CRYSTALLIZATION TO THE SQUARE LATTICE FOR A TWO-BODY POTENTIAL

LAURENT BÉTERMIN, LUCIA DE LUCA, AND MIRCEA PETRACHE

ABSTRACT. We consider two-dimensional zero-temperature systems of N particles to which we associate an energy of the form

$$\mathcal{E}[V](X) := \sum_{1\leq i<j\leq N} V(|X(i)-X(j)|),$$

where $X(j)\in\mathbb{R}^2$ represents the position of the particle j and $V(r)\in\mathbb{R}$ is the pairwise interaction energy potential of two particles placed at distance r. We show that under suitable assumptions on the single-well potential V, the ground state energy per particle converges to an explicit constant $\overline{\mathcal{E}}_{\rm sq}[V]$ which is the same as the energy per particle in the square lattice infinite configuration. We thus have

$$N\overline{\mathcal{E}}_{\rm sq}[V] \leq \min_{X:\{1,\dots,N\}\to\mathbb{R}^2} \mathcal{E}[V](X) \leq N\overline{\mathcal{E}}_{\rm sq}[V] + O(N^{\frac{1}{2}}).$$

Moreover $\overline{\mathcal{E}}_{\rm sq}[V]$ is also re-expressed as the minimizer of a four point energy.

In particular, this happens if the potential V is such that $V(r)=+\infty$ for $r<1$, $V(r)=-1$ for $r\in[1,\sqrt{2}]$, $V(r)=0$ if $r>\sqrt{2}$, in which case $\overline{\mathcal{E}}_{\rm sq}[V]=-4$.

To the best of our knowledge, this is the first proof of crystallization to the square lattice for a two-body interaction energy.

CONTENTS

1. Introduction 2
1.1. Our energy minimization problem 2
1.2. Description of the main results 3
1.3. Previous results on the optimality of the square lattice 7
1.4. Previous literature on the triangular lattice and comparison with our results 7
1.5. Summary of hypotheses on V used throughout the paper 9
2. Proof of Theorem 1.1 11
3. Smoothed potentials and proof of Theorem 1.2 13
3.1. Minimum distance between points for minimizers 13
3.2. Combinatorial setup 15
3.3. Local rigidity of configurations 17
3.4. Minima of 4-point energy and perturbed potentials 19

Date: October 23, 2019.

Acknowledgments: LB acknowledges support by VILLUM FONDEN via the QMATH Centre of Excellence (grant no. 10059) during his stay at University of Copenhagen and by the WWTF research project "Variational Modeling of Carbon Nanostructures" (no. MA14-009) at University of Vienna. LDL is a member of the INdAM-GNAMPA group and wishes to thank the Scuola Internazionale di Studi Superiori Avanzati where she worked in the early stage of this project. MP is supported by the Fondecyt Iniciación grant number 11170264 entitled "Sharp asymptotics for large particle systems and topological singularities".

3.5. Crystallization under smooth one-well potentials with finite range 25
4. Long-range potentials and proof of Theorem 1.3 29
4.1. Distortion estimates at larger scales 30
4.2. Boundary error bounds 38
4.3. Control of large-scale deformation errors by short-scale deformations 40
4.4. Proof of Theorem 4.16 43
Appendix A. Proof of Lemmas 3.5 and 3.8 49
Appendix B. List of Notations 55
References 56

1. Introduction

1.1. **Our energy minimization problem.** If $X_N := \{x_1, \dots, x_N\}$ $(N \in \mathbb{N})$ is a finite subset of $\mathbb{R}^2$, referred to as *configuration*, and $V : [0, +\infty) \to \mathbb{R} \cup \{+\infty\}$ is a function, referred to as *pairwise interaction potential*, the V-energy of X_N is defined by

$$\mathcal{E}[V](X_N) := \frac{1}{2} \sum_{i \neq j} V(|x_i - x_j|). \tag{1.1}$$

We are interested in the minimization of the energy $\mathcal{E}[V]$ amongst N-point configurations under *isotropic singular one-well potentials* V which decay as $|x| \to \infty$ (this means that $\lim_{r \downarrow 0} V(r) = +\infty, \lim_{r \to \infty} V(r) = 0$ and $r \mapsto V(r)$ is decreasing on $(0, r_0)$ and increasing on (r_0, ∞), for some $r_0 > 0$). We will normalize V below and assume that

$$\min_{r>0} V(r) = -1. \tag{1.2}$$

Since $\mathcal{E}[V]$ is invariant under isometries of $\mathbb{R}^2$, we study minimizers up to isometry, and we are interested in properties which hold for large N. We find here conditions (see Theorems 1.1, 1.2 and 1.3) under which in three different situations the minimum energy problem for (1.1) is asymptotically solved by a *square lattice* $t\mathbb{Z}^2$, for some $t > 0$. This means that, setting

$$\mathcal{E}[V](N) := \min\{\mathcal{E}[V](X_N) \ : \ \sharp X_N = N\}, \tag{1.3}$$

it holds $\mathcal{E}[V](N) = N\overline{\mathcal{E}}_{\rm sq}[V] + \mathrm{O}(N^{1/2})$ as $N \to \infty$, where $\overline{\mathcal{E}}_{\rm sq}[V]$ is the minimum energy per point taken amongst all square lattices:

$$\overline{\mathcal{E}}_{\rm sq}[V] := \min_{t>0} \lim_{R \to \infty} \frac{\mathcal{E}[V](t\mathbb{Z}^2 \cap B_R)}{\sharp(t\mathbb{Z}^2 \cap B_R)}. \tag{1.4}$$

Here and throughout the paper $B_R = B(0, R)$, where $B(x, \rho)$ denotes the open ball centered at x and having radius equal to ρ.

We note that for some pairwise interaction potentials V the minimizer of the energy (1.1) is a *triangular lattice*, i.e., a rescaled copy of $\mathsf{A}_2 = (1, 0)\mathbb{Z} + (1/2, \sqrt{3}/2)\mathbb{Z}$. We refer to Subsection 1.4 for a more detailed description of such results and for a general discussion on the optimization problems solved by A_2. To the best of our knowledge this seems to be the first rigorous proof of crystallization to a square lattice for a two-body potential, a result suggested already in [48, p. 212] in 2006, and towards which more evidence appeared recently in [6, Section 1.3]. We refer to Section 1.3 for more details about results on the optimality of a square lattice. Our three main theorems are stated in Subsection 1.2 below.

1.2. **Description of the main results.** We highlight the basic geometric phenomenon at work in our result by considering a very simple V. Let

$$V(r) := \begin{cases} +\infty, & r \in [0,1), \\ -1, & r \in [1, r_{max}], \\ 0, & r > r_{max}. \end{cases} \tag{1.5}$$

This is a simple family including the Heitmann-Radin "sticky disk" potential [31] for $r_{max} = 1$, a case in which the interval of "favourable distances" on which $V(r) = -1$ is reduced to the single point $\{1\}$, giving A_2 as the asymptotical optimizer of $\mathcal{E}[V]$. Our starting consideration was that for $r_{max} = \sqrt{2}$, asymptotically $\mathbb{Z}^2$ is instead the optimizer (further discussion of potentials including (1.5) will be the aim of a separate paper [42]). This follows from two elementary geometry considerations:

(a1) If no points are allowed to get closer than distance 1 then the maximum number of points $x_i \neq x_j$ from X_N that are within $\sqrt{2}$-distance of a given x_j, needs to be at most 8.

(a2) If x_i has precisely 8 "neighbors" at distances lying in $[1, \sqrt{2}]$, and each one of these neighbors has precisely 8 neighbors as well, then the neighbors of x_i must form a perfect square, i.e. they form, together with x_i itself, configuration isometric to $\{-1, 0, 1\}^2 \subset \mathbb{R}^2$.

These two ingredients give the basic rigidity result on which our paper is based. The main new idea that we exploit, compared to other energy-minimization problems, is to "look beyond the next neighbors". It is worth to mention an equivalent rigidity result, also useful later, which says that "small energy quadrilaterals are squares" (see Lemma 2.2):

(b) If a quadrilateral Q has sidelengths ≥ 1 and lengths of diagonals $\leq \sqrt{2}$ then Q is a square.

The proof of (b) uses the same kind of methods as (a1)-(a2). Lemma 2.2 also describes a way to obtain it as a corollary of (a1)-(a2) directly.

This rigidity argument gives our first result (see Theorem 2.1 for a full statement).

Theorem 1.1. *Let $r_{max} = \sqrt{2}$ in (1.5). Then, with the notation (1.3) and (1.4), we have*

$$N\overline{\mathcal{E}}_{\rm sq}[V] \leq \mathcal{E}[V](N) \leq N\overline{\mathcal{E}}_{\rm sq}[V] + O(N^{1/2}) \qquad \text{as } N \to +\infty,$$

where

$$\overline{\mathcal{E}}_{\rm sq}[V] = -4.$$

In the above statement and throughout all the paper $O = O(T)$ denotes a continuous function on $\mathbb{R}^+$ such that $\lim_{T\to+\infty} \frac{|O(T)|}{T}$ is finite.

The fact that rigidity is ensured once we look up to a large enough number of next-neighbors, is a natural idea, exploited successfully in the work by Hales on the best-packing in 3 dimensions [28]. However, as shown in that work, it could lead to somewhat tedious case examinations, in the absence of a machinery which allows to streamline the bookkeeping of the energy during the optimization (a striking example of such machinery, in which all layers are studied at the same time via Fourier analysis, are the recent papers [12, 13, 49, 14, 15]).

In order to deal with interaction potentials that are more regular than the one in (1.5) we follow the idea (b) above, introducing as a building block the 4-point energy defined as

$$\mathcal{E}_4[V](x_1,x_2,x_3,x_4) := \frac{1}{2}\sum_{j=1}^{2}\sum_{i=1}^{4} V(|x_i - x_{i+j}|), \quad \forall i \in \{1,2,3,4\}, x_i \in \mathbb{R}^2, \tag{1.6}$$

where indices are considered modulo 4. Note that "diagonal pairs" $(x_1,x_3),(x_2,x_4)$ are counted twice in the above sum, while "nearest neighbors" are counted only once.

Calling *elementary square* a 4-ple of points whose vertices form a "small" deformation of a unit square (see Definition 3.4), the use of $\mathcal{E}_4[V]$ is clear in view of the following considerations:

- Up to boundary contributions, the energy of a square-lattice configuration is the sum over all elementary squares of $\mathcal{E}_4[V]$ (see Figure 1).
- On the other hand, (as in point (b) above) if V is a "short-enough-range" potential, a minimizing configuration is the one for which each elementary square separately optimizes $\mathcal{E}_4[V]$ (see Section 3.4).

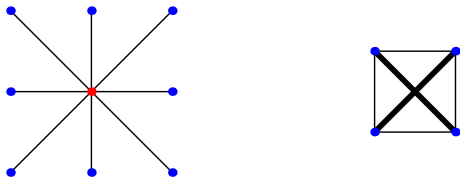


FIGURE 1. We will use the fact that energy contributions appearing in $\mathcal{E}_4[V]$ correspond to energy contributions of a single point as indicated in the above figure. This resummation trick will be used for regions of our configuration which are small deformations of regions in $\mathbb{Z}^2$.

Since the 4-point energy functional $\mathcal{E}_4[V]$ plays a fundamental role in our anlysis, we focus on convexity and minimality properties of $\mathcal{E}_4[V]$; such an analysis has appeared in [27] in the case of a potential modeling elastic responses, and more general calculations of the type that we perform in Section 3.4 seem to have a long history, starting from Maxwell's work [39] (see also [11]), and appear in the study of stability and oscillation modes of frameworks, see e.g. [33] for a geometric introduction to this subject, and the references therein.

Now we state our second result which holds for more regular finite-range potentials V. We assume that V satisfies the following properties, for suitable $0 < \alpha' < \alpha < \alpha''$, $\epsilon' > 0$ (small) and $K > 0$ (large):

(A) $\mathcal{E}_4[V]$ has a strict minimum at the unit square, and this is its unique minimum amongst all 4-point configurations with interpoint distances in $E_{\alpha''}$. This happens in particular if V is piecewise-C^2 in $(0,\infty)$, i.e. $V \in C^2_{pw}((0,\infty))$, and satisfies the explicit derivative bounds (1) and (2) from Section 1.5 below);

(B) $-1 = \min V \leq V(r) \leq -1+\epsilon'$, for $r \in E_{\alpha'}$, where

$$E_\beta := E^1_\beta \cup E^2_\beta, \quad E^1_\beta := (1-\beta, 1+\beta) \text{ and } E^2_\beta := (\sqrt{2}-\beta, \sqrt{2}+\beta) \quad \text{for any } \beta > 0; \tag{1.7}$$

(C) $V(r) > -\frac{1}{2}$ if $r \notin (1-\alpha, \sqrt{2}+\alpha)$;

(D) $V(r) \geq K$ for $r \leq 1-\alpha$;

(E) $V(r) = 0$ for $r \geq \sqrt{2}+\alpha''$.

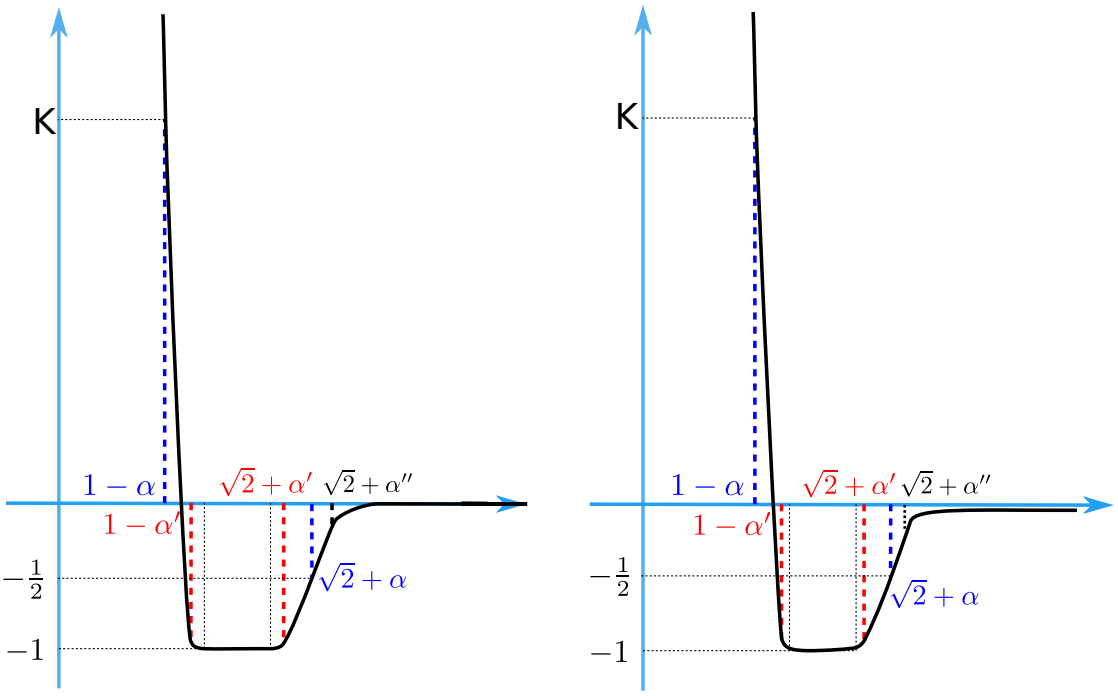


FIGURE 2. A potential satisfying properties (A)-(E) required for Theorem 1.2, and one satisfying properties (A)-(E') needed for Theorem 1.3 (note that the values of $\alpha, \alpha', \alpha''$ are exaggerated).

See Figure 2(left) for a potential satisfying these properties. This control allows us to get a result similar to Theorem 1.1 (see Theorem 3.16 for a more complete statement).

