x')| \leq 1 + \alpha$. *Alternatively we say* x' *is a neighbor of* x. *Denote by* $\mathcal{N}(x)$ *the set of neighbors of* x*, i.e.*

$$\mathcal{N}(x) = \{x' \neq x, |y(x') - y(x)| \leq 1 + \alpha\}.$$

It is also useful to introduce extended neighbors:

$$\mathcal{N}^{(2)}(x) = \mathcal{N}(\mathcal{N}(x)) = \bigcup_{y \in \mathcal{N}(x)} \mathcal{N}(y),$$

and similarly

$$\mathcal{N}^{(k)}(x) = \mathcal{N}(\mathcal{N}^{(k-1)}(x)), \quad k \geq 3.$$

One can then use the notion of neighbor to define regular or defected atoms as follows.

Definition 3.3 (*Regular and defected atoms*)**.** *An atom* $x \in X_N$ *is said to be regular if* $\#\mathcal{N}(x) = 3$. *Otherwise it is called defected. We denote*

$$\partial X_N = \{x \in X_N : x \textit{ is defected}\}. \tag{3.1}$$

The following definition shows in what sense we can map the neighborhood of regular atoms into the perfect Hex lattice.

Definition 3.4 (*Imbedding into perfect hexagonal lattices*). *Let $\omega \subset X_N \backslash \partial X_N$. A map $\Phi : \omega \to Hex$ is said to be an imbedding if*

(1) *Φ preserves neighboring relations: If $x \neq x' \in \omega$ are neighbors, then $|\Phi(x) - \Phi(x')| = 1$.*
(2) *Φ preserves (local) orientations: If $x_1, x_2 \in \mathcal{N}(x)$, then*

$$\left(\frac{(y(x_1) - y(x)) \cdot (y(x_2) - y(x))}{|y(x_1) - y(x)| \cdot |y(x_2) - y(x)|}\right) \cdot \left(\frac{(\Phi(x_1) - \Phi(x)) \cdot (\Phi(x_2) - \Phi(x))}{|\Phi(x_1) - \Phi(x)| \cdot |\Phi(x_2) - \Phi(x)|}\right) > 0.$$

The following combinatorial lemma plays an important role in the proof of the Main Theorem 1.2.

Lemma 3.5.

$$\#\mathcal{S} \leq \frac{3}{2}N - \frac{1}{2}\#\partial X_N.$$

Proof. Let $n(x) = \#\mathcal{N}(x)$ = the number of neighboring pairs which contain the atom x. Then

$$\begin{aligned}\#\mathcal{S}(y_N) &= \frac{1}{2}\sum_{x \in X_N} n(x) = \frac{1}{2}\sum_{x \in X_N \backslash \partial X_N} n(x) + \frac{1}{2}\sum_{x \in \partial X_N} n(x)\\ &\leq \frac{3}{2}(N - \#\partial X_N) + \#\partial X_N\\ &= \frac{3}{2}N - \frac{1}{2}\#\partial X_N.\end{aligned}$$

□

4. The Renormalized Potential Energy, Deformed Hexagons and Partition of Pairs

4.1. The renormalized two-body potential energy. To introduce the renormalized potential, we recall that

$$Hex = \{\xi = ma_1 + na_2 + lb : m, n \in \mathbb{Z}, l = 0 \text{ or } 1\},$$

where $a_1 = (\sqrt{3}, 0)$, $a_2 = (\frac{\sqrt{3}}{2}, \frac{3}{2})$, $b = (\sqrt{3}, 1)$. The renormalized potential V_* is given by

$$V_*(r) = \frac{1}{3}\sum_{0 \neq \xi \in Hex} V_2(r|\xi|).$$

This is the energy per bond in a homogeneously dilated perfect lattice. To simplify this expression further, define

$$\begin{aligned}m(\lambda) &= \frac{1}{3}\#\left(Hex \cap \{|\xi| = \lambda\}\right)\\ &= \frac{1}{3}\#\left\{(m, n, l) : m, n \in \mathbb{Z}, l = 0 \text{ or } 1, \text{ and } 3(m + \frac{n}{2} + l)^2 + (m + \frac{3}{2}n + l)^2 = \lambda^2\right\}\\ &= \frac{2}{3}\#\left\{k \in \mathbb{Z}^2 : k \cdot \begin{pmatrix} 4 & 3 \\ 3 & 3 \end{pmatrix} k = \lambda^2\right\}. \qquad (4.1)\end{aligned}$$

The countable set $\Lambda = \{\lambda > 0 : \ m(\lambda) \neq 0\}$ is the set of distances. From the above derivation we obtain an equivalent expression of the renormalized potential:

$$V_*(r) = \sum_{\lambda \in \Lambda} m(\lambda) V_2(\lambda r). \tag{4.2}$$

It follows easily from Assumption 1.1 that if α is sufficiently small, then V_* is uniformly convex on $(1-\alpha, 1+\alpha)$, i.e. for some constant $\theta > 0$, we have

$$V_*(r) \geq V_*(1) + \frac{\theta}{2}|r-1|^2, \quad \forall\, r \in (1-\alpha, 1+\alpha). \tag{4.3}$$

4.2. Deformed hexagons and splitting of pairs. The whole proof is centered around the concept of "deformed hexagons". To this end we introduce

Definition 4.1 (*Deformed hexagons*). *Let $H \subset X_N$ be such that $\#H = 6$ and $\lambda \in \Lambda$. We say that H is a deformed hexagon with side length λ for the configuration y satisfying 3.1 and write shortly $H \in H_\lambda$ if either of the following two conditions holds:*

A. $\lambda = 1$. $H = \{x_i\}_{i=0}^5$. x_i and x_{i+1} are α-bonded (see 2.5) for $i = 0, \cdots, 5$. Here we denote $x_i := x_{i+6}$. $z = \frac{1}{6}\sum_{x\in H} y(x)$. $B(z, 20) \cap y(\partial X_N) = \emptyset$, and the Bond angles $\theta_{x_{i+1}x_i x_{i-1}}$ satisfy

$$|\theta_{x_{i+1}x_i x_{i-1}} - \frac{2\pi}{3}| \leq \frac{C}{\sqrt{\beta}}.$$

B. $\lambda > 1$. $H = \{x_i\}_{i=0}^5$. $z = \frac{1}{6}\sum_{x\in H} y(x)$. $B(z, 100\lambda) \cap y(\partial X_N) = \emptyset$. There exists a patch $\omega_H \subset X_N \backslash \partial X_N$ and a discrete imbedding $\Phi_H : \omega_H \to Hex$ such that the image $\{\Phi(x_i)\}_{i=0}^5$ is the vertex of a hexagon in the perfect lattice Hex with side length λ and positive orientation. Here we say $\{\Phi(x_i)\}_{i=0}^5$ is positively oriented in the sense that they are aligned in the plane counterclockwise. Furthermore

$$B(z, 5\lambda) \cap y(Hex) \supset y(\omega_H) \supset B(z, 3\lambda) \cap y(Hex). \tag{4.4}$$

Lemma 4.2. *There exist constants α_0, β_0, $K > 0$ such that the following holds for any $0 < \alpha < \alpha_0$, $\beta > \beta_0$ and any configuration y satisfying* 3.1:
If $\lambda \in \Lambda\backslash\{1\}$, $H \in H_\lambda$, then for any $\{x, x'\} \subset H$ with $|\Phi(x) - \Phi(x')| = \lambda$, the following estimate holds:

$$\left| \frac{1}{\lambda}|y(x) - y(x')| - 1 \right| \leq K \min\{\alpha, \frac{1}{\sqrt{\beta}}\}.$$

Proof. See the Appendix. □

Proposition 4.3 (*Partition of long edges*)**.** *There exist constants α_0, $\beta_0 > 0$ such that the following holds for any $0 < \alpha < \alpha_0$, $\beta > \beta_0$ and any configuration y satisfying 3.1: For all pairs $\{x_1, x_2\} \subset X_N$ with the property $|y(x_1) - y(x_2)| > 1 + \alpha$, the set*

$$\mathcal{H}(x_1, x_2) = \left\{ H \in \cup_{\lambda \in \Lambda\backslash\{1\}} H_\lambda | \{x_1, x_2\} \subset H, \ |\Phi(x_1) - \Phi(x_2)| = \lambda \right\}$$

satisfies the following assertions:

(1) *$\#\mathcal{H}(x_1, x_2) \leq 2$ and there exists a unique number $\lambda \in \Lambda$ such that $\mathcal{H}(x_1, x_2) \subset H_\lambda$.*

(2) *If* $B(\frac{1}{2}(y(x_1)+y(x_2)), 300|y(x_1)-y(x_2)|)\cap y(\partial X_N)=\emptyset$, *then* $\#\mathcal{H}(x_1,x_2)=2$.
(3) *Conversely if* $\#\mathcal{H}(x_1,x_2)\le 1$, *then* $y(\partial X_N)\cap B\neq\emptyset$, *where* $B=(\frac{1}{2}(y(x_1)+y(x_2)), 300|y(x_1)-y(x_2)|)$.

Proof. See the Appendix. □

Proposition 4.4 (*Partition of short edges*)**.** *There exist constants* α_0, $\beta_0>0$ *such that the following holds for any* $0<\alpha<\alpha_0$, $\beta>\beta_0$ *and any configuration* y *satisfying 3.1: For all pairs* $\{x_1,x_2\}\subset X_N$ *with the property* $|y(x_1)-y(x_2)|\le 1+\alpha$, *the set*

$$\mathcal{H}(x_1,x_2)=\{H\in H_1|\{x_1,x_2\}\subset H,\ |\Phi(x_1)-\Phi(x_2)|=1\}$$

satisfies the following assertions:

(1) $\#\mathcal{H}(x_1,x_2)\le 2$.
(2) *If* $B(\frac{1}{2}(y(x_1)+y(x_2)), 40)\cap y(\partial X_N)=\emptyset$, *then* $\#\mathcal{H}(x_1,x_2)=2$.
(3) *Conversely if* $\#\mathcal{H}(x_1,x_2)\le 1$, *then* $y(\partial X_N)\cap B\neq\emptyset$, *where* $B=(\frac{1}{2}(y(x_1)+y(x_2)), 40)$.

Proof. See the Appendix. □

Proposition 4.5. *There exist constants* α_0, β_0, $C>0$ *such that the following holds for any* $0<\alpha<\alpha_0$, $\beta>\beta_0$, $\lambda\in\Lambda$ *and any configuration* y *satisfying* 3.1:

1. *The number of hexagons rescales:*

$$0\le \#H_1-\frac{1}{m(\lambda)}\#H_\lambda\le C\lambda^2\#\partial X_N, \tag{4.5}$$

2. *The area covered by hexagons of different side-lengths also rescales:*

$$0\le\sum_{H\in H_1} meas(conv(y(H)))-\frac{1}{\lambda^2 m(\lambda)}\sum_{H\in H_\lambda} meas(conv(y(H)))\le C\lambda^2\#\partial X_N, \tag{4.6}$$

3. *There are only finitely many hexagons with given side-length which cover a vertex* x*:*

$$\#\{H\in H_\lambda|x\in\omega_H\}\le C\lambda^2 m(\lambda)\quad \text{for any } x\in X_N. \tag{4.7}$$

Proof. See the Appendix. □

We now use the notion of deformed hexagons to define splitting of pairs. First introduce

$$\mathcal{L}_1=\Big\{\{x_1,x_2\}\subset X_N:\ |y(x_1)-y(x_2)|>1+\alpha,\\ B(\frac{1}{2}(y(x_1)+y(x_2)), 300|y(x_1)-y(x_2)|)\cap y(\partial X_N)\neq\emptyset\Big\}. \tag{4.8}$$

The set $\mathcal{L}_1$ contains "long edges" which are close to the defected atoms. Also introduce

$$\mathcal{L}_2=\Big\{\{x_1,x_2\}\subset X_N:\ |y(x_1)-y(x_2)|\\ \le 1+\alpha,\ B(\frac{1}{2}(y(x_1)+y(x_2)), 40)\cap y(\partial X_N)\neq\emptyset\Big\}. \tag{4.9}$$

The set $\mathcal{L}_2$ contains "short edges" which are close to the defected atoms. We shall define

$$\mathcal{L} = \mathcal{L}_1 \cup \mathcal{L}_2 = \text{"bad pairs" that are close to defects.}$$

Observe that for any $p \notin \mathcal{L}$, by Proposition 4.3 and 4.4, p must belong to exactly two deformed hexagons. In this sense we have obtained a partition of the set of pairs. The partitioning of the set of pairs also induces a partitioning of the energy:

$$\sum_{p \in \mathcal{P}} e(p) = \Big(\frac{1}{2} \sum_{\lambda \in \Lambda} \sum_{H \in H_\lambda} \sum_{\substack{\{x,x'\} \subset H \\ |\Phi(x)-\Phi(x')|=\lambda}} e(p) \Big) + \sum_{p \in \mathcal{L}} e(p).$$

As we shall see in the next section, the last term which corresponds to the contribution by "bad edges" can be estimated by small surface terms. The first term carries the dominating part of the energy.