Theorem 1.2. *There exists $\bar{\alpha}, \bar{\epsilon} > 0$ such that for all $\alpha'' \in (0, \bar{\alpha}]$ and all $\epsilon' \in (0, \bar{\epsilon}]$ there exist $0 < \alpha' < \alpha < \alpha''$ and $K = K(\alpha, \epsilon')$ such that if $V \in C^2_{pw}((0,\infty))$ satisfies above conditions (A)-(E) then*

$$N\overline{\mathcal{E}}_{\rm sq}[V] \le \mathcal{E}[V](N) \le N\overline{\mathcal{E}}_{\rm sq}[V] + O(N^{1/2}) \qquad \text{as } N \to +\infty, \tag{1.8}$$

where

$$\overline{\mathcal{E}}_{\rm sq}[V] = \min \mathcal{E}_4[V]. \tag{1.9}$$

The above theorem uses, besides the thorough study of $\mathcal{E}_4[V]$ which we already mentioned, also the quantitative version of the phenomena valid for (1.5), which are included in a geometric rigidity result (Lemma 3.5). This result, whose proof is based on an elementary study of configurations close to $\{-1,0,1\}^2 \subset \mathbb{R}^2$, is another ingredient of the proofs which is new compared to the A_2-crystallization results. It plays an important role, allowing to avoid losing the combinatorial order between neighbors lying in the "interior" of a configuration, i.e. in a "neighborhood" of a point having 8 "nearest neighbors". Special emphasis on the combinatorial setup is included in Section 3.2: to keep track of this structure we use a differential-geometric language allowing to keep the model-space $\mathbb{Z}^2$ from the actual energy competitor at hand. Using geometric ideas for organizing energy contributions was an idea

already present in [48] and further developped e.g. in [18] and [17] in the 2-dimensional setup adapted to the study of A_2-crystallization (see also [19] for an application of this setting to the study of polycrystals made by A_2 grains).

The final result we prove is for long-range potentials V. The required assumptions on V coincide with conditions (A)-(D) above, plus an assumption on the "fast decay" of the tail, i.e., condition (E)

We can now state our theorem, whose detailed statement is Theorem 4.16.

Theorem 1.3. *There exists $\bar{\alpha}, \bar{\epsilon}, \bar{\epsilon}_0 > 0$ such that for all $\alpha'' \in (0, \bar{\alpha}]$, $\epsilon' \in (0, \bar{\epsilon}]$ and $\epsilon \in [0, \bar{\epsilon}_0]$ there exist $0 < \alpha' < \alpha < \alpha''$ and $K = K(\alpha, \epsilon')$ such that if $V \in C^2_{pw}((0,\infty))$ satisfies the above conditions (A)-(E') then*

$$N\overline{\mathcal{E}}_{\rm sq}[V] \leq \mathcal{E}[V](N) \leq N\overline{\mathcal{E}}_{\rm sq}[V] + O(N^{1/2}) \qquad \text{as } N \to +\infty, \tag{1.10}$$

where

$$\overline{\mathcal{E}}_{\rm sq}[V] = \min_{t>0} \lim_{R\to\infty} \frac{\mathcal{E}[V](t\mathbb{Z}^2 \cap B_R)}{\sharp(t\mathbb{Z}^2 \cap B_R)}. \tag{1.11}$$

Notice that condition (E') with $\epsilon = 0$ gives exactly condition (E); therefore Theorem 1.2 is implied by Theorem 1.3, once provided that, if (E) holds, then the right hand sides of (1.11) and of (1.9) coincide. In this paper, we do not pursue this strategy. Instead we find more instructive to give first the proof of Theorem 1.2, since in this case the scheme of the proof is somehow "cleaner" and does not require all the tools needed in the proof of Theorem 1.3 to account for long-range interactions.
Roughly speaking, the starting point in the proof of Theorem 1.3 consists in showing that $\overline{\mathcal{E}}_{\rm sq}[V] = \min \mathcal{E}_4[V_*]$, where V_* is a kind of "long-range potential defined on the distances of $\mathbb{Z}^2$" (see (4.36)). The main phenomenon at work in the above result is that the tail of our potential V is decaying so fast that actually V_* is nothing but a small enough perturbation of V so that the proof of Theorem 1.3 can be reduced to the one of Theorem 1.2 for V_*. The same method was also at the base of the main result of [48] for the triangular lattice (see also [21, 22] for applications of the same ideas to the honeycomb lattice with an additional three-body potential), however in our case new difficulties arise due to the fact that we have to account for energies coming from "sides" and "diagonals" of squares of different scales in our configurations. Thus we need new tools such as Lemma 4.12 which then allow resummation methods that yield a lower bound of the energy $\mathcal{E}[V]$ via the sum of 4-point energies on r-squares.

For the proof of Theorem 1.3 we have at the same time done an exercise of simplifying and extending to our situation the methods of proofs from [48]. The main technical improvements compared to [48] are that:

- we put a focus on separating the use of the combinatorial information, the metric information and the information about the embedding to $\mathbb{R}^2$ of our configurations;
- we avoid the use of the Friesecke-James-Müller rigidity estimate, employed in [48]: instead, we use a rougher estimate based on John's earlier result (see Lemma 4.7), which makes the proof self-contained without changing the decay hypotheses needed on V;
- we make more explicit the method of proof started in [48], i.e. the idea of controlling long-range deformations via the Hessian of the microscale energy, by separating the

self-contained result of the existence of minimizers for small perturbations of the potential V (Proposition 3.15).

1.3. **Previous results on the optimality of the square lattice.** Only few rigorous results exist about the crystallization on a square lattice, i.e. the fact that $\mathbb{Z}^2$ is a ground state of an interaction energy, with either one or several types of particles. Also note that, in 3 dimensions, there is only one chemical element which has a simple cubic structure (i.e. Polonium) and the only ionic solid having a simple cubic basis is the Sodium Chloride NaCl (rock-salt structure). However, in dimensions 2 and 3, $\mathbb{Z}^2$ and $\mathbb{Z}^3$ are some of the very few lattices (together with the triangular, the BCC and the FCC lattices) that are "density-stable", i.e. they can be critical points of the lattice energy per point associated with any absolutely summable interaction potential V for densities in an open interval (see [5] for a proof). It is then reasonable to think that they are good candidates for ground states of energies such as $\mathcal{E}[V]$ for two-body isotropic one-well potentials V.

The first rigorous result in this direction seems to be the work of Mainini, Piovano and Stefanelli [37], who proved the optimality of a subset of $\mathbb{Z}^2$ for a combination of (short-range) two-body and three-body angular potentials which favour right angles. Regarding the analogy with two-ion compounds, Friedrich and Kreutz [25] have shown the energy-optimality of a subset of $\mathbb{Z}^2$ composed of two types of particles under short-ranged repulsive/attractive interactions (modelling a rock-salt structure, in two dimensions).

Several potentials have been designed for stabilizing a square or a cubic lattice. Exploring the different structures that can be obtained by using a decreasing convex potential, Marcotte, Stillinger and Torquato have defined in [38, Section III.A] an example of potential such that $\mathbb{Z}^2$ is a ground state at fixed density 1, the same being also done in [3]. In [44], Rechtsman, Stillinger and Torquato proposed the potential $V(r) = r^{-12} - 2.7509e^{-32.2844(r-\sqrt{2})}$ that has (numerically) $\mathbb{Z}^3$ as the ground state of the pairwise energy.

Concerning the search of ground states amongst periodic configurations, it has been numerically shown in [4] that the square lattice is the ground state of the Lennard-Jones potential $V(r) = r^{-12} - 2r^{-6}$ among Bravais lattices of fixed density belonging to $(0.79, 0.87)$. This was conjectured to still hold true for general differences of completely monotone functions in [4] and was investigated for the Morse potential in [5]. For the 3-block copolymer case, Luo, Ren and Wei [36] proved in 2-dimensions the optimality among Bravais lattices of a square lattice of alternating types of species (two kinds with different sizes, a third one being considered as a background) under Coulomb interactions, under the condition that the parameter b of their system – depending on the size and a weight associated to each species – belongs to a certain explicit interval. Finally, two of the authors of this paper have constructed in [6] several examples of two-body one-well potentials V such that a square lattice has lower V-energy per point than a triangular one.

1.4. **Previous literature on the triangular lattice and comparison with our results.** Many two-dimensional optimization problems give as a (proved or conjectured) minimizer A_2. These include the best-packing problem [23], optimal-transport type problems [10], the best-covering problem [35] and the quantizer problem [24] (see also [32] for more examples). Furthermore A_2 is conjectured to be asymptotically minimizing for (1.1) when V is any Lennard-Jones type potential (i.e. a difference of inverse power laws), see [8, 3, 4, 6], as well

as for the Morse potential [5]. It was recently conjectured in [13] that in fact A_2 is *universally optimal*, i.e. it optimizes among fixed-density configurations all energies for which W defined such that $V(r) = W(r^2)$ has nonnegative Laplace transform (W is called completely monotone), a result so far known only for algebraically simpler to treat lattices in 8 and 24 dimensions [15]. A related conjecture is the *Abrikosov conjecture*, which again postulates that A_2 is optimal at any fixed density for the renormalized energy, i.e. under potentials V with heavy tails such as the Coulomb potential from Electrostatics [1, 46, 45, 40, 7]. Recently such a conjecture was shown to be equivalent to the Cohn-Kumar conjecture in [41] for Coulomb potentials and some Riesz potentials, and further extension to all Riesz potentials may be possible.

Concerning crystallization, the first rigorous proof of crystallization in two dimensions under a one-well isotropic potential seems to be the one by Heitmann and Radin [31] of 1980, who consider the potential from (1.5) with $r_{max} = 1$, called the "sticky disk" potential. Such a result is actually a finite crystallization result, i.e. Heitmann and Radin proved that for every $N \in \mathbb{N}$ all the minimizers of the sticky disc energy lie, up to rotations and translations, on A_2, using the minimal value of the energy, which was found in turn by Harborth [29] (see [18] for a more transparent proof).

Later, Radin [43] considered a slightly different version of the potential from [31]

$$V_{Rad}(r) := \begin{cases} +\infty, & r < 1, \\ 24r - 25, & 1 \leq r < 25/24, \\ 0, & r > 25/24. \end{cases}$$

In this case it is shown that all nearest-neighbors of the minimizers are at distance precisely 1 and then apply the basic rigidity principle that selects the triangular lattice ground state configuration, however the techniques are not sufficient for allowing smoother V. Our Theorems 1.1 and 1.2 can be considered as the asymptotic versions of the results [31] and [43] in the square lattice case. Actually, the basic rigidity principle on which such proofs are based, is analogous to points (a1)-(a2) and (b) in Section 1.2 and seems to be older. Indeed, it appears in the solution of the 2 dimensional packing problem, appearing e.g. in the paper [23] by Fejes Tóth from 1943.

Finally, the result about A_2 which is perhaps closer in spirit to our Theorems 1.2 and 1.3 is the 2006 paper [48] by Theil, in which the main theorem assumes that $V \in C^2((1-\alpha, \infty))$, for some $\alpha > 0$ sufficiently small, satisfies the following conditions:

(i) $V''(r) \geq 1$ for $r \in (1-\alpha, 1+\alpha)$;
(ii) $V(r) \geq -\alpha$ for $r \in [1+\alpha, 4/3]$;
(iii) $V(r) \geq \frac{1}{\alpha}$ for $r \leq 1-\alpha$;
(iv) $|V''(r)| \leq \alpha r^{-7}$ for $r > 4/3$;
(v) The minimal energy per point $\min_{r>0} \frac{1}{2} \sum_{p \in \mathbb{Z}^2 \setminus \{0\}} V(r|p|)$ is achieved for $r = 1$.

Under these conditions, the conclusion of the main theorem in [48] gives crystallization to A_2 in exactly the same sense as expressed in the conclusions of our Theorem 1.3 for the square lattice.

We note that the above conditions (ii), (iii) and (iv) above are triangular lattice equivalents of conditions (C), (D), (E') respectively. Here, as in [48], the role of these conditions is to suitably normalize V and to allow to apply the basic rigidity principles as appearing in e.g. [23] for the triangular lattice, and the apparently new ones (a1)-(a2), (b) for our new result on

the square lattice. Furthermore, assumption (v) is here to force the minimizer to be exactly A_2, which is not the case in our case where $t\mathbb{Z}^2$ (t given by (1.11)) is an asymptotic minimizer of our energy.

On the other hand, assumption (i) above, similarly to condition (A), has the main role of allowing precise Hessian bounds. For a comparison to [48], note that the Hessian of $\mathcal{E}_4[V]$ used here would correspond to the one of the 2-point energy $\mathcal{E}_2[V](\{x,y\}) := V(|x-y|)$ in the triangular lattice setup [48], in which case it is sufficient to use the quantity V'' instead.

Finally, condition (B) from Theorem 1.3 is still related to (i) above, and it appears due to the fact that we need to get coercivity control at interpoint distances lying in a whole interval $[1,\sqrt{2}]$ and not just near a minimum point of V as in the study of A_2.

1.5. **Summary of hypotheses on V used throughout the paper.** We include here, and briefly discuss, several requirements on V that will be useful during the proofs. Firstly, we will use the change of variables

$$W(s) := W(r^2) := V(r), \quad s := r^2, \quad r > 0, \tag{1.12}$$

which allows slightly more elegant Hessian computations.

Furthermore, note that in the rest of the paper we will use three small deformation parameters which will satisfy

$$0 < \alpha' < \alpha < \alpha'' < \frac{2-\sqrt{2}}{4},$$

and whose use will be the following:

(a) The parameter α will be used to measure the deformation of distances from a configuration X, with respect to the distances in the model space $\mathbb{Z}^2$.
(b) The parameter α' will measure the small neighborhood $E_{\alpha'} \subset E_\alpha$ on which the potential under consideration only takes values very close to its absolute minimum.
(c) The parameter α'' will give us a larger neighborhood $E_{\alpha''} \supset E_\alpha$ on which we have convexity bounds on V giving good growth control, and allowing to say that perturbing the distances to stay in $E_{\alpha'}$, decreases the energy.

We are now ready to enumerate the various conditions which we will impose on V, W in order to get the results in Theorems 1.2 and 1.3 (which correspond to the more precise statements in Theorems 3.16 and 4.16). We assume that $V, W \in C^2_{pw}((0,\infty))$ are related by (1.12) and satisfy:

(0) $\min_{s>0} W(s) = -1$.
It is just a renormalization, that actually does not affect our results.
(1) V is convex in $E_{\alpha''}$ and V satisfies $\inf_{r \in E_{\alpha''} \setminus [1,\sqrt{2}]} V''_{\pm}(r) \geq c$.
Such a condition provides good quantified convexity bounds on V, ensuring that $\mathcal{E}_4[V]$ and $\mathcal{E}_4[V_*]$ admit at most one global minimizer among the configurations whose interpoint distances lie in $E_{\alpha''}$, whenever V_* is a C^2-small enough perturbation of V. Condition (1) appears for the first time in Lemma 3.12 and then in Lemma 3.14.
(2) W satisfies

$$W'(1) + 2W'(2) = 0 \tag{1.13}$$

and there exists $c'>0$ such that

$$\begin{aligned} &W_-''(1)+W_+''(1)+2W'(1)>C_4c', \qquad && W_-''(2)+W_+''(2)>C_4c',\\ &W_-''(1)+W_+''(1)>C_4c', && W_\pm''(1)+4W_\pm''(2)>C_4c', \end{aligned} \tag{1.14}$$

where C_4 is a constant depending only on the dimension.
Condition (1.14) ensures that the configuration formed by the vertices of a unit square, from now on denoted by $\boxtimes$, is a strict local minimum - up to rotations and translations - of $\mathcal{E}_4[V]$; in particular, (1.13) guarantees that $\boxtimes$ is a critical point for $\mathcal{E}_4[V]$, whereas (1.14) reduces to the requirement of Hessian eigenvalues being strictly larger than C_4c' if V is smooth, but extends to piecewise-C^2 potentials V which seem easier to construct explicitly; more precisely (1.14) guarantees that $\nabla\mathcal{E}_4[V]$ is c'-monotone at $\boxtimes$. The considerations above give precisely the content of Lemma 3.11, where the existence of the constant C_4 is proven. Condition (2) appears also in Proposition 3.13, Lemma 3.14, Proposition 3.15.