5. Resummation of the Potential Energy V_2

This section is devoted to the proof of the following lemma.

Lemma 5.1 (Resummation of the potential energy V_2)**.** *We have*

$$\begin{aligned} &\frac{1}{2} \sum_{\lambda \in \Lambda} \sum_{H \in H_\lambda} \sum_{\{x,x'\} \subset H} e(\{x, x'\}) \\ &\quad \geq \frac{1}{2} \sum_{H \in H_1} \sum_{\{x,x'\} \subset H} \Big[e_*(\{x, x'\}) - C\alpha(|y(x) - y(x')| - 1)^2 \Big] - C\alpha \# \partial X_N \\ &\quad\quad - C\alpha \sum_{H \in H_1} \sum_{\substack{|\Phi(x)-\Phi(x')|=\sqrt{3} \\ \{x,x'\} \subset H}} (|y(x) - y(x')| - \sqrt{3})^2. \end{aligned}$$

Lemma 5.2. *There exist three constants $\alpha_0 > 0$, $C > 0$, $c_1 > 0$ such that the following holds for any $0 < \alpha < \alpha_0$, $\lambda > 0$: Let H be a hexagon in $\mathbb{R}^2$ with vertices A_i, $i = 1, \ldots, 6$, and side lengths l_i, $1 \leq i \leq 6$. Denote the cord lengths (see Fig. 4) $|A_1 - A_3| = f_1$, $|A_3 - A_5| = f_2$, $|A_1 - A_5| = f_3$. Assume that:*

(1) $\left| \frac{l_i}{\lambda} - 1 \right| \leq \alpha, \quad 1 \leq i \leq 6.$

(2) $\left| \frac{f_i}{\lambda} - \sqrt{3} \right| \leq \alpha, \quad 1 \leq i \leq 3.$

Then

$$\left| \frac{1}{\lambda} \left(\sum_{i=1}^{6} l_i - 6\lambda \right) - \frac{S(H) - S(H_0)}{c_1 \lambda^2} \right| \leq \frac{K}{\lambda^2} \left(\sum_{i=1}^{6} |l_i - \lambda|^2 + \sum_{i=1}^{3} |f_i - \sqrt{3}\lambda|^2 \right),$$

where in the above $S(H)$ is the area of the hexagon, $S(H_0)$ is the area of the undeformed hexagon, i.e. when side lengths $l_i = \lambda$ and $f_i = \sqrt{3}\lambda$. It is not difficult to find that $S(H_0) = \frac{3\sqrt{3}}{2}\lambda^2$.

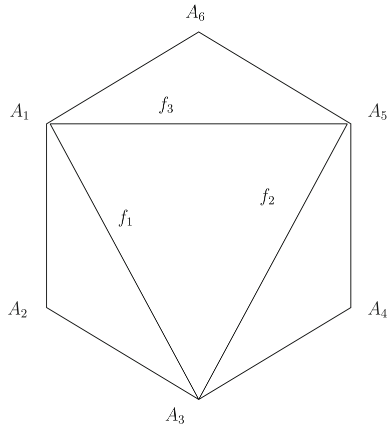

Fig. 4. The deformed hexagon H

Proof. Denote by $S(l_1, l_2, f_1)$ the area of the triangle $A_1A_2A_3$. By Heron's formula the area of the triangle can be expressed in terms of its side lengths. Furthermore it is clear that $S(l_1, l_2, f_1) = \lambda^2 S(\frac{l_1}{\lambda}, \frac{l_2}{\lambda}, \frac{f_1}{\lambda})$. Therefore it is enough to prove the inequality assuming $\lambda = 1$. To this end we have

$$S(l_1, l_2, f_1) = S(1, 1, \sqrt{3}) + c_1(l_1 + l_2 - 2) + c_2(f_1 - \sqrt{3}) \\ +O(|l_1 - 1|^2 + |l_2 - 1|^2 + |f_1 - \sqrt{3}|^2), \tag{5.1}$$

where the O-constant is bounded by a universal number, $c_1 = \frac{\sqrt{3}}{2}$, $c_2 = -\frac{1}{2}$. Similarly for triangle $A_3A_4A_5$ we have

$$S(l_3, l_4, f_2) = S(1, 1, \sqrt{3}) + c_1(l_3 + l_4 - 2) + c_2(f_2 - \sqrt{3}) \\ +O(|l_3 - 1|^2 + |l_4 - 1|^2 + |f_2 - \sqrt{3}|^2), \tag{5.2}$$

and for triangle $A_5A_6A_1$,

$$S(l_5, l_6, f_3) = S(1, 1, \sqrt{3}) + c_1(l_5 + l_6 - 2) + c_2(f_3 - \sqrt{3}) \\ +O(|l_5 - 1|^2 + |l_6 - 1|^2 + |f_3 - \sqrt{3}|^2). \tag{5.3}$$

Lastly for the triangle $A_1A_3A_5$, we have

$$S(f_1, f_2, f_3) = S(\sqrt{3}, \sqrt{3}, \sqrt{3}) + c_3(f_1 + f_2 + f_3 - 3\sqrt{3}) + O(\sum_{i=1}^{3} |f_i - \sqrt{3}|^2), \tag{5.4}$$

where $c_3 = \frac{1}{2}$. Adding (5.1), (5.2), (5.3), (5.4) together and noting that $c_2 + c_3 = 0$ yields the desired inequality. $\square$

Corollary 5.3. *Let $f \in C^2(0,\infty)$. Under the same hypothesis as in Lemma 5.2, we have*

$$\left|\sum_{i=1}^{6} f(l_i) - \left(6f(\lambda) + f'(\lambda)\cdot\frac{S(H)-S(H_0)}{c_1\lambda}\right)\right|$$
$$\leq K\left(\frac{|f'(\lambda)|}{\lambda} + \|f''(\lambda)\|_{L^\infty((1-\alpha)\lambda,(1+\alpha)\lambda)}\right)\left(\sum_{i=1}^{6}|l_i-\lambda|^2 + \sum_{i=1}^{3}|f_i-\sqrt{3}\lambda|^2\right).$$

Proof. This is straightforward by using Taylor expansion. □

The next lemma shows that in the main order of magnitude, the two-body potential V_2 can be "renormalized".

Lemma 5.4. *We have*

$$\sum_{\lambda\in\Lambda\backslash\{1\}}\sum_{H\in H_\lambda}\sum_{\substack{\{x,x'\}\subset H\\ |\Phi(x)-\Phi(x')|=\lambda}} V_2(|y(x)-y(x')|$$
$$\geq (\sum_{\lambda\in\Lambda\backslash\{1\}} m(\lambda)\sum_{H\in H_1}\sum_{\substack{\{x,x'\}\subset H\\ |\Phi(x)-\Phi(x')|=1}} V_2(\lambda|y(x)-y(x')|)) - e_1 - e_2 - e_3,$$

where

$$e_1 = C\sum_{\lambda\in\Lambda\backslash\{1\}}\sum_{H\in H_\lambda}\left(\frac{|V_2'(\lambda)|}{\lambda} + \|V_2''(\cdot)\|_{L^\infty((1-\alpha)\lambda,(1+\alpha)\lambda)}\right)$$
$$(\sum_{\substack{\{x,x'\}\subset H\\ |\Phi(x)-\Phi(x')|=\lambda}} ||y(x)-y(x')|-\lambda|^2 + \sum_{\substack{\{x,x'\}\subset H\\ |\Phi(x)-\Phi(x')|=\sqrt{3}\lambda}} ||y(x)-y(x')|-\sqrt{3}\lambda|^2),$$

also

$$e_2 = C\sum_{\lambda\in\Lambda\backslash\{1\}} m(\lambda)(|V_2(\lambda)|\lambda^2 + |V_2'(\lambda)|\lambda^3)\#\partial X_N,$$

and

$$e_3 = C\sum_{\lambda\in\Lambda\backslash\{1\}}\lambda^2 m(\lambda)\sum_{H\in H_1}\left(\frac{|V_2'(\lambda)|}{\lambda} + \|V_2''(\cdot)\|_{L^\infty((1-\alpha)\lambda,(1+\alpha)\lambda)}\right)$$
$$(\sum_{\substack{\{x,x'\}\subset H\\ |\Phi(x)-\Phi(x')|=1}} ||y(x)-y(x')|-1|^2 + \sum_{\substack{\{x,x'\}\subset H\\ |\Phi(x)-\Phi(x')|=\sqrt{3}}} ||y(x)-y(x')|-\sqrt{3}|^2).$$

In the above C denotes generic constants.

Proof. We have for each $H \in H_\lambda$, $\lambda \in \Lambda\backslash\{1\}$, by Corollary 5.3:

$$\sum_{\substack{\{x,x'\}\subset H\\ |\Phi(x)-\Phi(x')|=\lambda}} V_2(|y(x)-y(x')|)$$
$$\geq 6V_2(\lambda) + \frac{V_2'(\lambda)}{c_1\lambda}(S(H)-S(H_0)) - K\left(\frac{|V_2'(\lambda)|}{\lambda} + \|V_2''(\cdot)\|_{L^\infty((1-\alpha)\lambda,(1+\alpha)\lambda)}\right)$$
$$\Big(\sum_{\substack{\{x,x'\}\subset H\\ |\Phi(x)-\Phi(x')|=\lambda}} ||y(x)-y(x')|-\lambda|^2 + \sum_{\substack{\{x,x'\}\subset H\\ |\Phi(x)-\Phi(x')|=\sqrt{3}\lambda}} ||y(x)-y(x')|-\sqrt{3}\lambda|^2\Big).$$

The last term in the above inequality contributes to the error term e_1. The next Proposition 4.5 gives that

$$\sum_{H\in H_\lambda} 6V_2(\lambda) + \frac{V_2'(\lambda)}{c_1\lambda}(S(H)-S(H_0))$$
$$\geq \left(m(\lambda)\sum_{H\in H_1} 6V_2(\lambda) + \frac{V_2'(\lambda)}{c_1\lambda}\lambda^2(S(H)-S(H_0))\right) - C\cdot m(\lambda)(V_2(\lambda)\lambda^2$$
$$+V_2'(\lambda)\lambda^3)\#\partial X_N.$$

Clearly the last term above contributes to the error term e_2. Finally apply Corollary 5.3 again; we have for each $H \in H_1$,

$$6V_2(\lambda) + \frac{V_2'(\lambda)}{c_1\lambda}\lambda^2(S(H)-S(H_0)) \geq \Big(\sum_{\substack{\{x,x'\}\subset H\\ |\Phi(x)-\Phi(x')|=1}} V_2(\lambda|y(x)-y(x')|)\Big)$$
$$-\lambda^2\sum_{H\in H_1}\left(\frac{|V_2'(\lambda)|}{\lambda} + \|V_2''(\cdot)\|_{L^\infty((1-\alpha)\lambda,(1+\alpha)\lambda)}\right)$$
$$\Big(\sum_{\substack{\{x,x'\}\subset H\\ |\Phi(x)-\Phi(x')|=1}} ||y(x)-y(x')|-1|^2 + \sum_{\substack{\{x,x'\}\subset H\\ |\Phi(x)-\Phi(x')|=\sqrt{3}}} ||y(x)-y(x')|-\sqrt{3}|^2\Big).$$

Summing the last term in the above inequality over $\lambda \in \Lambda\backslash\{1\}$ gives us e_3. The lemma is proved. □

Lemma 5.5 (Bounding the error term e_1)**.** *We have*

$$|e_1| \leq C\alpha\Big(\sum_{H\in H_1}\sum_{\substack{\{x,x'\}\subset H\\ |\Phi(x)-\Phi(x')|=1}} (|y(x)-y(x')|-1)^2$$
$$+\sum_{H\in H_1}\sum_{\substack{\{x,x'\}\subset H\\ |\Phi(x)-\Phi(x')|=\sqrt{3}}} (|y(x)-y(x')|-\sqrt{3})^2\Big).$$

Proof. By Proposition 10.6, we have for each $\lambda \in \Lambda \backslash \{1\}$,

$$\sum_{H \in H_\lambda} \Big(\sum_{\substack{\{x,x'\} \subset H \\ |\Phi(x)-\Phi(x')|=\lambda}} ||y(x)-y(x')|-\lambda|^2 + \sum_{\substack{\{x,x'\} \subset H \\ |\Phi(x)-\Phi(x')|=\sqrt{3}\lambda}} ||y(x)-y(x')|-\sqrt{3}\lambda|^2 \Big)$$

$$\leq C \log \lambda \sum_{H \in H_\lambda} \sum_{\substack{S \in H_1 \\ y^{-1}(S) \subset \omega_H}} \Bigg(\sum_{\substack{\{x,x'\} \subset S \\ |\Phi(x)-\Phi(x')|=1}} \Big| |y(x)-y(x')| - 1 \Big|^2$$

$$+ \sum_{\substack{\{x,x'\} \subset S \\ |\Phi(x)-\Phi(x')|=\sqrt{3}}} \Big| |y(x)-y(x')| - \sqrt{3} \Big|^2 \Bigg).$$

Now by (4.7), there are at most $C\lambda^2 m(\lambda)$ deformed hexagons of side length λ whose ω_H contains a given $S \in H_1$. This gives us that

$$|e_1| \leq C \cdot D \cdot \Bigg(\sum_{H \in H_1} \sum_{\substack{\{x,x'\} \subset H \\ |\Phi(x)-\Phi(x')|=1}} (|y(x)-y(x')|-1)^2 + \sum_{H \in H_1} \sum_{\substack{\{x,x'\} \subset H \\ |\Phi(x)-\Phi(x')|=\sqrt{3}}} (|y(x)-y(x')|-\sqrt{3})^2 \Bigg),$$

where C is a constant and

$$D = \sum_{\lambda \in \Lambda \backslash \{1\}} \log \lambda \cdot m(\lambda)\lambda^2 \left(\frac{|V_2'(\lambda)|}{\lambda} + \|V_2''(\cdot)\|_{L^\infty((1-\alpha)\lambda,(1+\alpha)\lambda)} \right).$$

It remains to estimate D. To this end by using the decay assumption of V_2 (see Assumption 1.1), we have

$$D \leq C\alpha \sum_{\lambda \in \Lambda \backslash \{1\}} m(\lambda)\lambda^{2-\gamma} \log \lambda.$$

By using the definition of $m(\lambda)$ (see (4.1)), we can further bound D by

$$D \leq C\alpha \sum_{0 \neq k \in \mathbb{Z}^2} \frac{1}{|k|^{\gamma-2}} \log(|k|+2).$$

Since by assumption $\gamma > 6$, it is not difficult to check that the last sum converges and the lemma is proved. □

Concerning the error term e_2 we have

Lemma 5.6 (*Bounding the error term e_2*).

$$|e_2| \leq C\alpha \# \partial X_N.$$

Proof. Again by the decay assumption of V_2, 1.1 and the definition of $m(\lambda)$ (4.1), we have

$$|e_2| \le C \left(\sum_{\lambda \in \Lambda \setminus \{1\}} m(\lambda) \lambda^{4-\gamma} \right) \# \partial X_N$$
$$\le C \left(\sum_{0 \ne k \in \mathbb{Z}^2} \frac{1}{|k|^{\gamma-4}} \right) \# \partial X_N.$$

The last sum converges due to the assumption $\gamma > 6$. The lemma is proved. □

Also for error term e_3 we have

Lemma 5.7 (*Bounding the error term* e_3).

$$|e_3| \le C\alpha \Big(\sum_{H \in H_1} \sum_{\substack{\{x,x'\} \subset H \\ |\Phi(x)-\Phi(x')|=1}} (|y(x) - y(x')| - 1)^2 + \sum_{H \in H_1} \sum_{\substack{\{x,x'\} \subset H \\ |\Phi(x)-\Phi(x')|=\sqrt{3}}} (|y(x) - y(x')| - \sqrt{3})^2 \Big).$$

Proof. We have

$$|e_3| \le C \cdot D \cdot \Big(\sum_{H \in H_1} \sum_{\substack{\{x,x'\} \subset H \\ |\Phi(x)-\Phi(x')|=1}} (|y(x) - y(x')| - 1)^2 + \sum_{H \in H_1} \sum_{\substack{\{x,x'\} \subset H \\ |\Phi(x)-\Phi(x')|=\sqrt{3}}} (|y(x) - y(x')| - \sqrt{3})^2 \Big),$$

where

$$D = \sum_{\lambda \in \Lambda \setminus \{1\}} m(\lambda) \lambda^2 \left(\frac{|V_2'(\lambda)|}{\lambda} + \|V_2''(\cdot)\|_{L^\infty((1-\alpha)\lambda,(1+\alpha)\lambda)} \right).$$

The estimate of D is almost the same as in the proof of Lemma 5.5 and we get $D \le Const \cdot \alpha$. The lemma is proved. □

Proof of Lemma 5.1. By Lemmas 5.4, 5.5, 5.6 and 5.7, we have

$$\frac{1}{2} \sum_{\lambda \in \Lambda \setminus \{1\}} \sum_{H \in H_\lambda} \sum_{\substack{\{x,x'\} \subset H \\ |\Phi(x)-\Phi(x')|=\lambda}} V_2(|y(x) - y(x')|)$$
$$\ge \frac{1}{2} \sum_{H \in H_1} \sum_{\substack{\{x,x'\} \subset H \\ |\Phi(x)-\Phi(x')|=1}} \Big(e_*(\{x, x'\}) - e(\{x, x'\}) - C\alpha (|y(x) - y(x')| - 1)^2 \Big)$$
$$-C\alpha \# \partial X_N - C\alpha \sum_{H \in H_1} \sum_{\substack{\{x,x'\} \subset H \\ |\Phi(x)-\Phi(x')|=\sqrt{3}}} (|y(x) - y(x')| - \sqrt{3})^2.$$

This immediately yields the lemma by adding the term corresponding to $\lambda = 1$. □

6. Proof of the main theorem

The following lemma says that the contribution of those pairs in $\mathcal{L}$ can be bounded by surface terms.

Lemma 6.1 (Bounding $\mathcal{L}$-edges by surface terms)**.**

$$\sum_{p\in\mathcal{L}} |e_*(p) - e(p)| \leq C\alpha \# \partial X_N.$$

Proof. We begin by observing that for any $r > 1-\alpha$, by (4.2) and the fact that $m(1) = 1$, we have

$$|V_*(r) - V_2(r)| \leq \sum_{\lambda\in\Lambda\setminus\{1\}} m(\lambda) V_2(\lambda r).$$

Since $\lambda \geq \sqrt{3}$ and $\alpha < \frac{1}{12}$, we have $\lambda r \geq (1-\alpha)r > \frac{3}{2}$. By the decay estimate on V_2 (see (1.1)), we get

$$|V_2(\lambda r)| \leq \frac{\alpha}{(\gamma-1)(\gamma-2)}(\lambda r)^{2-\gamma}.$$

From this we obtain that

$$|V_*(r) - V_2(r)| \leq C_1 \alpha r^{2-\gamma}, \quad \forall\, r > 1-\alpha, \tag{6.1}$$

where C_1 is a constant.

Next for any $\{x, x'\} \in \mathcal{L}_1$ (see (4.9)) we have that if $d \leq |y(x) - y(x')| < d+1$ and $d \in \mathbb{N}$, then $y(x) \in B(y(x_b), 600d)$ for some atom $x_b \in \partial X_N$. Since the configuration y satisfies Assumption (2.1), there are at most $C_2 d^2$ atoms $x \in X$ such that $y(x) \in B(y(x_b), 600d)$. For each x such that $y(x) \in B(y(x_b), 600d)$, there are at most $C_3 d$ atoms $x' \in X$ for which $d \leq |y(x') - y(x)| < d+1$. After all these considerations and using (6.1), we obtain the inequality

$$\begin{aligned}\sum_{p\in\mathcal{L}_1} |e_*(p) - e_(p)| &\leq \sum_{x\in\partial X}\sum_{d=1}^{\infty} C_1 C_2 d^3 C_3 \alpha d^{2-\gamma}\\ &\leq C\alpha\#\partial X.\end{aligned}$$

In the first inequality above the sum over d converges due the assumption $\gamma > 6$. Finally for short edges $p \in \mathcal{L}_2$, by similar considerations and (6.1), we also obtain

$$\sum_{p\in\mathcal{L}_2} |e_*(p) - e(p)| \leq C\alpha\#\partial X.$$

The lemma is proved. □

Lemma 6.2. *There exist constants* $\epsilon_0 > 0$, $\delta_0 > 0$, $K > 0$ *such that the following holds for any* $0 < \epsilon < \epsilon_0$, $0 < \delta < \delta_0$*: Let* Δ *be a triangle in* $\mathbb{R}^2$ *with side lengths* l_1, l_2, l_3 *satisfying:*

(1) $|l_1 - 1| \leq \epsilon$, $|l_2 - 1| \leq \epsilon$.
(2) *Let* θ *be the angle between the sides* l_1 *and* l_2*, then* $|\cos\theta + \frac{1}{2}| \leq \delta$.

Then for l_3 we have:

$$|l_3 - \sqrt{3}|^2 \le K \cdot \left(|l_1 - 1|^2 + |l_2 - 1|^2 + |\cos\theta + \frac{1}{2}|^2 \right).$$

Proof. Since $l_3 = l_1^2 + l_2^2 - 2l_1 l_2 \cos\theta$, think of l_3 as a function of l_1, l_2 and $\cos\theta$. Then l_3 is continuously differentiable and the result follows by using Taylor's expansion. □

Lemma 6.3. *There exists constants $\alpha_0 > 0$, $\lambda_0 > 0$ and $C > 0$ such that the following holds for any $0 < \alpha < \alpha_0$ and $\beta > \beta_0$:*

$$\begin{aligned}
&\sum_{H \in H_1} \sum_{\substack{\{x,x'\} \subset H \\ |\Phi(x)-\Phi(x')|=\sqrt{3}}} \left(|y(x) - y(x')| - \sqrt{3} \right)^2 \\
&\le C \Bigg(\sum_{H \in H_1} \sum_{\substack{\{x,x'\} \subset H \\ |\Phi(x)-\Phi(x')|=1}} \left(|y(x) - y(x')| - 1 \right)^2 \\
&\quad + \sum_{H \in H_1} \sum_{\substack{\{x_0,x_1,x_2\} \subset H \\ |\Phi(x_1)-\Phi(x_0)|=|\Phi(x_2)-\Phi(x_0)|=1}} \left(\cos\theta_{x_2 x_0 x_1} + \frac{1}{2} \right)^2 \Bigg),
\end{aligned}$$

where in the above $\theta_{x_2 x_0 x_1}$ is the bond angle (see also 2.5).

Proof. Observe that for any $H \in H_1$ and $\{x, x'\} \subset H$ with $|\Phi(x) - \Phi(x')| = \sqrt{3}$, one can always find a unique triple $\{x_0, x_1, x_2\} \in H$ such that $\{x, x'\} = \{x_1, x_2\}$. The rest of the argument is rather straightforward using Lemma 6.2. □

Our next lemma says that if the three-body potential V_3 is sufficiently strong, then the total energy V can be bounded below purely in terms of the renormalized two-body potential e_*.

Lemma 6.4. *There exist constants $\alpha_0, \beta_0 > 0$ such that if $0 < \alpha < \alpha_0$, $\beta > \beta_0$, then the following holds for the potential $V = V_2 + V_3$ (with α, β as parameters in the definition of V_2 and V_3), and any ground state $y : X_N \to \mathbb{R}^2$:*

$$\begin{aligned}
&V(\{y_1, \cdots, y_N\}) \\
&\ge \frac{1}{2} \Bigg(\sum_{H \in H_1} \sum_{\substack{\{x,x'\} \subset H \\ |\Phi(x)-\Phi(x')|=1}} e_*(\{x, x'\}) - C\alpha(|y(x) - y(x')| - 1)^2 \Bigg) - C\alpha \# X_N.
\end{aligned}$$

Proof. By Lemma 5.1 we have

$$\begin{aligned}
\sum_{p \in \mathcal{P}} e(p) &= \frac{1}{2} \sum_{\lambda \in \Lambda} \sum_{H \in H_\lambda} \sum_{\{x,x'\} \subset H} e(\{x, x'\}) + \sum_{p \in \mathcal{L}} e(p) \\
&\ge \frac{1}{2} \sum_{H \in H_1} \sum_{\{x,x'\} \subset H} \left[e_*(\{x, x'\}) - C\alpha(|y(x) - y(x')| - 1)^2 \right] - C\alpha \# \partial X_N \\
&\quad - C\alpha \# \partial X_N - C\alpha \sum_{H \in H_1} \sum_{\substack{\{x,x'\} \subset H \\ |\Phi(x)-\Phi(x')|=\sqrt{3}}} (|y(x) - y(x')| - \sqrt{3})^2.
\end{aligned}$$

Next we use Lemma 6.3 to bound the last term in the above inequality. We have (by increasing the constant C slightly),

$$\sum_{p\in\mathcal{P}} e(p) \geq \frac{1}{2}\sum_{H\in H_1}\sum_{\{x,x'\}\subset H}\left[e_*(\{x,x'\}) - C\alpha(|y(x)-y(x')|-1)^2\right] - C\alpha\#\partial X_N$$
$$-C\alpha\sum_{H\in H_1}\sum_{\substack{\{x_0,x_1,x_2\}\subset H\\ |\Phi(x_1)-\Phi(x_0)|=|\Phi(x_2)-\Phi(x_0)|=1}}\left(\cos\theta_{x_2x_0x_1}+\frac{1}{2}\right)^2.$$

By the definition of V_3, it is clear that there exist β_0, $\alpha_0 > 0$, such that if $\beta > \beta_0$, $\alpha < \alpha_0$, then

$$C\alpha\sum_{H\in H_1}\sum_{\substack{\{x_0,x_1,x_2\}\subset H\\ |\Phi(x_1)-\Phi(x_0)|=|\Phi(x_2)-\Phi(x_0)|=1}}\left(\cos\theta_{x_2x_0x_1}+\frac{1}{2}\right)^2 \leq \frac{1}{3!}\sum_{i,j,k}V_3(y_i,y_j,y_k).$$

The lemma is now proved. □

Remark 6.5. It is not difficult to see that if we make α_0 even smaller, we can obtain a slightly stronger inequality:

$$\begin{aligned} &V(\{y_1,\cdots,y_N\})\\ &\geq \frac{1}{2}\Bigg(\sum_{H\in H_1}\sum_{\substack{\{x,x'\}\subset H\\ |\Phi(x)-\Phi(x')|=1}} e_*(\{x,x'\}) - C\alpha(|y(x)-y(x')|-1)^2\Bigg) - C\alpha\#X_N\\ &\quad+\frac{1}{12}\sum_{i,j,k}V_3(y_i,y_j,y_k). \end{aligned} \tag{6.2}$$

This more refined inequality will be needed later in the proof of Theorem 1.3 (see Lemma 7.6).