(3) $\sup_{r\in E_{\alpha'}} V(r) < -\frac{15}{16} - c''$, for some constant $c''\in[0,\frac{1}{16})$.
Condition (3) requires V not to be much higher than its negative minimum in $E_{\alpha'}$. Such a condition appears for the first time in Proposition 3.15. Loosely speaking, the combination of (1) and (3) implies that the well of the potential is "large enough".

(4) $V(r)>-\frac{1}{2}$ if $r\notin(1-\alpha,\sqrt{2}+\alpha)$.
Also this condition appears for the first time in Proposition 3.15. The combination of conditions (3) and (4) implies that V "increases" passing from $E_{\alpha'}$ to $\mathbb{R}^+\setminus(1-\alpha,\sqrt{2}+\alpha)$.

(5) $V(r)\geq K$ if $0<r\leq 1-\alpha$, for some suitable constant $K>0$.
This assumption allows to say that the distance between two points of a minimal configuration is strictly larger than $1-\alpha$. The value of the constant K is determined in Lemma 3.1; it depends on α'' and on the constants ϵ and p of assumption (6') below.

(6) $V(r)=0$ if $r\geq\sqrt{2}+\alpha''$.
This is just a short-range assumption.

(6') $V(r)\leq 0$ if $r\geq 1$ and $|V(r)|$, $r|V'(r)|$, $r^2|V''(r)|<\epsilon r^{-p}$ if $r\geq\sqrt{2}+\alpha''$, for some $\epsilon>0$ small enough and $p>4$.
This assumption is the long-range version of (6). It ensures that the tail of the potential V goes fast enough to 0. Notice that, up to changing ϵ by a constant factor, it is equivalent to require

$$|V''(r)|\leq\epsilon r^{-p-2} \text{ for } r\geq\sqrt{2}+\alpha'', \quad V(r)\to 0 \quad (r\to\infty).$$

Finally, we note that a one-well potential $V(r)=W(r^2)$ which satisfies the above (0)-(5) and (6') can be given by the following formulas, for $1\leq r_1\leq r_2\leq r_3\leq\sqrt{2}$ and parameters

$q>0$, $p>4$, $a_i>0$ and $C>0$ chosen in such a way that W is C^1.

$$W(s)=\begin{cases} a_1 s^{-q/2} & \text{for } s\in\left(0,(1-\alpha'')^2\right],\\ -C+a_2(s-r_1^2)^2 & \text{for } s\in\left[(1-\alpha'')^2,r_1^2\right],\\ -C & \text{for } s\in\left[r_1^2,r_3^2\right],\\ -C+a_3(s-r_3^2)^2 & \text{for } s\in\left[r_3^2,(\sqrt{2}+\alpha'')^2\right],\\ a_4(s-r_2^2)^{-p/2} & \text{for } s>(\sqrt{2}+\alpha'')^2. \end{cases} \tag{1.15}$$

In particular, one can verify through a tedious verification that conditions (0)-(5) and (6') hold for suitable choices of the parameters, and can be achieved even for $r_1=1, r_3=\sqrt{2}$ yielding $W\in C^2_{pw}$, whereas if we leave the parameters r_1, r_3 a bit more free we can achieve $W\in C^2$ as well.

2. Proof of Theorem 1.1

In this section we prove Theorem 1.1. Therefore the interaction potential V is the one defined in (1.5) with $r_{max}=\sqrt{2}$.
For every $N\in\mathbb{N}\cup\{+\infty\}$ we denote by

$$\mathcal{X}_N(\mathbb{R}^2):=\{X\subset\mathbb{R}^2:\ \sharp X=N\}, \tag{2.1}$$

the set of N-point configurations. Notice that if $X_N=\{x_1,\dots,x_N\}\in\mathcal{X}_N(\mathbb{R}^2)$ with $\mathcal{E}[V](X_N)<+\infty$, then $|x_i-x_j|\geq 1$ for every $i\neq j$.
Therefore we define the families of configurations having locally finite energy as

$$\mathcal{C}:=\left\{X\subset\mathbb{R}^2:\ \inf_{x\neq x'\in X}|x-x'|\geq 1\right\},\qquad \mathcal{C}_N:=\mathcal{C}\cap\mathcal{X}_N(\mathbb{R}^2). \tag{2.2a}$$

We define square-lattice configurations of locally finite energy as follows:

$$\mathcal{C}^{\mathbb{Z}^2}:=\left\{X\subset\mathbb{Z}^2:\ \inf_{x\neq x'\in X}|x-x'|\geq 1\right\},\qquad \mathcal{C}^{\mathbb{Z}^2}_N:=\mathcal{C}_N\cap\mathcal{C}^{\mathbb{Z}^2}=\mathcal{C}^{\mathbb{Z}^2}\cap\mathcal{X}_N(\mathbb{R}^2). \tag{2.2b}$$

We define $\mathcal{E}[V](N)$ as in (1.3) and

$$\mathcal{E}^{\mathbb{Z}^2}[V](N):=\min_{X_N\in\mathcal{C}^{\mathbb{Z}^2}_N}\mathcal{E}[V](X_N). \tag{2.3}$$

Then clearly we have $\mathcal{E}[V](N)\leq\mathcal{E}^{\mathbb{Z}^2}[V](N)$. In order to prove Theorem 1.1, we introduce the graph associated to a configuration in $\mathcal{C}$. For every $X\in\mathcal{C}$, we set

$$\mathcal{S}_0(X):=\{\{x,y\}\ :\ x,y\in X,\ |x-y|\in[1,\sqrt{2}]\}$$

and we denote by $\mathcal{G}_0(X)$ the graph $(X,\mathcal{S}_0(X))$ whose sets of nodes and edges are given by X and $\mathcal{S}_0(X)$ respectively. We say that the points $x,y\in X$ are nearest neighbors if they are connected by an edge. Moreover, we denote by

$$\partial\mathcal{G}_0(X):=\{x\in X:\ x \text{ has less than 8 nearest neighbors }\}. \tag{2.4}$$

Our first result states that to leading order $\mathcal{E}[V](N)$ and $\mathcal{E}^{\mathbb{Z}^2}[V](N)$ have the same asymptotics equal to $-4N+o(N)$, and that an infinite configuration is locally minimal if and only if it is an isometric copy of $\mathbb{Z}^2$.

Theorem 2.1. *Let V be as in (1.5) with $r_{max} = \sqrt{2}$.*

(i) *It holds*

$$-4N \leq \mathcal{E}[V](N) \leq -4N + O(N^{\frac{1}{2}}) \tag{2.5a}$$

where

$$-4 = \lim_{N\to\infty} \frac{\mathcal{E}^{\mathbb{Z}^2}[V](N)}{N} = \lim_{R\to\infty} \frac{\mathcal{E}[V](\mathbb{Z}^2 \cap B_R)}{\sharp(\mathbb{Z}^2 \cap B_R)}. \tag{2.5b}$$

(ii) *If $X \in \mathcal{C}$ and if a point $x \in X$ has 8 nearest neighbors in $\mathcal{G}_0(X)$, each of which in turn has 8 nearest neighbors in $\mathcal{G}_0(X)$, then $\overline{B}(x,\sqrt{2}) \cap X$ equals up to rotation and translation $\overline{B}(0,\sqrt{2}) \cap \mathbb{Z}^2 = \{-1,0,1\}^2$.*

In the theorem above and throughout the paper $\overline{B}(x,\rho)$ denotes the closed ball centered at x and having radius ρ. Although we prove more general results which imply the above theorem below, we give a direct proof of (i), whereas we refer the reader to Corollary A.4 in Appendix A for the proof of (ii). The proof uses some elementary geometry arguments developed in Appendix A.

Proof. We first prove (2.5a).
Let $N \in \mathbb{N}$. Trivially, it is enough to prove the first inequality only for configurations in $\mathcal{C}_N$ and the second inequality only for configurations in $\mathcal{C}_N^{\mathbb{Z}^2}$.
Let $X_N \in \mathcal{C}_N$. Notice that every $x \in X_N$ has at most 8 neighbors in $\mathcal{G}_0(X_N)$. Indeed, if there were $x \in X$ and 9 points $x_0, \dots, x_8 \in X_N \setminus \{x\}$ such that $|x - x_i| \in [1, \sqrt{2}]$ for all $i \in \{0,\dots,8\} \simeq \mathbb{Z}/9\mathbb{Z}$ then, assuming that the points are ordered such that the angular coordinate centered at x is increasing and indices are taken modulo 9, then there exists $i \in \mathbb{Z}/9\mathbb{Z}$ such that $\widehat{x_i x x_{i+1}}$ is smaller than $360°/9 = 40°$, thus contradicting Corollary A.2 in the Appendix A. As a consequence, for every $N \in \mathbb{N}$ and for every $X_N \in \mathcal{X}_N(\mathbb{R}^2)$, it holds

$$\mathcal{E}[V](X_N) \geq -4N, \tag{2.6}$$

i.e. the first inequality in (2.5a).

Let $X_N \in \mathcal{C}_N^{\mathbb{Z}^2}$. We first note that each point in the neighbor graph $\mathcal{G}_0(\mathbb{Z}^2)$ has precisely 8 neighbors. Thus we have, by (2.6), with notation (2.4), for any $X_N \subset \mathbb{Z}^2$,

$$-4N \leq \mathcal{E}[V](X_N) \leq -4\sharp\left(X_N - \partial\mathcal{G}_0(X_N)\right) = -4N + 4\sharp\partial\mathcal{G}_0(X_N), \tag{2.7}$$

and since we may find a sequence $X_N \subset \mathbb{Z}^2$ such that $\sharp(\partial\mathcal{G}_0(X_N)) = O(N^{\frac{1}{2}})$ as $N \to \infty$, the second equality in (2.5a) follows. This concludes the proof of (2.5a) and shows the first equality in (2.5b).
For proving the second equality (2.5b), it is enough to notice that $\mathcal{E}[V](\mathbb{Z}^2 \cap B_R) = -4\sharp(\mathbb{Z}^2 \cap B_R) + O(R)$. □

The content of the following lemma, whose proof is obtained directly by Theorem 2.1(ii), is nothing but property (b) in Subsection 1.2.

Lemma 2.2. *Let $\{x_1, x_2, x_3, x_4 \equiv x_0\} \in \mathcal{C}_4$ be such that $[x_{i-1}, x_i]$ are the sides of a quadrilateral Q for $i = 1,\dots,4$. Assume moreover that $\{x_1, x_3\}, \{x_2, x_4\}, \{x_{i-1}, x_i\} \in \mathcal{S}_0$ for every $i = 1,\dots,4$. Then Q is a square with sidelength equal to one.*

Proof. We first note that Q is convex, as can be seen by applying the law of cosines. Therefore tiles congruent to $Q, -Q$ can tile the plane (to find the neighbors of Q, apply a reflection with respect to the midpoint of each side, and using the fact that the internal angles of Q sum to 360° obtain that this procedure can be iterated without generating overlaps). Let X denote the vertices of such tessellation and let $x \in X$. By construction, we have that there exist eight points $x_1, \dots, x_8$ such that $|x - x_i| \in \mathcal{S}_0$ for every $i = 1, \dots, 8$. Moreover, for the same reason for every $i = 1, \dots, 8$ there are eight points $x_{i1}, \dots, x_{i8}$ in X with $|x_i - x_{ij}| \in \mathcal{S}_0$ for every $j = 1, \dots, 8$. By Theorem 2.1(ii), we get that $B(x, \sqrt{2}) \cap X$ equals up to a rotation and a translation $B(0, \sqrt{2}) \cap \mathbb{Z}^2$, so that the original Q was a unitary square. □

3. Smoothed potentials and proof of Theorem 1.2

The goal of this section is to prove the crystallization in the sense of the thermodynamic limit for a perturbation of (1.5).

3.1. **Minimum distance between points for minimizers.**

Lemma 3.1. *For every $C_1 > 0, C_2 > 0$, $r_{min} > 0$, $r_0 > r_{min}$, and $p > 2$, there exists $K > 0$, depending on $C_1, C_2, r_{min}, r_0, p$ such that if*

$$\begin{cases} V(r) \geq K & \text{for } 0 < r \leq r_{min}\,, \\ V(r) \geq -C_1 r^{-p} & \text{for } r \geq r_0\,, \\ V(r) \geq -C_2 & \text{for } r > 0, \\ \lim\limits_{r\to\infty} V(r) = 0, \end{cases} \tag{3.1}$$

then for every $N \in \mathbb{N}$ all the minimizers $X_N = \{x_1, \dots, x_N\}$ of $\mathcal{E}[V]$ in $\mathcal{X}_N(\mathbb{R}^2)$ satisfy

$$\min_{i\neq j} |x_i - x_j| > r_{min}. \tag{3.2}$$

Moreover, there exists a constant $K' > 0$, depending on C_2, r_{min}, r_0 such that if

$$\begin{cases} V(r) \geq K' & \text{for } 0 < r \leq r_{min}\,, \\ V(r) \geq -C_2 & \text{for } r > 0\,, \\ V(r) = 0 & \text{for } r \geq r_0, \end{cases} \tag{3.3}$$

then for every $N \in \mathbb{N}$ all the minimizers $X_N = \{x_1, \dots, x_N\}$ of $\mathcal{E}[V]$ in $\mathcal{X}_N(\mathbb{R}^2)$ satisfy (3.2).

Remark 3.2. Note that assumptions (0) and (6') in Subsection 1.5 give exactly (3.1) with $r_{min} = 1 - \alpha$, $r_0 = \sqrt{2} + \alpha''$, $C_1 = \epsilon$ and $C_2 = 1$, whereas conditions (0) and (6) are the same as (3.3) for the same choice of parameters.

Proof. We prove the claim only in the case $C_1 > 0$ whereas the proof for $C_1 = 0$ is left to the reader. For simplicity, we will denote in the below by C any constant depending only on C_1, C_2 from the theorem, which may change from line to line.

We follow along the lines of [48, Lemma 2.2], but for the benefit of the reader we include the proof in self-contained form. For every $N \in \mathbb{N}$ we set

$$M = M(r_{min}, N) := \max \sharp \left\{ X_N \cap B\left(y, \frac{r_{min}}{2}\right) :\ y \in \mathbb{R}^2, \quad \begin{array}{l} X_N \text{ is a minimizer of } \mathcal{E}[V] \\ \text{in } \mathcal{X}_N(\mathbb{R}^2) \end{array} \right\}.$$

For the remainder of the proof we fix $N \in \mathbb{N}$ and a minimizer $X_N = \{x_1, \dots, x_N\} \subset \mathbb{R}^2$ of $\mathcal{E}[V]$ in $\mathcal{X}_N(\mathbb{R}^2)$ which achieves the above maximum M. By translation invariance, we may assume that $y = 0$ and we write $B = B\left(0, \frac{r_{min}}{2}\right)$.

We need to show that $M = 1$ for K large enough.