Proof of the Main Theorem. By Lemma 6.4, we have

$$\begin{aligned} &V(\{y_1,\ldots,y_N\})\\ &\geq \frac{1}{2}\sum_{H\in H_1}\sum_{\{x,x'\}\subset H}\left[e_*(\{x,x'\}) - C\alpha(|y(x)-y(x')|-1)^2\right] - C\alpha\#\partial X_N. \end{aligned}$$

Now since the set of neighboring pairs which are not the edges of some hexagon are necessarily bad edges, i.e.,

$$\mathcal{S}(y_N)\backslash\{p : p\subset H, \text{ for some } H\in H_1\}\subset\mathcal{L},$$

we can use Lemma 6.1 again to find

$$V \geq \sum_{\{x,x'\}\in\mathcal{S}}\left[e_*(\{x,x'\}) - C\alpha(|y(x)-y(x')|-1)^2\right] - C\alpha\#\partial X_N.$$

Since our renormalized potential e_* is uniformly convex on $(1-\alpha, 1+\alpha)$ (see (4.3)), we have

$$e_*(\{x,x'\}) \geq e_*(1) + \frac{\theta}{2}(|y(x)-y(x')|-1)^2$$
$$= -1 + \frac{\theta}{2}(|y(x)-y(x')|-1)^2.$$

This together with the assumption $4C\alpha \leq \theta$ immediately gives us

$$V \geq -\#\mathcal{S} - C\alpha\#\partial X_N + \sum_{\{x,x'\}\in\mathcal{S}} \frac{\theta}{4}(|y(x)-y(x')|-1)^2.$$

Finally use Lemma 3.5 and we have

$$V \geq -\frac{3}{2}N + (\frac{3}{2} - C\alpha)\#\partial X_N + \sum_{\{x,x'\}\in\mathcal{S}} \frac{\theta}{4}(|y(x)-y(x')|-1)^2. \tag{6.3}$$

Since by assumption $C\alpha < 3/2$, we conclude

$$V \geq -\frac{3}{2}N.$$

The theorem is proved. □

7. Proof of theorem 1.3

Let $L \in \mathbb{N}$. A set $X \subset Hex$ is called L-periodic if $X + LHex = X$. We introduce an equivalence relation $\sim$ on subsets of an L-periodic set X such that: two subsets $\omega, \omega' \subset X$ satisfy $\omega \sim \omega'$ if there is a vector $\tau \in LHex$ for which $\omega' = \omega + \tau$. We say a map $y :, X \to \mathbb{R}^2$ is L-periodic if $y(x+\tau) = y(x) + \tau$ for all $x \in X$, $\tau \in LHex$. For an L-periodic map, the defects ∂X, neighbors $\mathcal{S}$ and deformed hexagons H_λ are periodic sets and one can define their natural quotient sets $\tilde{X} := X/\sim$, $\partial\tilde{X} := \partial X/\sim$, $\tilde{\mathcal{S}} = \mathcal{S}/\sim$, $\tilde{\mathcal{P}} = \mathcal{P}/\sim$, $\tilde{H}_\lambda = H_\lambda/\sim$.

In the periodic case since the definition of E_L^{per} does not allow particles to be moved to infinity, we have to relax the minimization problem in order to get (2.1). A natural idea is to remove L-periodic sets from Hex: if $X \subset Hex$ is L-periodic, we set

$$\tilde{E}_L^{per}(X,\{y\}) = \sum_{\substack{x\in X\cap Q_L\\ x'\in Hex\setminus\{x\}}} V_2(|y(x)-y(x')|) + \sum_{\substack{x_1\in X\cap Q_L\\ x_2\in Hex\setminus\{x_1\}\\ x_3\in Hex\setminus\{x_1,x_2\}}} V_3(y(x_1), y(x_2), y(x_3)).$$

It is clear that $\tilde{E}_L^{per}(Hex,\cdot) = E_L^{per}(\cdot)$. In this sense $\tilde{E}_L^{per}$ is a relaxed version of the original minimization problem. In what follows we drop the tildes and write $\tilde{E}_L^{per}$ as E_L^{per}. The existence of a minimizer (X_{min}, y_{min}) of E_L^{per} is easy since there are only 2^{L^2} possible L-periodic sets. First we have the following periodic version of Lemma 2.3:

Lemma 7.1 (*Minimum distance, periodic version*)**.** *Let $V = V_2 + V_3$ and let V_2 satisfy the same assumption as in Lemma 2.3. Assume only that V_3 is nonnegative (see Remark 7.2). Then there exists a constant $\alpha_0 \in (0, \frac{1}{3})$ such that for any $0 < \alpha < \alpha_0$, $L \in \mathbb{N}$ and all minimizers (X_{min}, Y_{min}) of $E_L^{per}(\cdot,\cdot)$ the minimum distance between the particles satisfies (2.1).*

Proof. WLOG we can assume $L \geq 4$ since the cases $L' = 1, 2, 3$ can be covered by $L = 4L'$. Let M and $\mathcal{A}$ be the same as in the proof of Lemma 2.3. Then clearly the two-body interaction energy of the particles in $\mathcal{A}$ and their periodic images are at least:

$$\sum_{\substack{\{x,x'\}\subset\mathcal{A}\\ x\neq x'}} e(\{x,x'\}) + \sum_{x\in\mathcal{A}} \sum_{x'\in(\mathcal{A}+LHex)\setminus\mathcal{A}} e(\{x,x'\}) \geq \frac{1}{2\alpha} M(M-1) - CM^2\alpha,$$

where $C = Const \sum_{\xi\in LHex\setminus\{0\}} \frac{1}{|\xi|^\beta}$. On the other hand the two-body interaction energy of the particles in $\mathcal{A}$ and other particles in $(X_{min} + LHex)\setminus(\mathcal{A} + LHex)$ can also be bounded from below (compare (2.5), (2.6)):

$$e(\mathcal{A}, (X_{min} + LHex)\setminus(\mathcal{A} + LHex)) \geq -M^2 CC_1 \left(\frac{4}{1-\alpha}\right)^\beta \sum_{k=1}^{\infty} \frac{1}{k^{\beta-1}}.$$

The proof of the above inequality is the same as the proof of (2.5) and (2.6). Finally since the three-body energy is always nonnegative we obtain that

$$\begin{aligned} &\text{total energy due to } \mathcal{A} \\ &\quad \geq \text{total two-body energy due to } \mathcal{A} \\ &\quad \geq \frac{1}{2\alpha} M(M-1) - CM^2\alpha - M^2 CC_1 \sum_{k=1}^{\infty} \frac{1}{k^{\beta-1}}. \end{aligned} \tag{7.1}$$

It is clear that there exists $\alpha_0 > 0$ such that if $\alpha < \alpha_0$ then the last term above is always positive if $M > 1$. Now since a competitor of the minimization problem $E_L^{per}(\cdot, \cdot)$ is $X_{min}\setminus(\mathcal{A} + LHex)$, i.e. the set obtained after removing $\mathcal{A}$ from X_{min}. Clearly by the minimization property of X_{min} we have

$$E(X_{min}, \cdot) \leq E(X_{min}\setminus(\mathcal{A} + LHex, \cdot),$$

which implies that the total energy due to $\mathcal{A}$ must be non-positive. From (7.1) it follows that if $\alpha < \alpha_0$ then $M = 1$, proving the lemma. □

Remark 7.2. It is worth mentioning that in the periodic situation considered here we don't need to assume V_2 or V_3 decay at infinity. However such a condition is needed in the proof of Lemma 2.3.

Definition 7.3 (*Bond and Bond angle, periodic case*)**.** *Two atoms x, x' are said to be α-bonded (w.r.t. the configuration $y : X \to \mathbb{R}^2$) if $1 - \alpha \leq \min_{\xi\in LHex} |y(x) - y(x' + \xi)| \leq 1+\alpha$. For any triple x_0, x_1, x_2, assume x_1, x_0 is α-bonded and x_2, x_0 is α-bonded. Then the bond angle of $\{x_0, x_1, x_2\}$ with center at x_0 is defined as the unique angle $\theta \in [0, \pi]$ such that $\cos\theta = \frac{(y(\tilde{x}_1)-y(x_0))\cdot(y(\tilde{x}_2)-y(x_0))}{|y(\tilde{x}_1)-y(x_0)|\cdot|y(\tilde{x}_2)-y(x_0)|}$. Here $\tilde{x}_i$ is the unique periodic image of x_i such that $|y(x_0) - y(\tilde{x}_i)| = \min_{\xi\in LHex} |y(x_0) - y(x_i + \xi)|$.*

We shall prove the following lemma for V_3 being of the Stillinger-Weber type (1.1). Similar lemmas can be proven for other potentials with necessary modifications.

Lemma 7.4 (*Uniform bond angle, periodic case*). *Assume V_2 satisfies the hypothesis in Lemma 7.1 with the parameter $\alpha < \alpha_0$. Let V_3 be the Stillinger-Weber potential* (1.1) *with the cut-off distance $1 < a < \sqrt{3}$ and β being the adjustable parameter. Assume $\alpha_0 < \alpha - 1$. Then there exist constants $\beta_0 > 0$, $C > 0$, such that if $\beta > \beta_0$, the following holds for any $L \in \mathbb{N}$, all minimizers (X_{min}, Y_{min}) of $E_L^{per}(\cdot, \cdot)$: If $\{x_0, x_1, x_2\} \subset X_{min}$ is such that x_0, x_1 is α-bonded and x_0, x_2 is α-bonded (see Definition 7.3), then the bond angle θ satisfies*

$$\left|\theta - \frac{2\pi}{3}\right| \leq \frac{C}{\sqrt{\beta}}.$$

Proof. WLOG we can assume $L \geq 4$ (see the beginning of the proof of Lemma 7.1). Let $\{x_0, x_1, x_2\}$ be such that $x_0 \in Hex \cap Q_L$, both x_0, x_1 and x_0, x_2 are α-bonded. If we remove x_0 from X_{min} and its periodic images, then we obtain a competitor of X_{min}. Since (X_{min}, y_{min}) is a minimizer of E_L^{per}, we have

$$\begin{aligned}
&\text{total energy due to } x_0 \\
&\quad = \text{total two-body energy due to } x_0 + \text{total three-body energy due to } x_0 \\
&\quad = V_2(x_0, X\backslash x_0) + V_3(x_0, X\backslash x_0) \\
&\quad \leq 0.
\end{aligned} \tag{7.2}$$

On the other hand, $V_2(x_0, X\backslash x_0)$ can be estimated in the same way as (7.1):

$$\begin{aligned}
V_2(x_0, X\backslash x_0) &\geq -C_1\alpha - C_2 \sum_{k=1}^{\infty} \frac{1}{k^{\beta-1}} \\
&\geq -C_3,
\end{aligned} \tag{7.3}$$

where C_1, C_2, C_3 are constants. Since V_3 is always nonnegative, $V_3(x_0, X\backslash x_0) \geq V_3(y(x_0), y(\tilde{x}_1), y(\tilde{x}_2))$, where $\tilde{x}_i$ is the unique periodic image of x_i such that $|y(x_0) - y(\tilde{x}_i)| = \min_{\xi \in LHex} |y(x_0) - y(x_i + \xi)|$. Since $\alpha_0 < a - 1$, by the definition of the Stillinger-Weber potential (1.1) we have

$$V_3(y(x_0), y(\tilde{x}_1), y(\tilde{x}_2)) \geq \lambda \cdot e^{\frac{2\gamma}{1+\alpha_0-\alpha}} (\cos\theta + \frac{1}{2})^2, \tag{7.4}$$

where θ is the bond angle defined in 7.3. From (7.2) (7.3) (7.4), we have

$$(\cos\theta + \frac{1}{2})^2 \leq \frac{C}{\beta}.$$

The lemma is now proved by taking β_0 sufficiently large. □

Combining both Lemmas 7.1 and 7.4, we obtain the following corollary.