Let $I \subset \{1, \dots, N\}$ be the indices such that $x_i \in B$, so that $\sharp I = M$. As $V(r) \geq K$ on $(0, r_{min})$, we have

$$\sum_{\substack{i,j \in I \\ i \neq j}} V(|x_i - x_j|) \geq K \ M(M-1). \tag{3.4}$$

We now claim that

$$\sum_{\substack{i \in I \\ j \notin I}} V(|x_i - x_j|) + \frac{1}{2} \sum_{\substack{i,j \in I \\ i \neq j}} V(|x_i - x_j|) \leq 0. \tag{3.5}$$

Since X_N is a minimizer of $\mathcal{E}[V]$ in $\mathcal{X}_N(\mathbb{R}^2)$, for every $Y_N = \{y_1, \dots, y_N\} \in \mathcal{X}_N(\mathbb{R}^2)$ we have

$$\begin{aligned} \mathcal{E}[V](X_N) &= \frac{1}{2} \sum_{i \neq j} V(|x_i - x_j|) \\ &= \frac{1}{2} \sum_{\substack{i,j \in I \\ i \neq j}} V(|x_i - x_j|) + \sum_{\substack{i \in I \\ j \notin I}} V(|x_i - x_j|) + \frac{1}{2} \sum_{\substack{i,j \notin I \\ i \neq j}} V(|x_i - x_j|) \\ &\leq \mathcal{E}[V](Y_N) = \frac{1}{2} \sum_{\substack{i,j \in I \\ i \neq j}} V(|y_i - y_j|) + \sum_{i \in I} \sum_{j \notin I} V(|y_i - y_j|). \end{aligned} \tag{3.6}$$

In particular we can construct configurations Y_N from X_N by keeping $y_j = x_j$ if $j \notin I$ while for $i \in I$ we can move y_i towards infinity and away from each other, so that the quantity

$$\min_{\substack{i \in I \\ j \neq i}} |y_i - y_j|$$

gets arbitrarily large. Since by hypothesis $V(r) \to 0$ as $r \to +\infty$, we obtain from (3.6)

$$\frac{1}{2} \sum_{i \neq j} V(|x_i - x_j|) \leq \frac{1}{2} \sum_{\substack{i,j \notin I \\ i \neq j}} V(|x_i - x_j|) + M \ (N-1) \ \lim_{r \to \infty} V(r) = \frac{1}{2} \sum_{\substack{i,j \notin I \\ i \neq j}} V(|x_i - x_j|),$$

which yields (3.5).

Combining (3.5) and (3.4), we get

$$\sum_{\substack{i \in I \\ j \notin I}} V(|x_i - x_j|) \leq -K \frac{M(M-1)}{2}. \tag{3.7}$$

We now rewrite $\mathbb{R}^2 \setminus B = \bigcup_{k=1}^{\infty} A_k$ where $A_k := \left\{ x \in \mathbb{R}^2 : \ |x| \in \left(k \frac{r_{min}}{2}, (k+1) \frac{r_{min}}{2} \right] \right\}$ for every $k \in \mathbb{N}$. It follows that

$$\sum_{\substack{i \in I \\ j \notin I}} V(|x_i - x_j|) = \sum_{i \in I} \sum_{k=1}^{\infty} \sum_{j : x_j \in A_k} V(|x_i - x_j|).$$

By the third condition of (3.1), for every $k \in \mathbb{N}$ it holds

$$\sum_{\substack{i\in I\\ x_j\in A_k}} V(|x_i - x_j|) \geq -CM\sharp(A_k \cap X_N). \tag{3.8a}$$

Let now k_0 be such that $\operatorname{dist}(B, A_k) = \frac{r_{min}(k-1)}{2} \geq r_0$ for $k \geq k_0$ with r_0 as in (3.1). By the second condition of (3.1), for every $k \geq k_0$, we have

$$\sum_{\substack{i\in I\\ x_j\in A_k}} V(|x_i - x_j|) \geq -\frac{C\ M\ \sharp(A_k \cap X_N)}{\operatorname{dist}(B, A_k)^p} = -\frac{2^p\ C\ M\ \sharp(A_k \cap X_N)}{r_{min}^p (k-1)^p}. \tag{3.8b}$$

Moreover, by covering A_k by copies of B and using the maximality property of B, one can easily check that $\sharp(A_k \cap X_N) \leq CMk$, for some geometric constant $C > 0$, independent of k. Thus, by appropriately summing the bounds (3.8) and inserting into (3.7), we have

$$\begin{aligned} -K\frac{M(M-1)}{2} &\geq \sum_{\substack{i\in I\\ j\notin I}} V(|x_i - x_j|) \\ &= \sum_{i\in I}\left(\sum_{k=1}^{k_0-1}\sum_{j:x_j\in A_k} V(|x_i - x_j|) + \sum_{k=k_0}^{+\infty}\sum_{j:x_j\in A_k} V(|x_i - x_j|)\right) \\ &\geq -C\ M\left(M\frac{k_0(k_0-1)}{2} + \frac{2^p M^2}{r_{min}^p}\sum_{k=k_0}^{\infty}\frac{k}{(k-1)^p}\right). \end{aligned} \tag{3.9}$$

Notice that if $M \geq 2$, then for $K \to +\infty$ the left-hand-side in (3.9) tends to $-\infty$ whereas the right-hand-side remains finite since $p > 2$; therefore, there exists $K = K(C_1, C_2, r_{min}, r_0, p) > 0$ large enough such that $M = 1$. □

3.2. **Combinatorial setup.** From now on we slightly change notations, in order to be able to think of our configurations optimizing the energy as *discrete manifolds*.

We have three types of data: labels of points, combinatiorial information (graphs, edges, boundaries, etc.) and metric information (distances, angles, etc.). To keep track of this we use the following notation conventions:

- Sets of labels, with no further structure useful to us, will be indicated by greek capital letters like $\Xi, \Lambda, \ldots$.
- Sets of which we are interested in the *combinatorial* structure will be indicated by capital calligraphic letters like $\mathcal{G}, \mathcal{Z}_{\boxtimes}, \mathcal{S}, \ldots$.
- Sets of which we are interested in the *metric* structure will be indicated by capital letters like $X, U, \ldots$.

The combinatorial model-space will be

$$\mathcal{Z}_{\boxtimes} = (\mathbb{Z}^2, \{\{a, b\} :\ a, b \in \mathbb{Z}^2,\ |a - b| \in \{1, \sqrt{2}\}\}). \tag{3.10}$$

In general, the notation $\mathcal{G} = (\Xi, \mathcal{S})$ will be used to denote a graph with vertex set Ξ and edge set $\mathcal{S}$.

The first notations we introduce are

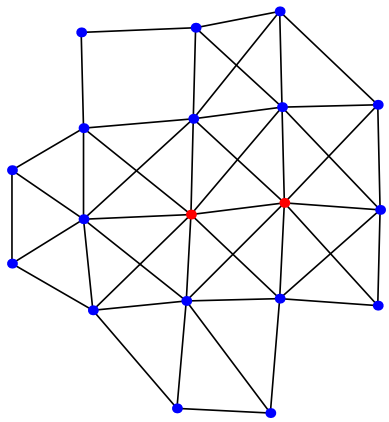


FIGURE 3. A configuration with 19 points, blue vertices correspond to $\partial\mathcal{G}_\alpha$ and red points are interior ones (with $\alpha = 0.3$ here).

- Ξ are the labels of our configurations. Till now we had $\Xi = \{1, \dots, N\}$, but putting an order structure on our labels could be confusing and we avoid it. We write Ξ_N when we want to stress that Ξ is a set of N labels.
- $X \subset \mathbb{R}^2$ will be a finite metric subspace. We also denote by X injective maps $\Xi \to \mathbb{R}^2$, whenever only the image $X(\Xi)$ is of interest to us and we use the notation $x_p := X(p)$ for every $p \in \Xi$. Till now we had $X_N = X(\Xi) = X(\{1, \dots, N\})$ and $x_i = X(i)$.

We next introduce some notations reminiscent of the ones of [48] adapted to our setting (see also Figure 3). Below X and Ξ are as above, and p denotes a point in Ξ:

$$\mathcal{S}_\alpha = \mathcal{S}_\alpha(X) := \Big\{\{p,q\} :\ p,q \in \Xi,\ |x_p - x_q| \in (1-\alpha, \sqrt{2}+\alpha)\Big\}, \tag{3.11a}$$

$$\mathcal{G}_\alpha = \mathcal{G}_\alpha(X) := (\Xi, \mathcal{S}_\alpha(X)), \tag{3.11b}$$

$$\mathcal{N}_\alpha(p) = \mathcal{N}_\alpha(X,p) := \{q \in \Xi : \{p,q\} \in \mathcal{S}_\alpha(X)\} \cup \{p\}, \tag{3.11c}$$

$$\partial\mathcal{G}_\alpha := \{p \in \Xi : \mathcal{N}_\alpha(p) \neq 9\}, \tag{3.11d}$$

$$\mathcal{G}_\alpha|_\Lambda = \mathcal{G}_\alpha(X)|_\Lambda := \big(\Lambda\ ,\ \{\{p,q\} : p,q \in \Lambda\} \cap \mathcal{S}_\alpha(X)\big). \tag{3.11e}$$

Notice that $p \in \mathcal{N}(p)$ by definition. Lemma 3.1, applied with $r_{\min} = 1-\alpha$ ensures that for energy-minimizing configurations there holds $|x_p - x_q| > 1-\alpha$ for $p \neq q \in \Xi$, thus the energy of any minimizer can be written as follows

$$\mathcal{E}[V](X) = \sum_{\{p,q\} \in \mathcal{S}_\alpha(X)} V(|x_p - x_q|) + \sum_{\substack{\{p,q\} \notin \mathcal{S}_\alpha(X) \\ p,q \in \Xi, p \neq q}} V(|x_p - x_q|). \tag{3.12}$$

Notice that the notation in (3.11) is coherent with the one introduced in Section 2 for $\alpha = 0$, since

$$\mathcal{S}_0 = \bigcap_{\alpha > 0} \mathcal{S}_\alpha = \lim_{\alpha \to 0^+} \mathcal{S}_\alpha.$$

Anyway, wherever not specified, all the results of the remainder of the paper refer to the case $\alpha > 0$. Whenever it is clear from the context, the dependence on α is omitted in the notations.

Lemma 3.3. *There exists $\bar{\alpha} \in (0,1)$ such that for every $\alpha \in [0, \bar{\alpha})$ the following holds: If X satisfies* (3.2) *with $r_{min} = 1-\alpha$, i.e.*

$$\min_{\substack{p,q\in\Xi \\ p\neq q}} |x_p - x_q| > 1-\alpha, \tag{3.13}$$

then $\sharp\mathcal{N}_\alpha(p) \leq 9$ for every $p \in \Xi$.

Proof. Let $p \in \Xi$ such that $\sharp\mathcal{N}_\alpha(p) \geq 10$, then there exists two points $q, q' \in \mathcal{N}_\alpha(p)\backslash\{p\}$ such that $\theta := \widehat{x_q x_p x_{q'}} \leq 40^\circ$. Therefore, by the cosine law and by the definition of $\mathcal{N}_\alpha(p)$, we deduce that

$$\begin{aligned} |x_q - x_{q'}|^2 &= |x_p - x_q|^2 + |x_p - x_{q'}|^2 - 2|x_p - x_q||x_p - x_{q'}|\cos\theta \\ &\leq (\sqrt{2}+\alpha)^2 - 2(1-\alpha)^2\cos 40^\circ. \end{aligned}$$

We now claim that, for α small enough,

$$(\sqrt{2}+\alpha)^2 - 2(1-\alpha)^2\cos 40^\circ \leq (1-\alpha)^2.$$

It is indeed straightforward to rewrite the inequality above as

$$2\cos 40^\circ\alpha^2 - \left(2\sqrt{2} + 2 + 4\cos 40^\circ\right)\alpha + 2\cos 40^\circ - 1 \geq 0$$

and to show that this inequality is true if and only if

$$\alpha \in [0, \overline{\alpha}] \cup [\tilde{\alpha}, \infty),$$

where, in particular,

$$\overline{\alpha} = \frac{\sqrt{2}+1+2\cos 40^\circ - \sqrt{(\sqrt{2}+1+2\cos 40^\circ)^2 - 2\cos 40^\circ(2\cos 40^\circ - 1)}}{2\cos 40^\circ} \approx 0.068.$$

and $\tilde{\alpha} > 5$.

Thus, for $\alpha \in [0, \overline{\alpha})$, we have $|x_q - x_{q'}| < 1-\alpha$ which contradicts (3.2) and thus proves the lemma. □

3.3. **Local rigidity of configurations.** To proceed, we next include a definition, which will help us to track the deformations of our model configurations:

Definition 3.4 (α-deformed distances)**.** Let $\alpha \in [0,1)$ be a constant and (X_1, d_1), (X_2, d_2) be two metric spaces. We say that (X_1, d_1) is an *α-deformation* of (X_2, d_2) and we write

$$X_1 \sim_\alpha X_2, \tag{3.14}$$

if there exists a bijection $\phi : X_1 \to X_2$, called the *α-deformation map* such that

$$\forall x, y \in X_1, \quad (1-\alpha)d_1(x,y) \leq d_2(\phi(x), \phi(y)) \leq (1+\alpha)d_1(x,y).$$

If $x, y \in X$ and ϕ is given, we denote the *ϕ-deformation of* $\{x, y\}$ by

$$\delta_\phi(x,y) := |d_2(\phi(x), \phi(y)) - d_1(x,y)|.$$

If ϕ is clear from the context, we omit it in the notation.

We also say that $A, B \subset \mathbb{R}^2$ are *congruent* and we write $A \simeq B$ if there exists an isometry $T : \mathbb{R}^2 \to \mathbb{R}^2$ such that $T(\mathrm{A}) = B$. This corresponds to the $A \sim_\alpha B$ in the case $\alpha = 0$, with the notation of Definition 3.4.

The next result tells us that whenever we have the combinatorial structure of a square lattice in $\mathcal{G}$ near a point, the metric structure is not much deformed. This will be our main tool for "transforming" combinatorial information to metric information.

In the following $O = O(\alpha)$ is a continuous function defined in a right neighborhood of the origin such that $\limsup_{\alpha \to 0^+} \frac{|O(\alpha)|}{\alpha}$ is finite.

Lemma 3.5 (combinatorics links to metric control)**.** *There exists $\alpha_0 \in (0,1)$ such that for all $\alpha \in (0, \alpha_0)$ the following fact holds true: For every X satisfying* (3.13) *and for every $p \in \Xi$ with $\mathcal{N}_\alpha(p) \cap \partial \mathcal{G}_\alpha = \emptyset$ there exists a bijection $\phi : \mathcal{N}_\alpha(p) \to \{-1,0,1\}^2$ such that $\phi(p) = (0,0)$ and*

$$\begin{array}{llllllll} \phi(p_1) & =(\ \ 1, 0), & \phi(p_2) & =(\ \ 1, \ \ 1), & \phi(p_3) & =(0, \ \ 1), & \phi(p_4) & =(-1, \ \ 1), \\ \phi(p_5) & =(-1, 0), & \phi(p_6) & =(-1, -1), & \phi(p_7) & =(0, -1), & \phi(p_8) & =(\ \ 1, -1), \end{array} \tag{3.15}$$

where $p_1, \dots, p_8$ are the nearest neighbors of p in $\mathcal{G}_\alpha$ ordered counterclockwise around p and such that $|X(p_1) - X(p)| = \min\{|X(p_j) - X(p)| \,:\, j = 1 \dots, 8\}$. Moreover,

$$\begin{aligned} 1 - \alpha \leq |X(p_{j+1}) - X(p_j)| = 1 + O(\alpha) \quad & \text{for every } j = 1, \dots, 7, \\ 1 - \alpha \leq |X(p_{2j+1}) - X(p)| = 1 + O(\alpha) \quad & \text{for every } j = 0, \dots, 3, \\ |X(p_{2j}) - X(p)| = \sqrt{2} + O(\alpha) \quad & \text{for every } j = 1, \dots, 4, \\ \sqrt{2} + O(\alpha) \leq |X(p_{2j-1}) - X(p_{2j+1})| \leq \sqrt{2} + \alpha \quad & \text{for every } j = 1, \dots, 4, \end{aligned} \tag{3.16}$$

with the convention that $p_9 \equiv p_1$.
In particular, there exists $C_3 = C_3(\alpha_0) \in [1, \frac{1}{\alpha_0})$ such that

$$X(\mathcal{N}_\alpha(p)) \sim_{C_3 \alpha} \{-1,0,1\}^2 \ , \tag{3.17}$$

where $\{-1,0,1\}^2$ is endowed with the induced metric from $\mathbb{R}^2$.