Corollary 7.5 (*Minimum distance and uniform bond angle, periodic version*)**.** *There exist positive numbers α_0, β_0, C, such that if $0 < \alpha < \alpha_0$ and $\beta > \beta_0$, then the following holds for any $L \in \mathbb{N}$, and all minimizers (X_{min}, Y_{min}) of $E_L^{per}(\cdot, \cdot)$:*

(1) (*Minimum distance property*).

$$\min_{x \neq x'} \left|y_{min}(x) - y_{min}(x')\right| > 1 - \alpha,$$

(2) (*Uniform bond angle*).
If $\{x_0, x_1, x_2\}$ *are such that both* x_0, x_1 *and* x_0, x_2 *are* α*-bonded* (*see* 7.3)*, then the bond angle* $\theta_{x_1 x_0 x_2}$ *satisfies*

$$\left|\cos\theta_{x_1x_0x_2} + 1/2\right| \le \frac{C}{\sqrt{\beta}}.$$

Proof. This follows directly from Lemmas 7.1 and 7.4. □

Lemma 7.6 (*Lower bound for the total energy, periodic version*)**.** *There exist constants* $C > 0$, $\alpha_0 > 0$, $\beta_0 > 0$ *such that the following holds for any minimizer* (X_{min}, y_{min}) *of the minimization problem* $E_L^{per}(\cdot,\cdot)$*:*

$$\begin{aligned} &E_L^{per}(X_{min}, \{y_{min}\}) \\ &\quad \ge -\frac{3}{2}\#\tilde{X}_{min} + \sum_{\{x,x'\}\in\tilde{\mathcal{S}}} \frac{\theta}{4}\left(|y_{min}(\tilde{x}) - y_{min}(\tilde{x}')| - 1\right)^2 \\ &\qquad + (\frac{3}{2} - C\alpha)\#\partial\tilde{X}_{min} + \frac{1}{12}\sum_{\{x_1,x_2,x_3\}/\sim} V_3(y_{min}(x_1), y_{min}(x_2), y_{min}(x_3)). \end{aligned} \tag{7.5}$$

Proof. This is almost the same as the proof of the main theorem. One simply replaces the sets X, ∂X, $\mathcal{S}$, H_λ by the corresponding quotients $\tilde{X}$, $\partial\tilde{X}$, $\tilde{\mathcal{S}}$, $\tilde{\mathcal{H}}_\lambda$ and the elements of those quotient sets by representatives. See (6.3) for a comparison. We note that the last term on the V_3 potential energy in the above inequality comes from a refined version of Lemma 6.4 (see Remark 6.5). □

Proof of Theorem 1.3. It is rather easy to obtain an upper bound for $E_L^{per}(\cdot,\cdot)$: we can just choose the identity map $y(x) = x$ which is L-periodic for any $L \in \mathbb{N}$, this gives us

$$E_L^{per}(X_{min}, \{y_{min}\}) \le -\frac{3}{2}L^2.$$

By using (7.5) we have

$$\begin{aligned} &\frac{3}{2}(L^2 - \#\tilde{X}_{min}) + (\frac{3}{2} - C\alpha)\#\partial\tilde{X}_{min} + \frac{\theta}{4}\left(|y_{min}(\tilde{x}) - y_{min}(\tilde{x}')| - 1\right)^2 \\ &\quad + \frac{1}{12}\sum_{\{x_1,x_2,x_3\}/\sim} V_3(y_{min}(x_1), y_{min}(x_2), y_{min}(x_3)) \le 0. \end{aligned}$$

For α_0 sufficiently small, this will imply that $L^2 = \#\tilde{X}_{min}$ ($\#\tilde{X}_{min} \le L^2$!), $\partial\tilde{X}_{min} = \emptyset$ and $|y_{min}(x) - y_{min}(x')| = 1$ for all $\{x, x'\} \in \mathcal{S}$. Moreover if any triple $\{x_0, x_1, x_2\}$ is such that $|y(x_0) - y(x_1)| = 1$, $|y(x_0) - y(x_2)| = 1$, then the bond angle $\theta_{x_2x_0x_1} = \frac{2\pi}{3}$. Putting all these together, we find that the set $\Omega = \{y_{min}(x) | x \in Hex\}$ satisfies the following properties:

(1) $\min_{y \ne y'} |y - y'| \ge 1$.
(2) $\left\{y' \in \Omega \,\middle|\, |y - y'| = 1,\ y' \ne y\right\} = 3$ for all $y \in \Omega$.
(3) If $|y_i - y_0| = 1$ for $i = 1, 2$, then the bond angle between the two vectors $y_1 - y_0$, $y_2 - y_0$ is $\frac{2\pi}{3}$.

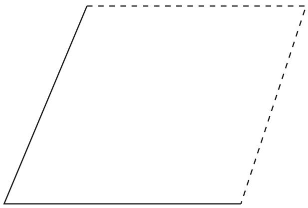

Fig. 5. The fundamental domain Y

It is not hard to show by elementary methods that any such set $\Omega \subset \mathbb{R}^2$ satisfying these properties is countable and there exists a rotation $R \in SO(2)$, a translation vector $\tau \in \mathbb{R}^2$ such that

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

Now since y_{min} is L-periodic, we can just choose $R = Id$ and the proof is finished. □

8. Proof of Corollary 1.4

In what follows it is useful to introduce the following notation: for any three countable sets $A_i \subset \mathbb{R}^2$, $i = 1, 2, 3$, define the two-body and three-body interaction energies:

$$\begin{aligned} V_2(A_1, A_2) &:= \sum_{(y_1, y_2) \in \mathcal{P}_2} V_2(y_1, y_2), \\ V_3(A_1, A_2, A_3) &:= \sum_{(y_1, y_2, y_3) \in A_1 \times A_2 \times A_3} V_3(y_1, y_2, y_3), \end{aligned} \tag{8.1}$$

where

$$\mathcal{P}_2 = (A_1 \times A_2) \backslash \{(y, y) : y \in A_1 \cap A_2\}.$$

The meaning of $\mathcal{P}_2$ is to avoid self-energies in the calculation of total two-body energies. No such restriction is needed for the three-body potential V_3 since its definition already eliminates such possibilities (see (1.1)).

Our first lemma is a simple decay estimate of the interaction energy V_2. Let L be an even natural number which is sufficiently large. Define Y to be the semi-open parallelogram (see Fig. 5) with vertices at $(\frac{3\sqrt{3}}{4}L, \frac{3}{4}L)$, $(-\frac{\sqrt{3}}{4}L, \frac{3}{4}L)$, $(-\frac{3\sqrt{3}}{4}L, -\frac{3}{4}L)$ and $(\frac{\sqrt{3}}{4}L, -\frac{3}{4}L)$. Y can be viewed as a fundamental domain for the periodic lattice $LHex$.

Lemma 8.1. *Let V_2 satisfy Assumption 1.1. Then for any finite set $A \subset \mathbb{R}^2$ and any $\epsilon > 0$, there exists $L_0 = L_0(\epsilon, A) \in \mathbb{N}$, such that if $L > L_\epsilon$, L is an even natural number, then*

$$|V_2(A, (A + LHex) \backslash Y)| < \epsilon, \tag{8.2}$$

and

$$\max_{B \in Y \cap Hex} |V_2(A, (B + LHex) \backslash Y)| < \epsilon. \tag{8.3}$$

Proof. From the decay property of V_2 we have for some constants $C_1, C_2 > 0$,

$$|V_2(A, (A + LHex)\backslash Y)| \leq C_2 \sum_{0 \neq \xi \in Hex} \frac{1}{|L\xi - C_1|^\beta} < \epsilon,$$

if L is sufficiently large. This proves (8.2). The inequality (8.3) is proved the same way. □

As in the proof of Theorem 1.3, to get the lower bound (2.1), we must slightly relax the minimization problem. To this end, define for each $\mathcal{A}' \subset \mathcal{A}$,

$$E(\mathcal{A}', \{y\}) = \sum_{\substack{\{x,x'\} \subset X \\ \{x,x'\} \cap \mathcal{A}' \neq \emptyset}} V_2(|y(x) - y(x')|) + \sum_{\substack{\{x_1,x_2,x_3\} \subset X \\ \{x_1,x_2,x_3\} \cap \mathcal{A} \neq \emptyset}} V_3(y(x_1), y(x_2), y(x_3)),$$

where $X = (Hex\backslash\mathcal{A}) \cup \mathcal{A}'$. As before $E(\mathcal{A}', \cdot) = E_{\mathcal{A}}(\cdot)$ if $\mathcal{A}' = \mathcal{A}$. Now let $(\mathcal{A}_{min}, y_{min})$ be the minimizer of $E(\cdot, \cdot)$. By repeating almost word by word the proof of Corollary 2.7, it is clear that y_{min} satisfies the minimum distance property (2.10) and the uniform bond angle property (2.11).

Having established the two properties (2.10), (2.11) of y_{min}, we can now use $(\mathcal{A}_{min}, y_{min})$ to define a competitor (X_{per}, y_{per}) for a related periodic problem. The idea here is to deduce the properties of $(\mathcal{A}_{min}, y_{min})$ from (X_{per}, y_{per}). To this end let $X_{per} = \mathcal{A}_{min} \cup (Y\backslash A) + LHex$. X_{per} contains the set $\mathcal{A}_{min} \cup (Y\backslash A)$ together with all its L-periodic images. We then define a L-periodic function $y_{per} : X_{per} \to \mathbb{R}^2$ as

$$y_{per}(x) = y_{min}(x - \tau) + \tau, \tag{8.4}$$

where τ is the unique vector in $LHex$ such that $x - \tau \in Y \cap LHex$. We think of (X_{per}, y_{per}) as an admissible function for the minimization problem $E_L^{per}(\cdot, \cdot)$ ($E_L^{per}(\cdot, \cdot)$ is defined in the previous section). The following lemma suggests that, due to the minimization property of (A_{min}, y_{min}) (for the original problem), (X_{per}, y_{per}) is very close to being the true minimizer.

Lemma 8.2 (Upper bound for $E_L^{per}(\mathcal{A}_{per}, y_{per})$). *For any $\epsilon > 0$, there exists $L_\epsilon \in \mathbb{N}$, such that for $L > L_\epsilon$, L being an even natural number, we have,*

$$E_L^{per}(\mathcal{A}_{per}, y_{per}) \leq -\frac{3}{2}L^2 + \epsilon.$$

Proof. Since (A_{min}, y_{min}) is a minimizer for the minimization problem $E(\cdot, \cdot)$, clearly $E(A_{min}, y_{min}) \leq E(A, Id)$, where Id is the identity map. This implies that, by using the notations (8.1),

$$
\begin{aligned}
&E(A_{min}, y_{min})\\
&= \frac{1}{2}V_2(y(A_{min}), y(A_{min})) + V_2(y(A_{min}), Hex\backslash A)\\
&\quad+\frac{1}{2}V_3(y(A_{min}), y(A_{min}), y(A_{min})) + V_3(y(A_{min}), y(A_{min}), (Y \cap Hex)\backslash A)\\
&\quad+\frac{1}{2}V_3(y(A_{min}), (Y \cap Hex)\backslash A, (Y \cap Hex)\backslash A) + \frac{1}{2}V_3((Y \cap Hex)\backslash A, y(A_{min}),\\
&\qquad y(A_{min}))\\
&\quad+V_3((Y \cap Hex)\backslash A, y(A_{min}), (Y \cap Hex)\backslash A)\\
&\le \frac{1}{2}V_2(A, A) + V_2(A, Hex\backslash A) + \frac{1}{2}V_3(A, A, A) + V_3(A, A, (Y \cap Hex)\backslash A)\\
&\quad+\frac{1}{2}V_3(A, (Y \cap Hex)\backslash A, (Y \cap Hex)\backslash A) + \frac{1}{2}V_3((Y \cap Hex)\backslash A, A, A)\\
&\quad+V_3((Y \cap Hex)\backslash A, A, (Y \cap Hex)\backslash A).
\end{aligned}
\tag{8.5}
$$

On the other hand, for $E_L^{per}(X_{per}, y_{per})$, by taking L sufficiently large, we have

$$
\begin{aligned}
&E_L^{per}(X_{per}, y_{per})\\
&= \frac{1}{2}V_2(y(A_{min}), y(A_{min})) + V_2(y(A_{min}), (Y \cap Hex)\backslash A)\\
&\quad+V_2(y(A_{min}), (y(A_{min}) + LHex)\backslash Y) + V_2(y(A_{min}), ((Y \cap Hex)\backslash A + LHex)\backslash Y)\\
&\quad+\frac{1}{2}V_2((Y \cap Hex)\backslash A, (Y \cap Hex)\backslash A) + V_2\left((Y \cap Hex)\backslash A, ((Y \cap Hex)\backslash A\right.\\
&\quad\left.+LHex)\backslash Y\right)\\
&\quad+\frac{1}{2}V_3(y(A_{min}), y(A_{min}), y(A_{min})) + V_3(y(A_{min}), y(A_{min}), (Y \cap Hex)\backslash A)\\
&\quad+\frac{1}{2}V_3(y(A_{min}), (Y \cap Hex)\backslash A, (Y \cap Hex)\backslash A)\\
&\quad+\frac{1}{2}V_3((Y \cap Hex)\backslash A, (Y \cap Hex)\backslash A + LHex, (Y \cap Hex)\backslash A + LHex)\\
&\quad+V_3((Y \cap Hex)\backslash A, (Y \cap Hex)\backslash A, y(A_{min}))\\
&\quad+\frac{1}{2}V_3((Y \cap Hex)\backslash A, y(A_{min}), y(A_{min})).
\end{aligned}
\tag{8.6}
$$