The proof of Lemma 3.5 is quite long and is postponed in the Appendix A.

Remark 3.6. In view of (3.15), it immediately follows that, writing $\phi_p = \phi$, it holds: $\phi_p(p) = (0,0)$, $\phi_p(p_{2j}) = \phi_p(p_{2j-1}) + \phi_p(p_{2j+1})$ and $\phi_p(p_{2j+1}) = \frac{1}{2}(\phi_p(p_{2j}) + \phi_p(p_{2j+2}))$, with the usual convention that the numbering of the p_i's is cyclic.

Remark 3.7. The bijection ϕ constructed in Lemma 3.5 is unique up to a composition of a graph endomorphism of $\mathcal{Z}_\boxtimes$.

The following result l is a generalization of Lemma 2.2 to the case $\alpha > 0$. It can be proved using the same tools as for Lemma 3.5, so that also its proof is postponed to Appendix A.

Lemma 3.8. *There exist $\alpha_0' > 0, C_3' > 1$ with $C_3' \alpha_0' < 1$ such that for all $\alpha \in (0, \alpha_0')$, if $\mathcal{G}_\alpha$ is isomorphic to the complete graph over 4 vertices, then*

$$X(\Xi) \sim_{C_3' \alpha} \{0,1\}^2 \subset \mathbb{R}^2. \tag{3.18}$$

3.4. **Minima of 4-point energy and perturbed potentials.** Now we study the 4-point energy problem. The goal is to formulate sufficiently general conditions on potential V under which the square is the unique minimizer. For the computations below it will be simpler to re-express as already mentioned in (1.12),

$$W(s) := V(\sqrt{s}), \quad \text{for} \quad s > 0, \tag{3.19}$$

and to perform the computations using the formula $W(|x-y|^2)$ rather than $V(|x-y|)$ for the pairwise interactions.

We assume that $V, W \in C^2_{pw}((0,\infty))$. In view of (3.19) we can rewrite the four-point energy $\mathcal{E}_4[V] : (\mathbb{R}^2)^4 \to \mathbb{R}$ defined in (1.6) as

$$\mathcal{E}_4[V](x_1,x_2,x_3,x_4) := \frac{1}{2}\sum_{i=1}^{4} W(|x_i - x_{i+1}|^2) + W(|x_1-x_3|^2) + W(|x_2-x_4|^2), \tag{3.20}$$

where we identify indices up to equivalence modulo 4. The vectors in $(\mathbb{R}^2)^4$ will be denoted by $\vec{h} = (h_1,h_2,h_3,h_4)$ and $\vec{k} = (k_1,k_2,k_3,k_4) \in (\mathbb{R}^2)^4$. Moreover we denote by $\{e_1,e_2\}$ the canonical orthonormal basis of $\mathbb{R}^2$ and we set

$$\vec{q} := (q_1,q_2,q_3,q_4) = \frac{1}{2}((-1,-1),(-1,1),(1,1),(1,-1)). \tag{3.21}$$

Lemma 3.9 (Taylor expansion of energy close to a square)**.** *For every $W \in C^2((0,\infty))$ we have*

$$\partial_{\vec{h}}\mathcal{E}_4[V](\vec{q}) = \big(W'(1)+2W'(2)\big)\left(\langle h_3-h_1, e_1+e_2\rangle + \langle h_2-h_4, e_2-e_1\rangle\right), \tag{3.22}$$

$$\begin{aligned}\partial^2_{\vec{h},\vec{k}}\mathcal{E}_4[V](\vec{q}) =& \sum_{i=1}^{4}\left(\sum_{j=1,2} W'(j)\langle h_i-h_{i+j}, k_i-k_{i+j}\rangle\right)\\ &+ 2\sum_{i=1}^{4}\left(\sum_{j=1,2} W''(j)\langle h_i-h_{i+j}, q_i-q_{i+j}\rangle\langle k_i-k_{i+j}, q_i-q_{i+j}\rangle\right).\end{aligned} \tag{3.23}$$

If $W \in C^2_{pw}((0,\infty))$, then (3.22) holds true whereas (3.23) is replaced by

$$\begin{aligned}\partial^2_{\vec{h},\vec{k}}\mathcal{E}_4[V](\vec{q}) =& \sum_{i=1}^{4}\left(\sum_{j=1,2} W'(j)\langle h_i-h_{i+j}, k_i-k_{i+j}\rangle\right)\\ &+ \sum_{i=1}^{4}\left(\sum_{j=1,2} W''_{\pm}(j)\langle h_i-h_{i+j}, q_i-q_{i+j}\rangle\langle k_i-k_{i+j}, q_i-q_{i+j}\rangle\right),\end{aligned} \tag{3.24}$$

where W''_+, W''_- are the second derivatives of W taken from the right and the left respectively and $\pm$ are chosen to match the sign of $\langle h_l-h_m, q_l-q_m\rangle$.

If $W \in C^2((0,\infty))$ then Hess $\mathcal{E}_4[V](\vec{q})$ *has the following eigenvectors and eigenvalues:*

- $(v,v,v,v), v \in \mathbb{R}^2$ *with eigenvalue* 0 *(corresponding to infinitesimal translations),*
- $(v,-v,v,-v), v \in \mathbb{R}^2$ *with eigenvalue* $4(W'(1)+W''(1))$ *(corresponding to translating diagonals in opposite directions),*
- $\vec{q} = (q_1,q_2,q_3,q_4)$*, with eigenvalue* $2W'(1)+4W'(2)+4W''(1)+16W''(2)$ *(corresponding to infinitesimal dilations),*

- (q_2, q_3, q_4, q_1) *with eigenvalue* $2W'(1) + 4W'(2)$ *(corresponding to infinitesimal rotations),*
- (q_4, q_3, q_2, q_1) *with eigenvalue* $2W'(1) + 4W'(2) + 4W''(1)$ *(infinitesimal deformation which rotates the diagonals with respect to each other),*
- (q_1, q_4, q_3, q_2) *with eigenvalue* $2W'(1)+4W'(2)+16W''(2)$ *(infinitesimal deformation which squeezes one diagonal and dilates the other while keeping sidelengths constant).*

The basic tool to prove Lemma 3.9 comes from the expansion of the $N = 4$ energy for configurations close to $\{0,1\}^2 \subset \mathbb{R}^2$. The proof is omitted because it is a direct computation. The lemma slightly generalizes the result of [27, Lemma 6.1], where only a special choice of potential modeling elastic springs was considered instead.

If $W \in C^2_{pw}((0,\infty))$ then we may still apply formula (3.24) to compute the second-order variations of $\mathcal{E}_4[V]$ along vectors $\vec{h}$ expressed in the above basis of infinitesimal deformations. We cannot call these vectors "eigenvectors" anymore, but we can use the geometric decomposition of the above basis in order to understand, for the case of $W \in C^2_{pw}$, what conditions ensure that $\vec{q}$ is a strict local minimum. The result of this computation is stated in Lemma 3.11 below.

We first introduce some notations. By abuse of notation we write $\mathcal{E}_4[V]$ also for the induced functional on 4-ples of points defined up to rotations and translations, thus we write

$$\mathcal{E}_4[V] : \mathcal{X}_4(\mathbb{R}^2)/\mathrm{Isom}(\mathbb{R}^2) = \{X_4 \subset \mathbb{R}^2 : \ \sharp X_4 = 4\}/\mathrm{Isom}(\mathbb{R}^2) \to \mathbb{R}. \tag{3.25}$$

We remark that this is possible since $\mathcal{E}_4[V]$ is invariant under permutations and under isometries of $\mathbb{R}^2$. Note that the above space $\mathcal{X}_4(\mathbb{R}^2)/\mathrm{Isom}(\mathbb{R}^2)$ is a manifold of dimension 5, because $\mathcal{X}_4(\mathbb{R}^2)$ has dimension 8 and it is quotiented by a free action of a group of dimension 3. The scalar product of $\mathbb{R}^8 = (\mathbb{R}^2)^4$ is also invariant thus induces a natural Riemannian manifold structure on $\mathcal{X}_4(\mathbb{R}^2)/\mathrm{Isom}(\mathbb{R}^2)$.

Recalling the definition of $\vec{q}$ in (3.21), we denote by $\boxtimes$ the equivalence class of $\vec{q}$ with respect to the isometries of $\mathbb{R}^2$, i.e. $\boxtimes$ is the undeformed square of sidelength 1 in $\mathcal{X}_4(\mathbb{R}^2)/\mathrm{Isom}(\mathbb{R}^2)$.

Recall that if T_pM is the tangent space at $p \in M$ where (M, g) is a Riemannian manifold, for each $v \in T_pM$ there exists a unique geodesic $\gamma_v : [0,1] \to M$ such that $\gamma_v(0) = p$ and $\gamma_v'(0) = v$. This allows to locally define the *exponential map* $\exp_p : B_r(0) \subset T_pM \to U \subset M$ by $\exp_p(v) := \gamma_v(1)$. For $r > 0$ small enough this map is bijective and is called an *exponential chart*. We use this terminology for $M := U$ where U is a neighborhood of $\boxtimes$ in $\mathcal{X}_4(\mathbb{R}^2)/\mathrm{Isom}(\mathbb{R}^2)$. Furthermore $\nabla\mathcal{E}_4[V]$ calculated at $\widetilde{\boxtimes}$ takes values into $T_{\widetilde{\boxtimes}}U$, and $\exp^*_{\boxtimes}\nabla\mathcal{E}_4[V]$ uses the differential of $\exp_{\boxtimes}$ to go back to corresponding vectors in $T_{\exp^{-1}_{\boxtimes}(\widetilde{\boxtimes})}\widetilde{U} \simeq \mathbb{R}^5$.

With the above notation, we will say that the gradient $\nabla\mathcal{E}_4[V] : U \to \mathbb{R}^5 \simeq T\mathcal{X}_4(\mathbb{R}^2)/\mathrm{Isom}(\mathbb{R}^2)$ is *c-monotone at* $\boxtimes$, if there exist $c \in \mathbb{R}$ and a small neighborhood $\widetilde{U} \ni \boxtimes$ such that the exponential chart $\exp_{\boxtimes} : \widetilde{U} \subset T_{\boxtimes}\mathcal{X}_4(\mathbb{R}^2)/\mathrm{Isom}(\mathbb{R}^2) \to U$ satisfies

$$\langle \exp^*_{\boxtimes}\nabla\mathcal{E}_4[V](\eta') - \exp^*_{\boxtimes}\nabla\mathcal{E}_4[V](\eta''), \eta' - \eta''\rangle > c \qquad \text{for all } \eta', \eta'' \in \widetilde{U} \text{ with } \eta' \neq \eta''. \tag{3.26}$$

We say that $\nabla\mathcal{E}_4[V]$ is *strictly monotone* if the above is satisfied with $c > 0$.

Remark 3.10. The above terminology, is usual in convex analysis or optimal transport theory. See [20] for more details.

The next lemma has as hypothesis condition (2) of Subsection 1.5.

Lemma 3.11 (Local minimum at the square)**.** *Let $V, W \in C^2_{pw}((0,\infty))$ be related by* (3.19)*. The undeformed square $\boxtimes$ is a critical point of $\mathcal{E}_4[V]$ if and only if*

$$W'(1) + 2W'(2) = 0. \tag{3.27}$$

There exists $C_4 > 0$ depending only on the dimension such that $\nabla\mathcal{E}_4[V]$ is c'-monotone at $\boxtimes$ if

$$\begin{aligned} &W''_-(1) + W''_+(1) + 2W'(1) > C_4c', && W''_-(2) + W''_+(2) > C_4c', \\ &W''_-(1) + W''_+(1) > C_4c', && W''_\pm(1) + 4W''_\pm(2) > C_4c'. \end{aligned} \tag{3.28}$$

In particular in this case $\boxtimes$ is a strict local minimum of $\mathcal{E}_4[V]$ up to rotations and translations.

Sketch of proof: It is sufficient to verify that the directional one-sided double derivatives of $\mathcal{E}_4[V]$ along any direction are strictly positive.

If in a neighborhood of $\{1,2\}$ the function W happens to be C^2 then the statement follows directly from Lemma 3.9. If not, note that the formulas (3.23) still hold separately for the cases that h_j infinitesimally increase/decrease the lengths of the sides of the square $\{-1/2, 1/2\}^2$ which we consider. We next discuss what happens along the infinitesimal deformations distinguished in the lemma, not coming from translations or rotations. Below, the constant C_4 accounts for deformations coming from bounds on $\exp_\boxtimes$ in U and from applying the chain rule, and thus ultimately depends only on the dimension.

- The infinitesimal dilations $\vec{h} = \lambda\vec{q}$ either contemporarily increase or contemporarily decrease all lengths of all sides and diagonals, thus we get the strict local minimum conditions $W''_+(1) + 4W''_+(2) > C_4c'$ and $W''_-(1) + 4W''_-(2) > C_4c'$.
- The infinitesimal perturbations along (q_4, q_3, q_2, q_1) infinitesimally preserve lengths of diagonals, squeeze two sides and dilate the other two, thus we get the condition $W''_-(1) + W''_+(1) > C_4c'$.
- The infinitesimal perturbations along (q_1, q_4, q_3, q_2) infinitesimally preserve lengths of sides, squeeze one diagonal and dilate the other, and give the strict local minimum condition $W''_-(2) + W''_+(2) > C_4c'$.
- Finally, the case $\vec{h} = (v, -v, v, -v)$ does not alter the lengths of diagonals, and thus contributes by only the term with $W''_\pm(1)$ in (3.23), which gives the contribution proportional to $I(v)$, where with notation $v := (v_1, v_2)$ and $\sigma_j := \mathrm{sign} v_j$ we have

$$\begin{aligned} I(v) &:= W''_{\sigma_2}(1)|v_2|^2 + W''_{-\sigma_1}(1)|v_1|^2 + W''_{-\sigma_2}(1)|v_2|^2 + W''_{\sigma_1}(1)|v_1|^2 \\ &= (W''_+(1) + W''_-(1))|v|^2, \end{aligned}$$

  where in the first above sum, the contributions of indices $(i,j) = (1,2), (2,3), (3,4), (4,1)$ are summed in this order. Summing the above to the $W'(1)$-term, we get the condition $W''_+(1) + W''_-(1) + 2W'(1) > C_4c'$.

The fact that $C_4 > 0$ as in the statement can be encountered follows by standard Taylor-type approximation of $\mathcal{E}_4[V]$. □

3.4.1. *Perturbations of $\mathcal{E}_4[V]$ near its minimum.* We recall that E_α, E^1_α and E^2_α are defined by (1.7). Taking indices $1,\dots,4$ modulo 4, we set

$$\begin{aligned}\mathscr{Q}_\alpha := \{\eta=\{\eta_1,\eta_2,\eta_3,\eta_4\equiv\eta_0\}\in\mathcal{X}_4(\mathbb{R}^2)\,:\,|\eta_i-\eta_{i+1}|\in E^1_\alpha \quad \text{for all } i=1,\dots,4,\\ |\eta_1-\eta_3|,|\eta_2-\eta_4|\in E^2_\alpha\},\qquad \overline{\mathscr{Q}}_\alpha := \mathscr{Q}_\alpha/\mathrm{Isom}(\mathbb{R}^2),\end{aligned} \tag{3.29}$$

and

$$\begin{aligned}\mathscr{S}_\alpha := \{\eta=\{\eta_1,\eta_2,\eta_3,\eta_4\equiv\eta_0\}\in\mathscr{Q}_\alpha\,:\,|\eta_i-\eta_{i+1}|=l \quad \text{for all } i=1,\dots,4,\\ |\eta_1-\eta_3|,|\eta_2-\eta_4|=\sqrt{2}l \text{ for some } l\in E^1_\alpha\cap\frac{1}{\sqrt{2}}E^2_\alpha\},\quad \overline{\mathscr{S}}_\alpha := \mathscr{S}_\alpha/\mathrm{Isom}(\mathbb{R}^2).\end{aligned} \tag{3.30}$$

With a little abuse of notations, we will call quadrilaterals the 4-ples η of $\mathscr{Q}_\alpha$; moreover, for every $\eta\in\mathscr{Q}_\alpha$ we refer to the quantities $|\eta_i-\eta_{i+1}|$ as side-lengths of η and to the quantities $|\eta_1-\eta_3|$ and $|\eta_2-\eta_4|$ as diagonal-lengths.
The following lemma holds under the hypothesis from condition (1) in Subsection 1.5.