The idea is to rewrite $E_L^{per}(X_{per}, y_{per})$ in terms of $E(A_{min}, y_{min})$. By using the above expressions, we have

$$
\begin{aligned}
E_L^{per}(X_{per}, y_{per}) = {}& E(A_{min}, y_{min}) + \frac{1}{2}V_3((Y \cap Hex)\backslash A, (Y \cap Hex)\backslash A\\
&+LHex, (Y \cap Hex)\backslash A + LHex)\\
&+ (V_2(y(A_{min}), (Y \cap Hex)\backslash A) - V_2(y(A_{min}), Hex\backslash A))\\
&+V_2(y(A_{min}), (y(A_{min}) + LHex)\backslash Y) + V_2(y(A_{min}),\\
&\quad ((Y \cap Hex)\backslash A + LHex)\backslash Y)\\
&+\frac{1}{2}V_2((Y \cap Hex)\backslash A, (Y \cap Hex)\backslash A)\\
&+V_2\left((Y \cap Hex)\backslash A, ((Y \cap Hex)\backslash A + LHex)\backslash Y\right).
\end{aligned}
$$

By using Lemma 8.1 and (8.5), taking L sufficiently large, we then get

$$\begin{aligned} &E_L^{per}(X_{per}, y_{per}) \\ &\leq 6\epsilon + \frac{1}{2}V_3((Y \cap Hex)\backslash A, (Y \cap Hex)\backslash A + LHex, (Y \cap Hex)\backslash A + LHex) \\ &\quad + \frac{1}{2}V_2(A, A) + V_2(A, Hex\backslash A) + \frac{1}{2}V_3(A, A, A) + V_3(A, A, (Y \cap Hex)\backslash A) \\ &\quad + \frac{1}{2}V_3(A, (Y \cap Hex)\backslash A, (Y \cap Hex)\backslash A) + \frac{1}{2}V_3((Y \cap Hex)\backslash A, A, A) \\ &\quad + V_3((Y \cap Hex)\backslash A, A, (Y \cap Hex)\backslash A) \\ &= -\frac{3}{2}L^2 + 6\epsilon. \end{aligned}$$

The last equality follows from writing out explicitly $E_L^{per}(Hex \cap Y, Id)$ (Id here is the identity map) and the fact that $E_L^{per}(Hex \cap Y, Id) = -\frac{3}{2}L^2$. The lemma is proved. □

We are now ready to prove Corollary 1.4.

Proof of Corollary 1.4. Define X_{per} and y_{per} as in (8.4). By Lemma 8.2 and Lemma 7.6, we have for any $\epsilon > 0$, if L is sufficiently large, then

$$\begin{aligned} &\frac{3}{2}(L^2 - \#\tilde{X}_{per}) + (\frac{3}{2} - C\alpha)\#\partial\tilde{X}_{per} + \frac{\theta}{4}\left(|y_{per}(\tilde{x}) - y_{per}(\tilde{x}')| - 1\right)^2 \\ &\quad + \frac{1}{12}\sum_{\{x_1,x_2,x_3\}/\sim} V_3(y_{per}(x_1), y_{per}(x_2), y_{per}(x_3)) \leq \epsilon. \end{aligned}$$

This immediately gives us that $\#\tilde{X}_{per} = L^2$ which in turn implies $A_{min} = A$. Also $\partial\tilde{X}_{per} = \emptyset$, $\big||y_{per}(x) - y_{per}(x')| - 1\big| < C\epsilon$, $\{x, x'\} \in \mathcal{S}$. Similarly any bond angles θ must satisfy $|\theta - \frac{2\pi}{3}| < C\epsilon$. It is clear that all these quantities are independent of L if L is taken sufficiently large. Therefore we conclude that $|y_{per}(x) - y_{per}(x')| = 1$ for all $\{x, x'\} \in \mathcal{S}$ and all bond angles are $\frac{2\pi}{3}$. By repeating the same argument as in the end of the proof of Theorem 1.3, we conclude that the set $\Omega = \{y_{per}(x) | x \in Hex\} = Hex + \tau$ for some $\tau \in \mathbb{R}^2$. Since $y_{per}(x) = y_{min}(x)$ for any $x \in A$. We obtain $\tau = 0$ and the proof of the corollary is finished. □

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9. Appendix

9.1. Geometric rigidity. The following lemma was proved in [14]. It is a generalization of an earlier result by F. John [6].

Proposition 9.1 (*Local rigidity implies global rigidity, L^∞ estimate*). *There exists a universal constant $\alpha \in (0, \frac{1}{2})$ such that for any pair of domains $\Omega' \subset \Omega \subset \mathbb{R}^d$ with the property $\inf_{x\in\Omega'} dist(x, \partial\Omega) \geq \frac{\sqrt{2\alpha}}{1-2\alpha} diam(\Omega')$ and all maps $u \in W^{1,\infty}(\Omega)$ satisfying $\|\nabla u - SO(d)\|_{L^\infty(\Omega)} \leq \alpha$ the estimate*

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

holds.

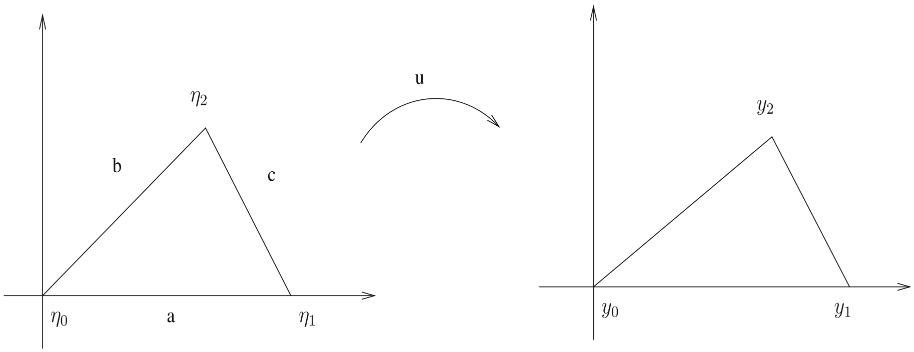

Fig. 6. The deformed triangles

Proof. See Proposition 4.1 of [14]. □

Lemma 9.2 (*Local distortion estimate*). *Let a, b, c be the side lengths of some triangle in $\mathbb{R}^2$. Then there exist constants $K = K(a, b, c)$, $\alpha_0 = \alpha_0(a, b, c)$ such that for each pair of triples $y_i, \eta_i \in \mathbb{R}^2$, $i = 0, 1, 2$, with the properties:*

(1) *η_i is the vertex of a triangle in $\mathbb{R}^2$ with side lengths a, b, c.*
(2) $\det(y_1 - y_0, y_2 - y_0)\det(\eta_1 - \eta_0, \eta_2 - \eta_0) \geq 0$.
(3) $\Big||y_i - y_j| - |\eta_i - \eta_j|\Big| \leq \alpha_0$, *for any $i \neq j$.*

The following inequality holds:

$$\min_{R\in SO(2)} \|F - R\|_F \leq K \max_{i\neq j}\Big||y_i - y_j| - |\eta_i - \eta_j|\Big|,$$

where $\|\cdot\|_F$ is the usual matrix Frobenius norm. The matrix $F \in \mathbb{R}^{2\times 2}$ is the gradient of the unique affine map $u : conv\{\eta_0, \eta_1, \eta_2\} \to \mathbb{R}^2$ satisfying $u(\eta_i) = y_i$ for $i = 0, 1, 2$.

Proof. WLOG we can assume $\eta_0 = y_0 = 0$ and they are aligned as in Fig. 6. Then the matrix $F = F(\epsilon_1, \epsilon_2, \epsilon_3; a, b, c)$ is a linear map such that $F\eta_i = y_i$, $i = 0, 1, 2$. Moreover $F(0, 0, 0; a, b, c)$ is the identity matrix. It is not difficult to see that $F(\cdot; a, b, c)$ is continuously differentiable in a small neighborhood of $(0, 0, 0)$. Then clearly we have

$$\|F - Id\|_F \leq K \max_i |\epsilon_i|.$$

The lemma is proved. □

9.2. Proof of Proposition 4.3. The first lemma gives the existence of local discrete imbedding into the perfect hexagonal lattice.

Lemma 9.3 (*Existence of local discrete imbedding*). *There exist constants $\alpha_0 > 0$, $\beta_0 > 0$ such that for any $0 < \alpha < \alpha_0$, $\beta > \beta_0$, the following holds true for any state y satisfying 3.1: Let x be a regular atom such that $\mathcal{N}^{(3)}(x)$ consists of regular atoms. Let $\xi, \xi' \in Hex$ such that $|\xi - \xi'| = 1$. Then there exists a unique imbedding $\Phi : \mathcal{N}^{(3)}(x) \to Hex$, such that $\Phi(x) = \xi$ and $\Phi(x') = \xi'$.*

Proof. This is not hard to show by elementary geometry. □

The next proposition says that when the patch is sufficiently away from the defected atoms ∂X_N, it is possible to imbed the defect free patch into the perfect hexagonal lattice Hex.

Proposition 9.4 (*Existence of global imbedding*). *There exist constants $\alpha_0 > 0$, $\beta_0 > 0$ and $K > 0$ such that for any $0 < \alpha < \alpha_0$, $\beta > \beta_0$, the following holds for any state y satisfying 3.1: Let $\Omega' \subset \Omega \subset \mathbb{R}^2$ with the properties $dist(\Omega', \partial\Omega) \geq 3diam(\Omega')+20$, Ω is convex and $\Omega \cap y(\partial X_N) = \emptyset$. Then there exists a discrete imbedding $\Phi : \omega \to Hex$, where $\omega = y^{-1}(\Omega')$ such that the following assertions hold:*

(1) *ϕ is unique up to rotation and translation, i.e. for any other imbedding $\phi' : \omega \to D$, there exists a rotation matrix $R \in SO(2)$ such that*

$$\phi(x) - \phi(x') = R(\phi'(x) - \phi'(x')) \qquad \forall\, x, x' \in \omega \tag{9.1}$$

(2) *ϕ satisfies the rigidity estimate*

$$\sup_{\{x,x'\}\subset\omega} \left| \frac{|\phi(x) - \phi(x')|}{|y(x) - y(x')|} - 1 \right| \leq K \min\{\alpha, \frac{1}{\sqrt{\beta}}\}. \tag{9.2}$$

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

$$\phi(\omega) \supset B(\phi(x), r/2) \cap Hex. \tag{9.3}$$

Proof. Step 1 (Existence and uniqueness of the imbedding Φ). Define $\Omega_2 = \{\eta \in \Omega | dist(\eta, \partial\Omega) \geq 2\}$. It can be shown by simple topological arguments that

$$\Omega_2 \subset \bigcup_{H\in H_1} conv(y(H)). \tag{9.4}$$

The map Φ can be defined on $y^{-1}(\Omega_2)$ which is larger than the set $\omega = y^{-1}(\Omega')$. The construction of the map Φ follows by extending the local imbedding map obtained for Lemma 9.3. The uniqueness of the map Φ can be proved using so called Burgers vectors and the fact that in defect-free patches the closed paths can be deformed to a point. Instead of repeating the existing arguments, we refer interested readers to Proposition 4.8 of [14] for more details.

Step 2 (Proof of the rigidity estimate and surjectivity). The affine map u is defined by interpolating the values $u(y(x)) = \Phi(x)$ for $x \in H$. By (9.4) the definition of u can then be extended continuously to Ω_2. Obviously $u \in W^{1,\infty}(\Omega_2)$. By Lemma 9.2 $\|\nabla u - SO(2)\|_{L^\infty(\Omega_2)} \leq K \min\{\alpha, \frac{1}{\sqrt{\beta}}\}$. Proposition 9.1 then gives

$$\sup_{\{\eta,\eta'\}\in\Omega'} \left| \frac{|u(\eta) - u(\eta')|}{|\eta - \eta'|} - 1 \right| \leq K \min\{\alpha, \frac{1}{\sqrt{\beta}}\},$$

which implies (9.2). The surjectivity (9.3) follows from the above estimate and the invariance of domain theorem. □

Proof of Lemma 4.2. Let $z = \frac{1}{6}\sum_{x\in H} y(x)$, $\Omega = B(z, 100\lambda)$ and $\Omega' = B(z, 10\lambda)$. It is clear that $dist(\Omega', \partial\Omega) \geq 90\lambda \geq 3diam(\Omega') + 20$. Consequently Proposition 9.4 implies that there exists a discrete imbedding $\Phi : y^{-1}(\Omega') \to Hex$ such that:

1) Φ coincides with Φ_T up to rotation and translation,
2) (9.2) is satisfied.