Lemma 3.12. *Let $V\in C^2_{pw}((0,\infty))$ and let $\alpha''\in(0,\alpha'_0)$ (with α'_0 given by Lemma 3.8) be such that*

1. *V is convex in $E_{\alpha''}$,*
2. *V is strictly convex in $E_{\alpha''}\setminus[1,\sqrt{2}]$.*

Then there exists at most one global minimizer $\tilde{Q}$ of $\mathcal{E}_4[V]$ in $\overline{\mathscr{Q}}_{\alpha''}$. Moreover, if such a minimizer exists, then it belongs to $\overline{\mathscr{S}}_{\alpha''}$. Furthermore, for every $\alpha'\in(0,\alpha'')$ there are no minimizers of $\mathcal{E}_4[V]$ in $\overline{\mathscr{Q}}_{\alpha'}\setminus\{\tilde{Q}\}$.

Proof. Let $\eta:=\{x_1,x_2,x_3,x_4\}\in\mathscr{Q}_{\alpha''}$ and let $a\le b\le c\le d$ denote the sidelengths of η.
Case 1. *V is strictly convex in $E_{\alpha''}$.* We will show that if $\eta\notin\mathscr{S}_{\alpha''}$, then the energy $\mathcal{E}_4[V](\eta)$ can be decreased to first order by infinitesimal perturbations.

- If $|x_1-x_3|<|x_2-x_4|$ then there exists an infinitesimal perturbation which increases $|x_1-x_3|$ and decreases $|x_2-x_4|$ while keeping the remaining distances fixed. The convexity of V for in $E^2_{\alpha''}$ shows that under this deformation $\mathcal{E}_4[V]$ decreases. Thus η has equal length diagonals.
- If $a<d$, then there exists an infinitesimal perturbation which preserves the length of the diagonals, preserves the ordering of sidelengths and increases a,b while diminishing c,d, and such that at least one of them increases/decreases is strict. The convexity of V in $E^1_{\alpha''}$ shows that $V(a)+V(d)$ and $V(b)+V(c)$ strictly decrease under this perturbation. Thus η has equal sidelengths.

The above two points show that $\eta\in\mathscr{S}_{\alpha''}$.

If there were two minima η,η' with sidelengths $r<r'\in E^1_{\alpha''}$ then we would have $2V(r)+2V(\sqrt{2}r)=2V(r')+2V(\sqrt{2}r')$ and by strict convexity of V in the intervals (r,r') and $(\sqrt{2}r,\sqrt{2}r')$ we would have that the square of any intermediate sidelength would have smaller energy $\mathcal{E}_4[V]$, thus giving a contradiction to the minimality of η,η'. This completes the proof of the uniqueness result. Finally, since the constraints defining E_α are open and V is continuous, the same reasoning proves also the last sentence of the statement.

Case 2. *General case.* To adapt the proof from case 1 to a proof under more general hypotheses (1),(2), we proceed in two steps.

- First note that a contradiction is reached if we know that V is strictly convex at *just a single* point of the subset $[a,d]\cup[|x_1-x_3|,|x_2-x_4|]$, while being convex on the whole subset.
- Finally, as a consequence of Lemma 3.8, if $\{x_1,x_2,x_3,x_4\}$ were not a unit square, then $[a,d]\cup[|x_1-x_3|,|x_2-x_4|]$ would intersect $(1-\alpha'',1]\cup[\sqrt{2},\sqrt{2}+\alpha'')$, and then the strict convexity hypothesis as described in the first item allows to find a contradiction, as desired.

□

By combining Lemma 3.11and Lemma 3.12, the first results insuring the undeformed square $\boxtimes$ to be a strict local minimizer of $\mathcal{E}_4[V]$ in $\overline{\mathscr{Q}}_{\alpha_0''}$ and the second one giving its uniqueness, we have the following result.

Proposition 3.13. *Let $V,W\in C^2_{pw}((0,\infty))$ be related as in* (1.12)*. Assume that V satisfies the assumptions of Lemma 3.12 and W satisfies* (3.27) *and* (3.28)*. Then, there exists $\alpha_0''\in(0,\alpha_0')$ (with α_0' given by Lemma 3.8) such that $\boxtimes$ is the only minimizer of $\mathcal{E}_4[V]$ in $\overline{\mathscr{Q}}_{\alpha_0''}$. Moreover, for every $\alpha''\in(0,\alpha_0'')$ there exists no minimizer of $\mathcal{E}_4[V]$ in $\overline{\mathscr{Q}}_{\alpha''}\setminus\{\boxtimes\}$.*

The following results Lemma 3.14 and Proposition 3.15 below are generalizations of Proposition 3.13 to perturbations of potentials W satisfying (3.27) and (3.28). Such results are used in the proof of Theorem 4.16 which deals with asymptotic crystallization for long-range potentials, but we decide to include them in this subsection since they concern the minimization of a 4-point energy.
For every $\alpha>0$, we set

$$E^{sq}_\alpha:=((1-\alpha)^2,(1+\alpha)^2)\cup((\sqrt{2}-\alpha)^2,(\sqrt{2}+\alpha)^2). \tag{3.31}$$

Lemma 3.14 (general perturbations of potentials)**.** *Let $c',\alpha'>0$. Let $W\in C^2_{pw}((0,\infty))$ satisfy* (3.27) *and* (3.28)*. Then there exists $c_5=c_5(c',\alpha',W)>0$ such that if W_* is a perturbation of W with $\|W'-W'_*\|_{C^1(E^{sq}_{\alpha'})}<c_5$, then the 4-point energy $\mathcal{E}_4[V_*]$ has precisely one local minimum $\overline{\boxtimes}$ in $\overline{\mathscr{Q}}_{\frac{\alpha'}{2}}$ and W_* satisfies* (3.28) *with $c=\frac{c'}{2}$.*

Proof. Due to the assumption that (3.27) holds, it follows from Lemma 3.11 that $\mathcal{E}_4[V]$ has a critical point at $\boxtimes$.

We can then apply the implicit function theorem for strictly monotone functions (see for instance [20, Thm. 1H.3], whose proof directly extends to the case of $F(w,x):=\nabla\mathcal{E}_4[v](\boxtimes+x)$, where w is a perturbation of W in C^2-norm, $v(r)=w(r^2)$, and $\mathcal{E}_4[v]$ is defined using formula (3.20) with w instead of W). This allows to verify that there exists $c_5=c_5(c',\alpha',W)>0$ such that for each W_* such that W'_* is closer than c_5 to W' in C^1-norm, there exists a unique zero of $\nabla\mathcal{E}_4[V_*]$ in $\overline{\mathscr{Q}}_{\frac{\alpha'}{2}}$. Up to restricting c_5, the bounds (3.28) hold also for W_* with $c=\frac{c'}{2}$ if $\|W'_*-W'\|_{C^1(E^{sq}_{\alpha'})}<c_5$. Thus the monotonicity conditions continue to hold for $\nabla\mathcal{E}_4[V_*]$ in $\overline{\mathscr{Q}}_{\frac{\alpha'}{2}}$ as well, allowing to verify the uniqueness and strict minimality claim of the lemma. □

By combining the above lemmas we have the following result, which applies to potentials V as in Figure 2. We recall that $\alpha_0'>0$ and $C_3'\in[1,\frac{1}{\alpha_0'})$ are the constants found in Lemma 3.8.

Proposition 3.15 (unique square minimum robust under C^2 perturbations)**.** *Let $\alpha'' \in (0, \alpha_0')$ and $0 < \alpha' \leq \alpha \leq \frac{\alpha''}{C_3'}$. Let $V, W \in C^2_{pw}((0,\infty))$ be related by (3.19). Assume that there exists $c, c', c'' > 0$ such that:*

(0) $\min_{s>0} W(s) = -1$;
(1) *V is convex in $E_{\alpha''}$ and V satisfies* $\inf_{r \in E_{\alpha''} \setminus [1,\sqrt{2}]} V''_{\pm}(r) \geq c$;
(2) *W satisfies (3.27) and (3.28) with constant c';*
(3) $\sup_{r \in E_{\alpha'}} V(r) < -\frac{15}{16} - c''$;
(4) $V(r) > -\frac{1}{2}$ *if* $r \notin (1-\alpha, \sqrt{2}+\alpha)$.

Recalling that c_5 is the constant defined in Lemma 3.14 and setting $c''' := \min\{c_5(c', \alpha', W), c''/2, c/2\}$, for every perturbation $V_* \in C^2_{pw}((0,\infty))$ of V with

$$\|W - W_*\|_{C^2((0,\infty))} < c''', \tag{3.32}$$

we have that the 4-point energy $\mathcal{E}_4[V_*]$ has exactly one global minimizer in $\mathcal{X}_4(\mathbb{R}^2)/\mathrm{Isom}(\mathbb{R}^2)$ and such a minimizer, denoted by $\boxtimes$, lies actually in $\mathscr{S}_{\frac{\alpha'}{2}}$.

If $V_* \in C^2_{pw}((0,\infty))$ satisfies only

$$\|W - W_*\|_{C^2(((1-\alpha'')^2,+\infty))} < c''', \tag{3.33}$$

then the energy $\mathcal{E}_4[V_*]$ has exactly one minimum with sidelengths in the interval $(1-\alpha, +\infty)$, which is a square.

Proof. We will only prove the first part of the statement, as the proof for the second part is analogous, restricting the domain to $(1-\alpha'', +\infty)$ instead.

We first show that all the points in a minimizer of $\mathcal{E}_4[V_*]$ stay at a distance in $(1-\alpha, \sqrt{2}+\alpha)$ from each other. Indeed, suppose we have a minimizing configuration Q which has two vertices x, x' whose distance is outside this interval. By using in order of appearance, (3.32), (3), and the fact that $c''' \leq \frac{c''}{2}$, we get

$$\mathcal{E}_4[V_*](\boxtimes) \leq 4 \sup_{r \in E_{\alpha'}} V(r) + 4c''' < -\frac{15}{4} - 4c'' + 4c''' \leq -\frac{15}{4} - 2c''; \tag{3.34}$$

moreover, by assumptions (0) and (4), (3.32), and using again the fact that $c''' < \frac{c''}{2}$, we obtain

$$\mathcal{E}_4[V_*](Q) \geq \frac{7}{2} \min_{\rho>0} V_*(\rho) + \frac{1}{2} V_*(|x - x'|) \geq -\frac{7}{2} - \frac{1}{4} - 4c''' \geq -\frac{15}{4} - 2c'', \tag{3.35}$$

which combined with (3.34) contradicts the assumption on the minimality of Q.
Since $\alpha < \alpha_0'$, by Lemma 3.8, the edge lengths of any minimizer are at most $C_3'\alpha$-deformed compared to the edge lengths of a unit square, which by the upper bound on α implies that all minimizers have edge lengths in $E_{\alpha''}$, as desired.
It follows that every minimizer of $\mathcal{E}_4[V_*]$ lies in $\mathscr{Q}_{\alpha''}$. Therefore, by assumption (1) and (3.32) we have that V_* still satisfies the assumptions of Lemma 3.12. Therefore, there exists at most one minimizer of $\mathcal{E}_4[V_*]$ in $\mathcal{X}_4(\mathbb{R}^2)/\mathrm{Isom}(\mathbb{R}^2)$ and that such minimizer, if exists, lies in $\overline{\mathscr{S}}_{\frac{\alpha'}{2}}$.
Finally, by assumption (2) and by (3.32), we can apply Lemma 3.14 thus obtaining that a unique minimizer of $\mathcal{E}_4[V_*]$ exists in $\overline{\mathscr{Q}}_{\frac{\alpha'}{2}}$; this fact together with the last part of Lemma 3.12 implies the full claim.

□

3.5. **Crystallization under smooth one-well potentials with finite range.** By using the tools from Sections 3.1, 3.2 and 3.3 we can prove our second main theorem, stated below in detail.

Recall that the constant $\overline{\alpha}$ is given by Lemma 3.3, the constants $\alpha_0 > 0$, $C_3 > 1$ are provided by Lemma 3.5, $\alpha_0' > 0$ is given by Lemma 3.8 , and α_0'' is given by Proposition 3.13.

Theorem 3.16 (crystallization under finite-range smooth potentials)**.** *Let $\alpha, \alpha', \alpha'' > 0$ be such that $\alpha' < \alpha < \frac{1}{C_3}\alpha'' < \frac{1}{C_3}\min\{(2-\sqrt{2})/4, \overline{\alpha}, \alpha_0, \alpha_0', \alpha_0''\}$.*
Set $r_{min} := 1-\alpha$, $C_2 := 1$ and $r_0 := \sqrt{2}+\alpha''$, and let $K' > 0$ be as in Lemma 3.1.
There exist constants $c', K'' > 0$ such that the following holds true: if $V, W \in C^2_{pw}((0,\infty))$ are related by (3.19) *and satisfy*

(0) $\min_{s>0} W(s) = -1$,
(1) *V is convex in $E_{\alpha''}$ and strictly convex in $E_{\alpha''} \setminus [1, \sqrt{2}]$,*
(2) *W satisfies* (3.27) *and* (3.28) *with constant c',*
(3) $\sup_{r \in E_{\alpha'}} V(r) < -\frac{15}{16}$;
(4) $V(r) > -\frac{1}{2}$ *if* $r \notin (1-\alpha, \sqrt{2}+\alpha)$,
(5) $V(r) > \max\{K', K''\}$ *for* $r \le 1-\alpha$,
(6) $V(r) = 0$ *for* $r \ge \sqrt{2}+\alpha''$,

then

$$N\overline{\mathcal{E}}_{\rm sq}[V] \le \mathcal{E}[V](N) \le N\overline{\mathcal{E}}_{\rm sq}[V] + O(N^{1/2}) \qquad \text{as } N \to +\infty, \tag{3.36}$$

and furthermore

$$\min \mathcal{E}_4[V] = \overline{\mathcal{E}}_{\rm sq}[V]. \tag{3.37}$$

Remark 3.17. *Assumption (3) corresponds to assumption (B) of the introduction with $\epsilon' = \frac{1}{16}$. Furthermore, the constant K'' is here to ensure that the minimal energy per point of a square $\overline{\mathcal{E}}_{\rm sq}[V]$ is achieved for some $\underline{t} > 1-\alpha$. The number $K > 0$ appearing in Theorem 1.2 and Figure 2(left) is then* $\max\{K', K''\}$.

Proof. We first prove (3.37). Let $\underline{t} > 0$ be the value at which the minimum from (1.4) in the definition of $\overline{\mathcal{E}}_{\rm sq}[V]$ is achieved.