The lemma is proved. □

Proof of Proposition 4.3. (1) *Step 1.* Let $H_1, H_2 \in \cup_{\lambda\in\Lambda\backslash\{1\}} H_\lambda$ such that $H_1 \neq H_2$. For $i = 1, 2$, denote by λ_i, ω_i and Φ_i the associated side-lengths, domains and discrete imbeddings. We first show that $\lambda_1 = \lambda_2$. WLOG assume that $\lambda_1 \leq \lambda_2$ and let $z = \frac{1}{2}(y(x_1) + y(x_2))$. For α sufficiently small and β sufficiently large, Lemma 4.2 implies that $\frac{2}{3}\lambda_2 \leq |y(x_1) - y(x_2)| \leq \frac{4}{3}\lambda_1$, $\lambda_2 \leq 2\lambda_1$ and $\max_{i=1,2}\left|z - \frac{1}{6}\sum_{x\in H_i} y(x)\right| \leq \lambda_2$. Let $\Omega = B(z, 30\lambda_1)$ and $\Omega' = B(z, 2\lambda_1)$. Clearly by (4.4) $\omega = y^{-1}(\Omega') \subset \omega_1 \cap \omega_2$ and $\{x_1, x_2\} \subset \omega$. By Proposition 9.4 there exists a discrete imbedding $\Phi : \omega \to Hex$ and matrices $Q_1, Q_2 \in SO(2)$ such that

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

for any $x' \in \omega$. In particular choosing $x' = x_2$ gives us $\lambda_1 = \lambda_2$.
Step 2. Let $H_3 \in H_\lambda$ be such that $\{x, x'\} \subset H_3$ with associated imbedding Φ_3 for which $|\Phi_3(x) - \Phi_3(x')| = \lambda$. We now show that H_3 either coincides with H_1 or H_2. By the same argument as in Step 1 above we can assume $\Phi_3(x) = \Phi(x)$ for all $x \in \omega$. Let $\{x_3\} = \left(H_3\backslash\{x, x'\}\right) \cap \mathcal{N}(x_1)$. Proposition 9.4 shows that $\Phi(x_3)$ either coincides with $\left(H_1\backslash\{x, x'\}\right) \cap \mathcal{N}(x_1)$ or $\left(H_2\backslash\{x, x'\}\right) \cap \mathcal{N}(x_1)$. It is an elementary fact to show that two (undeformed) hexagons sharing three vertices necessarily coincide with each other. We conclude that $\Phi(H_3) = \Phi(H_1)$ or $\Phi(H_3) = \Phi(H_2)$. Equivalently H_3 coincides with H_1 or H_2.
(2) Let $z = \frac{y(x_1)+y(x_2)}{2}$, $\Omega = B(z, 300|y(x_1) - y(x_2)|)$ and $\Omega' = B(z, 30|y(x_1) - y(x_2)|)$. Proposition 9.4 implies that there exists a discrete imbedding $\Phi : \omega = y^{-1}(\Omega') \to Hex$ such that $B(\Phi(x_1), 10\lambda) \cap Hex \subset \Phi(\omega)$, where $\lambda = |\Phi(x_1) - \Phi(x_2)|$. Let $Q_\pm \in SO(2)$ be the rotation by $\frac{2\pi}{3}$ in the clockwise (+) and counter-clockwise (−) direction. Since the perfect hexagonal lattice Hex is invariant under $Q_\pm$, it is not difficult to check that there exist two (undeformed) hexagons $\tilde{H}_1, \tilde{H}_2 \subset Hex$ with side-lengths λ and such that $\{\Phi(x_1), \Phi(x_2)\} \subset \tilde{H}_1 \cap \tilde{H}_2$. Clearly $\tilde{H}_1 \cup \tilde{H}_2 \subset B(\Phi(x_1), 10\lambda) \cap Hex$ and this implies that $\Phi^{-1}(\tilde{H}_1), \Phi^{-1}(\tilde{H}_2)$ are the desired two hexagons.
(3) This claim follows directly from (2) above. □

Proof of Proposition 4.4. The proof is identical to the proof of Proposition 4.3 above and therefore will be omitted here. □

Proof of Proposition 4.5. We divide the proof into three parts.
Proof of (4.5): For each $x \in X$ and $\lambda \in \Lambda$ define

$$s(x, \lambda) = \#\{H \in H_\lambda | x \in H\}.$$

$s(x, \lambda)$ records the number of deformed hexagons with side length approximately λ and having x as a vertex. First we have the identity

$$\sum_{x\in X} s(x, \lambda) = 6\# H_\lambda$$

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

$$s(x, \lambda) \leq m(\lambda)s(x, 1), \tag{9.5}$$

where $m(\lambda)$ was defined in (4.1). Inequality (9.5) is trivial if $s(x, \lambda) = 0$ or $\lambda = 1$. Therefore now assume $s(x, \lambda) \geq 1$ and $\lambda > 1$. First we show that $s(x, 1) = 3$. Let $\Omega = B(y(x), 60\lambda)$, $\Omega' = B(y(x), 4\lambda)$ and $\omega = y^{-1}(\Omega')$. The definition of H_λ gives that $\Omega \cap y(\partial X_N) = \emptyset$ and therefore by Proposition 9.4 we can construct a discrete imbedding $\Phi : \omega \to Hex$. This immediately gives $s(x, 1) = 3$. On the other hand by using again the imbedding Φ, any $H \in H_\lambda$ containing the vertex x is uniquely determined by a pair $\{\eta_1, \eta_2\} \subset Hex$ which satisfies $|\eta_1 - \Phi(x)| = |\eta_2 - \Phi(x)| = \lambda$. (We only need three vertices to determine uniquely a hexagon!) The number of such pairs can be expressed as $\#\{Hex \cap \{|\xi| = \lambda\}\}$. By formula (4.1) this gives $s(x, \lambda) \leq 3m(\lambda)$ which is the bound (9.5).

For the other direction, consider $\lambda > 1$, $x \in X$ with $s(x, \lambda) < 3m(\lambda)$. By Proposition 4.3 there exists $x_b \in \partial X_N$ such that $y(x_b) \in B(y(x), 310\lambda)$. Since the minimum distance between particles is bounded from below by $1/2$, we have

$$\#y^{-1}(B(y(x_b), 310\lambda)) \leq C\lambda^2. \tag{9.6}$$

By inequality (9.5) we have that the number of deformed hexagons H in H_λ which have at least one vertex lying in $B(y(x_b), 310\lambda)$ is bounded by $C\lambda^2 m(\lambda)$. The proof of (4.5) is now finished.

Proof of (4.6). For each $H \in H_\lambda$ and $S \in H_1$, we define

$$\mu(S, H) = \frac{meas(conv(y(S)) \cap conv(y(H)))}{meas(conv(y(S)))},$$

and also

$$n(S, \lambda) = \sum_{H \in H_\lambda} \mu(S, H).$$

If $dist(y(S), y(\partial X_N)) > 300\lambda$, then by applying again Proposition 9.4 we obtain a discrete imbedding $\Phi : \ \omega = y^{-1}(B(y(x), 10\lambda)) \to Hex$, where $x \in S$ is a vertex. In the perfect hexagonal lattice there are precisely $3m(\lambda)$ different hexagons with side length λ which contains a given vertex x. This implies that

$$n(S, \lambda) = m(\lambda)\lambda^2.$$

If $dist(y(S), y(\partial X_N)) \leq 300\lambda$, then clearly $n(S, \lambda) \leq m(\lambda)\lambda^2$ since we have fewer hexagons with side length λ. Now we have for each $\lambda \in \Lambda \backslash \{1\}$:

$$\begin{aligned}
&\sum_{H \in H_\lambda} meas(conv(y(H))) \\
&= \sum_{H \in H_\lambda} \sum_{S \in S_1} meas(conv(y(S)) \cap conv(y(H))) \\
&= \sum_{S \in H_1} n(S, \lambda) meas(conv(y(S)) \\
&\leq m(\lambda)\lambda^2 \sum_{S \in H_1} meas(conv(y(S))).
\end{aligned}$$

The opposite direction is proved similarly:

$$\begin{aligned}
&\sum_{H\in H_\lambda} meas(conv(y(H)))\\
&\geq \lambda^2 m(\lambda)\Big(\sum_{S\in H_1} meas(conv(y(S))) - \sum_{\substack{S\in H_1\\ dist(y(S),y(\partial X_N))\leq 300\lambda}} meas(conv(y(S)))\Big)\\
&\geq \lambda^2 m(\lambda)\Big(\sum_{S\in H_1} meas(conv(y(S))) - C\lambda^2\#\partial X\Big),
\end{aligned}$$

where the last inequality is due to the fact that for each $x\in\partial X_N$ there are at most $C\lambda^2$ hexagons with side length 1 within a disk of radius λ^2.
Proof of (4.7). This follows easily from the inequality (9.5) and (9.6). □

10. Distortion Estimates

Lemma 10.1. *Let $L\geq 2$ be an integer. Assume $v:[0,L]\to\mathbb{R}^2$ is piecewise linear in the sense that for any $n=0,1,\cdots,L-1$ and any s with $n\leq s<n+1$, the value of $v(s)$ is a linear interpolation of $v(n)$ and $v(n+1)$, i.e.:*

$$v(s)=v(n)+(s-n)\left(v(n+1)-v(n)\right). \tag{10.1}$$

Assume $v(0)=v(L)$. Then there exists an absolute constant $C>0$, such that

$$\|v-\bar v\|_{L^\infty([0,L])}\leq C\sqrt{\log L}\,\|v\|_{\dot H^{\frac12}([0,L])},$$

where $\bar v$ is the average of v on $[0,L]$, i.e.:

$$\bar v=\frac{1}{L}\int_0^L v(s)ds,$$

also

$$\|v\|^2_{\dot H^{\frac12}([0,L])}=\sum_{k\in\mathbb{Z}}|k||\hat v(k)|^2,$$

and

$$\hat v(k)=\frac{1}{L}\int_0^L v(s)e^{-2\pi ik\frac{s}{L}}ds.$$

Proof. WLOG we can assume that $\bar v=0$. By using (10.1), it is not difficult (after some algebra) to find that for any $k\in\mathbb{Z}$, $k\neq 0$:

$$\hat v(k)=\left(\frac{\sin\frac{\pi k}{L}}{\frac{\pi k}{L}}\right)^2\cdot\frac{1}{L}\sum_{n=0}^{L-1}v(n)e^{-2\pi i\frac{k}{L}n}.$$

This implies that if $k \in \mathbb{Z}$, $-\frac{L}{2} + 1 < k \leq \frac{L}{2}$, then

$$\sum_{m\in\mathbb{Z}} |\hat{v}(k+mL)| \leq \left(\sum_{m=1}^{\infty} \frac{C_1}{m^2}\right) |\hat{v}(k)| \\ \leq C_2 |\hat{v}(k)|,$$

where C_1 and C_2 are absolute constants. Now by using the definition of Fourier transform and use of the fact that $\hat{v}(mL) = 0$ for any $m \in \mathbb{Z}$, we have

$$\begin{aligned}\|v\|_{L^\infty([0,L])} &\leq \sum_{k\in\mathbb{Z}} |\hat{v}(k)| = \sum_{-\frac{L}{2}+1<k\leq\frac{L}{2}, k\neq 0} \sum_{m\in\mathbb{Z}} |\hat{v}(k+mL)| \\ &\leq C_3 \sum_{-\frac{L}{2}+1<k\leq\frac{L}{2}, k\neq 0} |\hat{v}(k)| \\ &\leq C_3 \Big(\sum_{-\frac{L}{2}+1<k\leq\frac{L}{2}, k\neq 0} |k||\hat{v}(k)|^2\Big)^{\frac{1}{2}} \cdot \Big(\sum_{-\frac{L}{2}+1<k\leq\frac{L}{2}, k\neq 0} \frac{1}{|k|}\Big)^{\frac{1}{2}} \\ &\leq C\sqrt{\log L}\, \|v\|_{\dot{H}^{\frac{1}{2}}([0,L])},\end{aligned}$$

where C_3 and C are absolute constants. The lemma is proved. □

Lemma 10.2. *Let Ω be a bounded Lipschitz domain in $\mathbb{R}^n$, $n \geq 2$. There exists a constant $C(\Omega)$ with the following property: For each $v \in W^{1,2}(\Omega, \mathbb{R}^n)$ there is an associated rotation $R \in SO(n)$ such that*

$$\|\nabla v - R\|_{L^2(\Omega)} \leq C(\Omega)\|dist(\nabla v, SO(n))\|_{L^2(\Omega)}.$$

Remark 10.3. As was also shown in [2], Lemma 10.2 is invariant under uniform scaling and translation of the domain. For example, the same constant C serves for $\lambda\Omega + c$, where $\lambda > 0$ is any constant and $c \in \mathbb{R}^n$. This important observation will be used below.

Proposition 10.4. *Let $M \in \mathbb{N}$ and $\Omega = conv\left\{\binom{0}{0}, M\binom{-\frac{3\sqrt{3}}{2}}{-\frac{3}{2}}, M\binom{\frac{\sqrt{3}}{2}}{-\frac{3}{2}}\right\}$ be a dilated right triangle. Then there exists an absolute constant $C > 0$ such that for all $u : \Omega \cap Hex \to \mathbb{R}^2$, we have the estimate:*

$$\begin{aligned}\min_{\substack{\tau\in\mathbb{R}^2\\ R\in SO(2)}} \max_{x\in\partial\Omega\cap Hex} |u(x) - \tau - Rx|^2 \leq C\log(M)\Big(&\sum_{\substack{x,x'\in\Omega\cap Hex\\ |x-x'|=1}} ||u(x) - u(x')| - 1|^2 \\ &+ \sum_{\substack{x,x'\in\Omega\cap Hex\\ |x-x'|=\sqrt{3}}} ||u(x) - u(x')| - \sqrt{3}|^2 + \sum_{\substack{x,x'\in\partial\Omega_1\cap Hex\\ |x-x'|=2}} \big||u(x) - u(x')| - 2\big|^2\Big),\end{aligned} \tag{10.2}$$

where $\partial\Omega_1$ is the line segment connecting $\binom{0}{0}$ and $M\binom{-\frac{3\sqrt{3}}{2}}{-\frac{3}{2}}$.

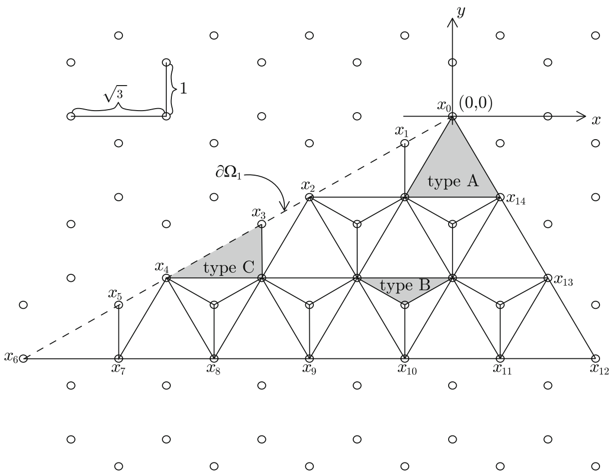

Fig. 7. The set Ω_M when $M = 3$

Proof. Define a triangulation as shown in Fig. 7. By using this triangulation, we can then extend u to a continuous map in $W^{1,\infty}(\Omega)$ by interpolation. We shall first estimate the local distortion of ∇u. As was shown in the figure, we label three different types of triangles by letters A, B and C. Using Lemma 9.2, we discuss three cases:

Case 1. Triangles of type A. Here $\{x_1, x_2, x_3\} \subset Hex$ is such that $|x_i - x_j| = \sqrt{3}$ whenever $i \neq j$. Then clearly for $x \in conv\{x_1, x_2, x_3\}$, we have

$$dist(\nabla u(x), SO(2)) \leq K \sum_{i \neq j} \Big| |u(x_i) - u(x_j)| - \sqrt{3} \Big|. \tag{10.3}$$

Case 2. Triangles of type B. In this case $\{x_1, x_2, x_3\} \subset Hex$ is such that $|x_2 - x_1| = |x_3 - x_1| = 1$ and $|x_2 - x_3| = \sqrt{3}$. Then for $x \in conv\{x_1, x_2, x_3\}$,

$$\begin{aligned} dist(\nabla u(x), SO(2)) \leq K \bigg(&\Big| |u(x_2) - u(x_1)| - 1 \Big| + \Big| |u(x_3) - u(x_1)| - 1 \Big| \\ &+ \Big| |u(x_2) - u(x_3)| - \sqrt{3} \Big| \bigg). \end{aligned} \tag{10.4}$$

Case 3. Triangles of type C. Here $\{x_1, x_2, x_3\} \subset Hex$ is such that $|x_1 - x_3| = 2$, $|x_1 - x_2| = \sqrt{3}$ and $|x_2 - x_3| = 1$. Then for $x \in conv\{x_1, x_2, x_3\}$,

$$\begin{aligned} dist(\nabla u(x), SO(2)) \leq K \bigg(&\Big| |u(x_1) - u(x_3)| - 2 \Big| + \Big| |u(x_1) - u(x_2)| - \sqrt{3} \Big| \\ &+ \Big| |u(x_2) - u(x_3)| - 1 \Big| \bigg). \end{aligned} \tag{10.5}$$

Next by Lemma 10.2, there exists a constant C independent of M and u, such that for each u, we can find $R \in SO(2)$ with the property

$$\int_\Omega |\nabla u - R|^2 \leq C \int_\Omega dist(\nabla u, SO(2))^2. \tag{10.6}$$

We now define

$$\tilde{u}(x) = u(x) - Rx,$$

and consider the set $\partial\Omega \cap Hex$. As shown in the figure, we can label the set in the counter-clockwise direction such that $\partial\Omega \cap Hex = \{x_i\}_{i=0}^{5M-1}$. It is convenient to denote $x_{5M} = x_0$. Finally we define a function $v : [0, 5M] \to \partial\Omega$ by interpolation as follows: for any $i = 0, 1, \cdots, 5M-1$ and any $i \le s \le i+1$,

$$v(s) = \tilde{u}(x_i) + (s-i)(\tilde{u}(x_{i+1}) - \tilde{u}(x_i)).$$

Roughly speaking, the function v can be regarded as the trace of the function $\tilde{u}$ on the boundary $\partial\Omega$. By the standard trace theorem, we have

$$\begin{aligned} \|v\|^2_{\dot{H}^{\frac{1}{2}}([0,5M])} &\le C \int_\Omega |\nabla \tilde{u}|^2 \\ &= C \int_\Omega |\nabla u - R|^2, \end{aligned}$$

where the constant C is independent of M. Finally by Lemma 10.1 and (10.6), we conclude that

$$\|v - \bar{v}\|_{L^\infty([0,5M])} \le C \int_\Omega dist(\nabla u, SO(2))^2.$$

Our desired inequality now follows easily by using (10.3), (10.4), (10.5) and writing everything out explicitly. The proposition is proved. □

The purpose of Proposition 10.4 is to bound global distortions in terms of the sum of all local distortions inside the domain. However the inequality (10.2) is not entirely satisfactory in the sense that the RHS still contains the distortions of edges of length 2. To eliminate such terms and upgrade Proposition 10.4, we make the following simple observation: for any $x, x' \in Hex$ such that $|x - x'| = 2$, there exists a unique (perfect) hexagon $H = \{x_i\}_{i=1}^6$ of side length 1 such that $\{x, x'\} \subset H$. Furthermore there are constants $K > 0$, $\delta_0 > 0$ such that if $0 < \delta < \delta_0$ and a map $u : Hex \to \mathbb{R}^2$ satisfies:

$$\sum_{\substack{\{x_i,x_j\}\subset H \\ |x_i - x_j| = 1}} \Big| |u(x_i) - u(x_j)| - 1 \Big| + \sum_{\substack{\{x_i,x_j\}\subset H \\ |x_i - x_j| = \sqrt{3}}} \Big| |u(x_i) - u(x_j)| - \sqrt{3} \Big| < \delta, \quad (10.7)$$

then we have

$$\begin{aligned} &\Big| |u(x) - u(x')| - 2 \Big| \\ &\quad \le K \Bigg(\sum_{\substack{\{x_i,x_j\}\subset H \\ |x_i - x_j| = 1}} \Big| |u(x_i) - u(x_j)| - 1 \Big| + \sum_{\substack{\{x_i,x_j\}\subset H \\ |x_i - x_j| = \sqrt{3}}} \Big| |u(x_i) - u(x_j)| - \sqrt{3} \Big| \Bigg). \end{aligned} \quad (10.8)$$

Inequality (10.8) expresses the obvious geometric fact (see Fig. 8) that if 6 side edges and 3 cord edges (edges of length approximately $\sqrt{3}$) of a deformed hexagon are held fixed, then the lengths of the rest of the edges are also fixed (or uniquely determined). From this we obtain the following more useful proposition:

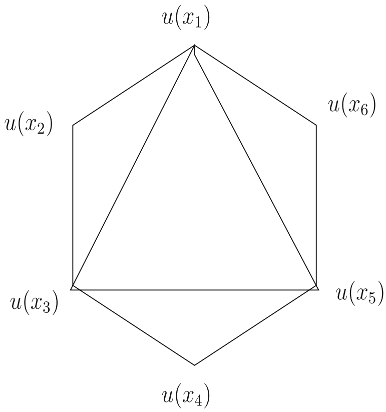

Fig. 8. The deformed hexagon

Proposition 10.5. *Let $M \in \mathbb{N}$ and $\Omega = conv\left\{\binom{0}{0}, M\binom{-\frac{3\sqrt{3}}{2}}{-\frac{3}{2}}, M\binom{\frac{\sqrt{3}}{2}}{-\frac{3}{2}}\right\}$ be a dilated right triangle. Let $u : \Omega \cap Hex$ be rigid on the boundary in the sense that u satisfies the estimate (10.8) for any hexagon H of side length 1 with $H \cap \partial\Omega_1 \neq \emptyset$. Then there exists an absolute constant $C > 0$ such that:*

$$\begin{aligned}\min_{\substack{\tau\in\mathbb{R}^2\\ R\in SO(2)}} \max_{x\in\partial\Omega\cap Hex} |u(x)-\tau-Rx|^2 &\le C\log(M)\Big(\sum_{\substack{x,x'\in\Omega\cap Hex\\ |x-x'|=1}} ||u(x)-u(x')|-1|^2\\ &+\sum_{\substack{x,x'\in\Omega\cap Hex\\ |x-x'|=\sqrt{3}}} ||u(x)-u(x')|-\sqrt{3}|^2+\sum_{H\cap\partial\Omega_1\neq\emptyset}\sum_{\substack{\{x,x'\}\subset H\\ |x-x'|=1}} ||u(x)-u(x')|-1|^2\\ &+\sum_{H\cap\partial\Omega_1\neq\emptyset}\sum_{\substack{\{x,x'\}\subset H\\ |x-x'|=\sqrt{3}}} ||u(x)-u(x')|-\sqrt{3}|^2\Big), \end{aligned} \tag{10.9}$$

where $\partial\Omega_1$ is the line segment connecting $\binom{0}{0}$ and $M\binom{-\frac{3\sqrt{3}}{2}}{-\frac{3}{2}}$.

Proof. This follows directly from Proposition 10.4 together with the estimate (10.8). □

Our next proposition bounds the deformation of any big deformed hexagon of side length λ in terms of the small deformed hexagons (of side length 1) inside.

Proposition 10.6. *There is an absolute constant $C > 0$ such that the following holds for any $H \in H_\lambda$ and $\lambda > 1$:*

$$\begin{aligned}&\sum_{\substack{\{x,x'\}\subset H\\ |\Phi(x)-\Phi(x')|=\lambda}} \Big||y(x)-y(x')|-\lambda\Big|^2+\sum_{\substack{\{x,x'\}\subset H\\ |\Phi(x)-\Phi(x')|=\sqrt{3}\lambda}} \Big||y(x)-y(x')|-\sqrt{3}\lambda\Big|^2\\ &\le C\log\lambda \sum_{\substack{S\in H_1\\ y^{-1}(S)\subset\omega_H}} \Bigg(\sum_{\substack{\{x,x'\}\subset S\\ |\Phi(x)-\Phi(x')|=1}} \Big||y(x)-y(x')|-1\Big|^2+\sum_{\substack{\{x,x'\}\subset S\\ |\Phi(x)-\Phi(x')|=\sqrt{3}}} \Big||y(x)-y(x')|-\sqrt{3}\Big|^2\Bigg),\end{aligned}$$

where ω_H is already defined in (4.4).

Proof. Let $H \in H_\lambda$ and $\{x, x'\} \subset H$. We discuss two cases.

Case 1. $|\Phi(x) - \Phi(x')| = \lambda$. Then by a geometric argument we can find an integer M with $M \le \lambda \le 2M$ and a translation vector $\tau \in Hex$ such that

$$\{t\Phi(x) + (1-t)\Phi(x') : 0 \le t \le 1\} \subset \tau + \Omega_M,$$

where $\Omega_M = conv\left\{\binom{0}{0}, M\binom{-\frac{3\sqrt{3}}{2}}{-\frac{3}{2}}, M\binom{\frac{\sqrt{3}}{2}}{-\frac{3}{2}}\right\}$. By the definition of ω_H, it is clear that if $S \in H_1$ satisfies $\Phi(S) \cap (\tau + \Omega_M) \ne \emptyset$, then we must have the inclusion $y^{-1}(S) \subset \omega_H$. By this and using Proposition 10.5, we conclude that

$$|\Phi(x) - \Phi(x')| \le C \log\lambda \sum_{\substack{S \in H_1 \\ y^{-1}(S) \subset \omega_H}} \Bigg(\sum_{\substack{\{x,x'\} \subset S \\ |\Phi(x) - \Phi(x')| = 1}} \Big| |y(x) - y(x')| - 1 \Big|^2 + \sum_{\substack{\{x,x'\} \subset S \\ |\Phi(x) - \Phi(x')| = \sqrt{3}}} \Big| |y(x) - y(x')| - \sqrt{3} \Big|^2 \Bigg),$$

where C is some absolute constant.

Case 2. $|\Phi(x) - \Phi(x')| = \sqrt{3}\lambda$. This is essentially the same as in Case 1. The proposition is proved. □

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