We first show that there exists $K'' > 0$, independent of the remaining parameters, so that $\underline{t} > 1-\alpha$. This will fix the choice of K'', and we use a strategy reminiscent of Lemma 3.1. Note first that $\overline{\mathcal{E}}_{\rm sq}[V] \le 0$, by considering condition (6) and testing the minimization over $t > 0$ with $t = 1$. Next, using assumptions (0), (4), (5) and (6), we write

$$\mathcal{E}[V](\underline{t}\mathbb{Z}^2 \cap B_R) = \frac{1}{2}\sum_{\substack{x \neq y \in \underline{t}\mathbb{Z}^2 \cap B_R \\ |x-y| \le 1-\alpha}} V(|x-y|) + \frac{1}{2}\sum_{\substack{x,y \in \underline{t}\mathbb{Z}^2 \cap B_R \\ |x-y| \in (1-\alpha, \sqrt{2}+\alpha'')}} V(|x-y|) \tag{3.38}$$

$$\ge \frac{1}{2}K''\sharp\{x \in \underline{t}\mathbb{Z}^2 \cap B_{R-1-\alpha}\}\left(\sharp\{x \in \underline{t}\mathbb{Z}^2 :\ |x| \le 1-\alpha\} - 1\right) \tag{3.39}$$

$$-\frac{1}{2}\sharp\{x \in \underline{t}\mathbb{Z}^2 \cap B_{R+\sqrt{2}+\alpha''}\}\sharp\{x \in \underline{t}\mathbb{Z}^2 :\ |x| \le \sqrt{2}+\alpha''\}. \tag{3.40}$$

To obtain (3.39) we used (5) and estimated the first sum in (3.38) from below by noting that for each $p \in \underline{t}\mathbb{Z}^2 \cap B_{R-1-\alpha}$, all points $x \in \underline{t}\mathbb{Z}^2 \cap \overline{B}_{1-\alpha}(p)$ contribute at least an energy of K'', and we double-count contributions at most twice. Similarly, for (3.40) we used (0) and

perform a similar bound from above, in which we do not account for the double-counting anymore. Now it remains to note that the first factors in (3.39), (3.40) are both of the form

$$\pi\left(\frac{R}{\underline{t}}\right)^2 + O\left(\frac{R}{\underline{t}}\right) \qquad \text{as } R\to\infty.$$

Finally, by a very rough packing bound, if $\underline{t} < 1-\alpha$ (condition required for the term (3.39) to be nonzero) the second factors in (3.39), (3.40) both lie in the interval $[c/\underline{t}^2, C/\underline{t}^2]$, where $0<c<C$ are constants which can be chosen independently of the choices of α, α'' in the interval $(0,(2-\sqrt{2})/4)$. These considerations allow to continue the estimate (3.38) and obtain

$$\mathcal{E}[V](\underline{t}\mathbb{Z}^2\cap B_R) \geq \left[\frac{1}{2}\pi\left(\frac{R}{\underline{t}}\right)^2 + O\left(\frac{R}{\underline{t}}\right)\right](cK''-C), \tag{3.41}$$

which for $K''>C/c$ contradicts our former conclusion $\overline{\mathcal{E}}_{\mathrm{sq}}[V]\leq 0$, as desired. It follows that $\underline{t}>1-\alpha$. Since $\alpha<\frac{\alpha''}{C_3}<\alpha''$ and $0<\alpha''<\frac{2-\sqrt{2}}{4}$, we get

$$2\underline{t} > 2(1-\alpha'') > 2-4\alpha''+\alpha'' > \sqrt{2}+\alpha'',$$

from which we deduce that only distances $\underline{t}, \underline{t}\sqrt{2}$ can participate to the computation of the energy and thus

$$\begin{aligned}\mathcal{E}[V]\left(\underline{t}\mathbb{Z}^2\cap B_R\right) &= \sharp\left(\underline{t}\mathbb{Z}^2\cap B_R\right)\mathcal{E}_4[V](\{0,\underline{t}\}^2) + O(R)\\ &\geq \sharp\left(\underline{t}\mathbb{Z}^2\cap B_R\right)\min\mathcal{E}_4[V] + O(R).\end{aligned} \tag{3.42}$$

Therefore, by dividing both terms by $\sharp\left(\underline{t}\mathbb{Z}^2\cap B_R\right)\sim O(R^2)$ and sending $R\to\infty$, we get the inequality "$\leq$" in (3.37). On the other hand, by assumptions (1) and (2), we can apply Proposition 3.13 thus obtaining $\min\mathcal{E}_4[V]=\mathcal{E}_4[V](\boxtimes)$. Then, doing the same computation as in the first line of (3.42) with $\underline{t}$ replaced by 1 we get the inequality "$\geq$" in (3.37).

We now prove the first inequality in (3.36). Let then $\mathcal{S}_\alpha$ be as in (3.11). By assumptions (0), (5) and (6), we can apply Lemma 3.1, thus getting that

$$\min_{\substack{p,q\in\Xi_N\\ p\neq q}} |x_p-x_q| > 1-\alpha \qquad \text{for any minimizer } X_N=X(\Xi_N) \text{ in } \mathcal{X}_N(\mathbb{R}^2). \tag{3.43}$$

Setting

$$\mathcal{S}_{\alpha'',\alpha} := \{\{p,q\} \,:\, p,q\in\Xi_N\,, \sqrt{2}+\alpha\leq|x_p-x_q|<\sqrt{2}+\alpha''\},$$

by (3.43) and by the fact that $V(r)=0$ for $r>\sqrt{2}+\alpha''$, we deduce that

$$\mathcal{E}[V](X_N) = \sum_{\{p,q\}\in\mathcal{S}_\alpha\cup\mathcal{S}_{\alpha'',\alpha}} V(|x_p-x_q|).$$

Then by Lemma 3.5 (in particular by (3.16)) following from the fact that $\alpha''<\alpha_0$, we find that for every $p\in\{1,\dots,N\}$ with $\mathcal{N}_\alpha(p)\cap\partial\mathcal{G}_\alpha=\emptyset$, the neighborhood $\mathcal{N}_\alpha(p)$ of p is locally a $C_3\alpha$-deformation of $\{-1,0,1\}^2$. We next write $\mathcal{E}[V](X_N)$ as a sum over $C_3\alpha$-deformations of $\{0,1\}^2$. We will use the following notation:

$$\mathcal{Q}_1 := \left\{Q\subset\Xi_N :\ X(Q)\sim_{C_3\alpha}\{0,1\}^2\right\}. \tag{3.44}$$

We then rewrite

$$\mathcal{E}[V](X_N) = \sum_{Q\in\mathcal{Q}_1}\mathcal{E}_4[V](Q) + \frac{1}{2}\sum_{\{x,y\}\in\mathcal{NC}^{(1)}} V(|x-y|) + \sum_{\{x,y\}\in\mathcal{NC}^{(2)}} V(|x-y|), \tag{3.45}$$

in which $\mathcal{NC}^{(j)}$ is the collection of all pairs $\{x, y\}$ which appear in the first sum on the right with multiplicity $2 - j$, for $j = 1, 2$. We will also denote $\mathcal{NC} := \mathcal{NC}^{(1)} \cup \mathcal{NC}^{(2)}$.

Since $C_3\alpha < \alpha'' < \alpha_0''$, we get that every $Q \in \mathcal{Q}_1$ satisfies $X(Q) \in \overline{\mathscr{F}}_{\alpha_0''}$, which in view of Proposition 3.13 implies

$$\mathcal{E}_4[V](Q) \geq \min \mathcal{E}_4[V] = \mathcal{E}_4[V](\boxtimes) \qquad \forall Q \in \mathcal{Q}_1, \tag{3.46}$$

and

$$\mathcal{E}_4[V](\boxtimes) \leq 4 \sup_{\rho \in E_{\alpha'}} V(\rho) := 4m_{\alpha',V}. \tag{3.47}$$

Note that if $\{p, q\} \in \mathcal{NC}$ then we have $\mathcal{N}_\alpha(p) \cap \partial\mathcal{G}_\alpha \neq \emptyset$ or $\mathcal{N}_\alpha(q) \cap \partial\mathcal{G}_\alpha \neq \emptyset$ or $\{p, q\} \in \mathcal{S}_{\alpha'',\alpha}$. We will use below without mention the consequences that all such edges belong to $\mathcal{S}_{\alpha''}$. Now we denote

$$\mathcal{E}^p[V](X_N) := \frac{1}{2} \sum_{\substack{q \in \Xi_N \\ q \neq p}} V(|x_p - x_q|) = \frac{1}{2} \sum_{\substack{q \in \mathcal{N}_{\alpha''}(p) \\ q \neq p}} V(|x_p - x_q|),$$

and we note that $\mathcal{E}[V](X_N)$ is the sum of $\mathcal{E}^p[V](X_N)$ over all labels p. Furthermore we have the following bound, which uses assumptions (0) and (4):

$$\begin{aligned} \mathcal{E}^p[V](X_N) \quad \geq \quad & \frac{1}{8}\mathcal{E}_4[V](\boxtimes)\ \sharp\{q \in \mathcal{N}_\alpha(p) \setminus \{p\} :\ \{p, q\} \notin \mathcal{NC}\} \\ & -\frac{1}{2}\sharp\{q \in \mathcal{N}_\alpha(p) \setminus \{p\} :\ \{p, q\} \in \mathcal{NC}\} \\ & -\frac{1}{4}\sharp\{q \in \mathcal{N}_{\alpha''}(p) \setminus \mathcal{N}_\alpha(p)\}. \end{aligned} \tag{3.48}$$

We concentrate first on p such that $\mathcal{N}_\alpha(p) \cap \partial\mathcal{G}_\alpha = \emptyset$. Note that due to the hypothesis $\alpha'' < \overline{\alpha}$, by Lemma 3.3 we have $\sharp\mathcal{N}_{\alpha''}(p) \leq 9$, and since $p \notin \partial\mathcal{G}_\alpha$, we have $\sharp\mathcal{N}_\alpha(p) = 9$, so that all 8 edges containing p in $\mathcal{G}_{\alpha''}$ are actually in $\mathcal{G}_\alpha$. By the hypothesis $\mathcal{N}_\alpha(p) \cap \partial\mathcal{G}_\alpha = \emptyset$ all such edges are covered with full multiplicity in the first sum on the right of (3.45), so they don't belong to $\mathcal{NC}$. Thus, the lower bound in (3.48) is in this case just $\mathcal{E}_4[V](\boxtimes)$.

Now consider the remaining points, for which we used the rough bounds corresponding to the last two lines in (3.48): either they have at least one "long" edge, with "good" energy bound $-1/4$ or this never happens and we have the "nasty" bound $-1/2$ for some edge. In the latter case, by the previous paragraph we also must have the "good" property $\mathcal{N}_\alpha(p) \cap \partial\mathcal{G}_\alpha \neq \emptyset$, and some $q \in \mathcal{N}_\alpha(p)$ has $\mathcal{N}_\alpha(q)$ of lower than maximum cardinality.

To make the reasoning of the previous paragraph rigorous, we enrich the graph $\mathcal{G}_\alpha$ by adding (i) the edges from $\mathcal{S}_{\alpha'',\alpha}$ and (ii) a set of $9 - \sharp\mathcal{N}_{\alpha''}(p)$ new vertices denoted $\bar{q}_p$, and together with each of them we add what we call a "missing edge" of the form $\{p, \bar{q}_p\}$. Let $\overline{\mathcal{G}}$ be the new graph and $\overline{\mathcal{N}}(p)$ the neighborhood of $p \in \Xi$ in $\overline{\mathcal{G}}$. Then (3.48) can be re-expressed as

$$\mathcal{E}^p[V](X_N) \geq \mathcal{E}_4[V](\boxtimes) + \sum_{q \in \overline{\mathcal{N}}(p) \setminus \{p\}} \overline{w}(\{p, q\}), \tag{3.49a}$$

where in order to recover (3.48) we define

$$\overline{w}(\{p,q\}) := \begin{cases} 0 & \text{if } \{p,q\} \in \mathcal{S}_\alpha \setminus \mathcal{NC}, \\ -\frac{\mathcal{E}_4[V](\boxtimes)}{2} - \frac{1}{2} & \text{if } \{p,q\} \in \mathcal{NC} \cap \mathcal{S}_\alpha, \\ -\frac{\mathcal{E}_4[V](\boxtimes)}{2} - \frac{1}{4} & \text{if } \{p,q\} \in \mathcal{S}_{\alpha'',\alpha}, \\ -\frac{\mathcal{E}_4[V](\boxtimes)}{2} & \text{if } \{p,q\} \text{ missing edge.} \end{cases} \tag{3.49b}$$

We concentrate on edges from $\mathcal{NC}$ only, and note that these edges only satisfy the last three cases in (3.49b). In these three cases we use the bound

$$-\frac{\mathcal{E}_4[V](\boxtimes)}{2} - \frac{1}{2} \geq -\frac{m_{\alpha',V}}{2} - \frac{1}{2}, \tag{3.50}$$

following from (3.47) and assumption (3) that implies the fact that $m_{\alpha',V} < 0$. The bound ensuing from (3.49b) via (3.50) for edges in $\mathcal{NC} \cap \mathcal{S}_\alpha$ is the most negative. Differences in the weight $\overline{w}$ compared to this value will be called "lost weight" and denoted $\mathrm{lw}(\{p,q\})$. In other words, edges in $\mathcal{S}_{\alpha'',\alpha}$ have lost weight $\frac{1}{4}$ and missing edges have lost weight $\frac{1}{2}$. The other edges from $\mathcal{NC}$ will have by definition zero lost weight, and the edges not contained in $\mathcal{NC}$.

With this terminology, we bound the total lost weight, amongst points p such that $\mathcal{N}_\alpha(p) \cap \partial\mathcal{G}_\alpha \neq \emptyset$ or $\mathcal{N}_{\alpha''}(p) \setminus \mathcal{N}_\alpha(p) \neq \emptyset$ (which, due to the previous discusson, include all the vertices participating to $\mathcal{NC}$), as follows:

$$\sum_{\{p,q\} \in \mathcal{NC}} \mathrm{lw}(\{p,q\}) + \sum_{\{p,\bar{q}_p\} \text{ missing edge}} \mathrm{lw}(\{p,\bar{q}_p\}) \geq \frac{1}{16} \sharp\{p : \mathcal{N}_\alpha(p) \cap \partial\mathcal{G}_\alpha \neq \emptyset \text{ or } \mathcal{N}_{\alpha''}(p) \setminus \mathcal{N}_\alpha(p) \neq \emptyset\}. \tag{3.51}$$

Let w be the map assigning to every p the total lost weight summed over edges containing p. In particular, $w(p) = 0$ if and only if $p \notin \partial\mathcal{G}_\alpha$, whereas $w(p) \geq \frac{1}{2}$, whenever $p \in \partial\mathcal{G}_\alpha$ and $w(p) \geq \frac{1}{4}$ whenever $\mathcal{N}_{\alpha''}(p) \setminus \mathcal{N}_\alpha(p) \neq \emptyset$. Then, moving, for every $p \in \partial\mathcal{G}_\alpha$, a weight of $1/16$ from p along each edge from $\mathcal{G}_\alpha$ containing it, will also leave at least a weight $1/16$ at p itself, since there are at most 7 such edges. We leave the weight at points having "long" edges fixed instead. If we do this operation contemporarily for each p we end up with a total weight of at least $1/16$ at each one of the points appearing on the left in (3.51). This proves (3.51).

Now, summing (3.49a) over $p \in \Xi_N$ and using (3.49b) and (3.51) together with the previous observation that $\mathcal{NC} \cup \mathcal{S}_{\alpha'',\alpha}$ has at most 8 edges per vertex, we have

$$\begin{aligned} \mathcal{E}[V](X_N) &\geq N\mathcal{E}_4[V](\boxtimes) \\ &\quad + \sharp\{p : \mathcal{N}_\alpha(p) \cap \partial\mathcal{G}_\alpha \neq \emptyset \text{ or } \mathcal{N}_{\alpha''}(p) \setminus \mathcal{N}_\alpha(p) \neq \emptyset\} \left(-4m_{\alpha',V} - 4 + \frac{1}{16}\right) \\ &\geq N\mathcal{E}_4[V](\boxtimes) = N \min \mathcal{E}_4[V], \end{aligned} \tag{3.52}$$

where now we used assumption (3). This, together with (3.37), proves the first inequality in (3.36).

To show the second inequality in (1.1), let $\underline{t}$ be the value which realizes the minimum in the definition of $\overline{\mathcal{E}}_{\mathrm{sq}}[V]$. It suffices to construct a competitor to the minimization problem solved by X_N, in which $\sharp\partial\mathcal{G}_\alpha = O(N^{1/2})$, by considering configurations given by a subset of $\underline{t}\mathbb{Z}^2$

of cardinality N. To see that such subset exists, simply note that there exists $\widetilde{X}_N \subset \underline{t}\mathbb{Z}^2$ of cardinality N such that

$$\{\underline{t}x : \ x \in \mathbb{Z}^2, \ |x| \leq \sqrt{N} - \sqrt{2}\} \subset \widetilde{X}_N \subset \{\underline{t}x : \ x \in \mathbb{Z}^2, \ |x| \leq \sqrt{N} + \sqrt{2}\},$$

for which all labels p such that $\mathcal{N}_\alpha(p) \cap \partial\mathcal{G}_\alpha \neq \emptyset$ are assigned to points in a - at most - $5\sqrt{2}$-neighborhood of $\partial B(0, \sqrt{N})$ for N large enough (note that we are considering here a metric neighborhood in $\mathbb{R}^2$). Such $\widetilde{X}_N$ forms a subset of $\underline{t}\mathbb{Z}^2$ of cardinality $O(N^{1/2})$. This allows to prove the second inequality in (1.1) and to conclude the proof. □

Actually, we can obtain an easier proof of Theorem 3.16 if we assume that

$$W(1) = W(2) = -1 = \min_{r>0} W(r), \tag{3.53}$$

as shown by the following result.

Proposition 3.18. *Let $0 < \alpha < \min\{\overline{\alpha}, \frac{2-\sqrt{2}}{2}\}$, with $\overline{\alpha}$ given by Lemma 3.3. Set $r_{min} := 1-\alpha$, $C_2 := 1$, $r_0 := \sqrt{2}+\alpha$ and let K' be given by Lemma 3.1. If $W : (0,\infty) \to \mathbb{R}$ satisfies* (3.53) *and* (3.3)*, then* (3.36) *holds true with*

$$\overline{\mathcal{E}}_{\rm sq}[V] = \min \mathcal{E}_4[V] = \mathcal{E}_4[V](\boxtimes) = -4. \tag{3.54}$$

Proof. The proof of (3.54), as well as the one of the second inequality in (3.36), is a triviality following from the fact that $\sqrt{2} < \sqrt{2} + \alpha < 2$ and is left to the reader.
We just prove the first inequality in (3.36). Let $N \in \mathbb{N}$ and let $X_N \in \mathcal{X}_N(\mathbb{R}^2)$ be a minimizer of $\mathcal{E}[V]$ in $\mathcal{X}_N(\mathbb{R}^2)$, i.e.,

$$\mathcal{E}[V](N) = \mathcal{E}[V](X_N). \tag{3.55}$$

Then, by (3.3) and by Lemma 3.1, we have

$$\mathcal{E}[V](X_N) = \sum_{\{p,q\}\in\mathcal{S}_\alpha} V(|x_p - x_q|). \tag{3.56}$$

Since $\alpha < \overline{\alpha}$, by Lemma 3.3, we deduce that $\sharp\mathcal{N}_\alpha(p) \leq 9$, so that

$$\sharp\mathcal{S}_\alpha = \frac{1}{2}\sum_{a\in\Xi_N} (\sharp\mathcal{N}_\alpha(a) - 1) \leq 4N. \tag{3.57}$$

By (3.56), (3.57), and (3.54) we get

$$\mathcal{E}[V](N) = \mathcal{E}[V](X_N) \geq -\sharp\mathcal{S}_\alpha \geq -4N = N\mathcal{E}_4[V] = N\mathcal{E}_{\rm sq}[V].$$

□

4. Long-range potentials and proof of Theorem 1.3

This section is devoted to the proof of the crystallization result in the thermodynamic limit for long-range potentials.

4.1. **Distortion estimates at larger scales.** We first organize the information from $\mathcal{G}_\alpha$ in order to be able to compare it to $\mathcal{Z}_\boxtimes$.

Definition 4.1 (combinatorial embedding)**.** Let $\mathcal{G}'_\alpha \subset \mathcal{G}_\alpha$ be a subgraph, with vertex labels $\Lambda \subset \Xi$ and edges $\mathcal{S}'_\alpha \subset \mathcal{S}_\alpha$. A map $\Phi : \Lambda \to \mathbb{Z}^2$ gives a *combinatorial embedding* if it is a graph isomorphism between $\mathcal{G}'_\alpha$ and a subgraph of $\mathcal{Z}_\boxtimes$, i.e. it is injective and $\{p,q\} \in \mathcal{S}'_\alpha$ if and only if $\{\Phi(p),\Phi(q)\}$ is an edge of $\mathcal{Z}_\boxtimes$.

Note that in [48] "discrete embeddings" were defined differently, with a slightly more complicated definition involving directly X and not only graphs. However, the graph-only Definition 4.1 does still allow to recover all the information relevant to our problem, and in our view makes the structure of the argument clearer.

We also need the following classical combinatorial definitions.

Definition 4.2 (elementary topology in $\mathcal{G}_\alpha$)**.**

(1) A *path in* $\mathcal{G}_\alpha$ is an sequence of edges of the form

$$\mathcal{P} = (\{p_0,p_1\},\{p_1,p_2\},\{p_2,p_3\},\dots,\{p_{n-1},p_n\}) \in (\mathcal{S}_\alpha)^n, n \in \mathbb{N}. \tag{4.1}$$

(2) Let $\Lambda \subset \Xi$. A path $\mathcal{P}$ as above is a path *through* Λ if $p_0,p_1,\dots,p_n \in \Lambda$. Equivalently $\mathcal{P}$ is also a path in $\mathcal{G}_\alpha|_\Lambda$.

(3) We say that a subset of vertices $\Lambda \subset \Xi$ is *path-connected* if for each $p \neq q \in \Lambda$ there exists a path $\mathcal{P}$ through Λ such that $p_0 = p, p_n = q$.

(4) An *elementary move in* $\mathcal{G}_\alpha$ consists in replacing successive edges $\{\{p,q\},\{q,r\}\} \to \{p,r\}$ or viceversa $\{p,r\} \mapsto \{\{p,q\},\{q,r\}\}$, provided $\{p,q,r\}$ forms a triangle (i.e. all pairs of points give an edge) in $\mathcal{G}_\alpha$.

(5) A *discrete homotopy* between two paths $\mathcal{P},\mathcal{Q}$ in $\mathcal{G}_\alpha$ is a sequence of paths connected by elementary moves, which starts at $\mathcal{P}$ and ends at $\mathcal{Q}$.

(6) A subset of vertices $\Lambda \subset \Xi$ is *simply connected* if in $\mathcal{G}_\alpha|_\Lambda$ any two paths in Λ are connected by a discrete homotopy.

Regions of $\mathcal{G}_\alpha$ which are away from $\partial\mathcal{G}_\alpha$ have a unique combinatorial embedding in the following sense:

Proposition 4.3 (combinatorial version of Theorem 2.1 part (ii))**.** *Let $\Lambda \subset \Xi$ be a path-connected subset such that for each $p \in \Lambda$ there holds $\mathcal{N}_\alpha(p) \cap \partial\mathcal{G}_\alpha = \emptyset$. Then:*

(1) *There exists a combinatorial embedding Φ of $\mathcal{G}_\alpha|_\Lambda$ into $\mathcal{Z}_\boxtimes$.*

(2) *Such Φ is unique up to composition with a combinatorial embedding of $\mathcal{Z}_\boxtimes$ into itself.*

Proof. For every $p \in \Lambda$ we set $\phi_p := \phi$, where ϕ is the bijection constructed in Lemma 3.5. If $\Lambda = \{p\}$, it is enough to consider $\Phi := \phi_p$ which in view of Remark 3.7 is unique up to a composition with a combinatorial embedding of $\mathcal{Z}_\boxtimes$ with itself. Otherwise, we construct Φ in the following way: Let $p \in \Lambda$, and let $\Phi(q) = \phi_p(q)$ for every $q \in \mathcal{N}_\alpha(p) \cap \Lambda$. For every $q \in \mathcal{N}_\alpha(p) \cap \Lambda$ we set $\Phi(r) = \phi_q(r) + \phi_p(q)$ and we proceed so forth. Since Λ is path-connected such a procedure stops after a finite number ($\leq \sharp\Lambda$) of steps.
Using Remark 3.6 one can easily check that the function Φ is well-defined, i.e., $\phi_p(r) = \phi_q(r) + \phi_p(q)$ for every $r \in \mathcal{N}_\alpha(p) \cap \mathcal{N}_\alpha(q) \cap \Lambda$. Moreover, Φ is a combinatorial embedding from $\mathcal{G}_\alpha$ into $\mathcal{Z}_\boxtimes$. The uniqueness in (2) is again a consequence of the fact that Λ is path-connected. □

The above proposition shows that under path-connectedness and neighborhood closure of Λ we actually have an identification of the whole Λ with a patch in $\mathcal{Z}_{\boxtimes}$. Thus we introduce the following concept:

Definition 4.4 (discrete $\mathcal{Z}_{\boxtimes}$-charts)**.** If $\Lambda \subset \Xi$ is such that

- $\mathcal{N}_\alpha(p) \cap \partial\mathcal{G}_\alpha = \emptyset$ for every $p \in \Lambda$,
- there exists a combinatorial embedding $\Phi : \Lambda \to \mathbb{Z}^2$ of $\mathcal{G}_\alpha|_\Lambda$ whose image is simply connected in $\mathcal{Z}_{\boxtimes}$, in the sense of Definition 4.2,

then we call (Φ, Λ) a *discrete $\mathcal{Z}_{\boxtimes}$-chart* of $\mathcal{G}_\alpha$ (or simply a *discrete chart*).
Moreover, we define a triangle in $\mathcal{Z}_{\boxtimes}$ as a triple of distinct vertices $\{z^1, z^2, z^3\}$ of $\mathcal{Z}_{\boxtimes}$ such that $\{z^i, z^j\}$ are bonds in $\mathcal{Z}_{\boxtimes}$ for every $i, j = 1, 2, 3$ with $i \neq j$. Let $\mathscr{T}'$ be the (non-planar) triangulation of $\Phi(\Lambda)$ induced by $\mathcal{Z}_{\boxtimes}$, i.e. $\mathscr{T}'$ is the set of all the triangles with vertices in $\Phi(\Lambda)$ that are half-unit-squares. A planar triangulation $\mathscr{T} = \mathscr{T}_{(\Phi,\Lambda)}$ associated to (Φ, Λ) is obtained by removing one arbitrarily chosen diagonal from each (unit) square of $\Phi(\Lambda) \cap \mathcal{Z}_{\boxtimes}$. Furthermore, we set $\mathscr{T}^{-1} := X^{-1}(\mathscr{T})$.

Now we introduce some notation that will be useful in the results of this section.

For every $d \in \mathbb{N}$ and for every $a, b \in \mathbb{R}^d$, we define the ellipsoid with foci a and b and ellipticity $\alpha > 0$ as

$$\mathrm{Ell}_\alpha(a, b) := \left\{ x \in \mathbb{R}^d : \ |x - a| + |y - b| \leq \frac{1+\alpha}{1-\alpha}|a - b| \right\}. \tag{4.2}$$

We denote by $\mathcal{D}$ the set of all (non-trivial) vectors in $\mathbb{Z}^2$, i.e.,

$$\mathcal{D} := \{|p| \ : \ p \in \mathbb{Z}^2 \setminus \{0\}\}. \tag{4.3}$$

For every $r \in \mathcal{D}$ we denote by Q'_r each square of sidelength r having vertices in $\mathbb{Z}^2$ and we denote by $\mathcal{Q}'_r$ the family of such squares Q'_r. Furthermore, we set

$$\begin{aligned}
&\mathrm{Sides}(Q'_r) := \{\{p, q\} \ : \ p, q \in Q'_r,\ |p - q| = r\} \quad \text{for every } Q'_r \in \mathcal{Q}'_r,\\
&\mathrm{Sides}(\mathcal{Q}'_r) := \bigcup_{Q'_r \in \mathcal{Q}'_r} \mathrm{Sides}(Q'_r),\\
&\mathrm{Diag}(Q'_r) := \{\{p, q\} \ : \ p, q \in Q'_r,\ |p - q| = \sqrt{2}r\} \quad \text{for every } Q'_r \in \mathcal{Q}'_r,\\
&\mathrm{Diag}(\mathcal{Q}'_r) := \bigcup_{Q'_r \in \mathcal{Q}'_r} \mathrm{Diag}(Q'_r).
\end{aligned} \tag{4.4}$$

Definition 4.5 (squares of scale r)**.** For $r \in \mathcal{D}$ we say that $Q_r \subset \Xi$ is a *square of scale r* if there exists a discrete $\mathcal{Z}_{\boxtimes}$-chart (Φ, Λ) such that

- $\Phi(Q_r) =: Q'_r \in \mathcal{Q}'_r$;
- $\mathbb{Z}^2 \cap \mathrm{Conv}(Q'_r) \subset \Phi(\Lambda)$;
- $\mathrm{Ell}_\alpha(X(p), X(q)) \subset \mathrm{Conv}(X(\Lambda))$ for every $p, q \in Q_r$ with $p \neq q$.

We denote by $\mathcal{Q}_r$ the families of the squares Q_r of sidelength r in $\mathcal{G}_\alpha$ and by $\mathcal{Q}$ the union of the families $\mathcal{Q}_r$, for r varying in $\mathcal{D}$. In analogy with (4.4) we also set

$$\begin{aligned}
\mathrm{Sides}(Q_r) &:= \{\{\Phi^{-1}(a),\Phi^{-1}(b)\} \,:\, \{a,b\}\in \mathrm{Sides}(\Phi(Q_r))\}\\
&= \{\{p,q\} \,:\, \{\Phi(p),\Phi(q)\}\in \mathrm{Sides}(\Phi(Q_r))\} \quad \text{for every } Q_r\in\mathcal{Q}_r,\\
\mathrm{Sides}(\mathcal{Q}_r) &:= \bigcup_{Q_r\in\mathcal{Q}_r} \mathrm{Sides}(Q_r),\\
\mathrm{Diag}(Q_r) &:= \{\{\Phi^{-1}(a),\Phi^{-1}(b)\} \,:\, \{a,b\}\in \mathrm{Diag}(\Phi(Q_r))\}\\
&= \{\{p,q\} \,:\, \{\Phi(p),\Phi(q)\}\in \mathrm{Diag}(\Phi(Q_r))\} \quad \text{for every } Q_r\in\mathcal{Q}_r\\
\mathrm{Diag}(\mathcal{Q}_r) &:= \bigcup_{Q_r\in\mathcal{Q}_r} \mathrm{Diag}(Q_r).
\end{aligned} \tag{4.5}$$

In the following, the *r-neighborhood* of a square at scale r is the set of all points in $\mathcal{G}_\alpha$ which can be connected to a point in Q_r through a combinatorial path of length $\leq r$.

Our next goal is to prove that X-images of squares $Q_r\in\mathcal{Q}_r$ are actually $L\alpha$-deformations of metric squares $Q_r\subset(\mathbb{Z}^2,\ell_2)$, with L independent of α. The case $r=1$ already follows from Lemma 3.5. Next, we consider the usual isometric embedding $\mathbb{Z}^2\subset\mathbb{R}^2$, seen here as a *labeling of a configuration*, with label set $\mathbb{Z}^2$:

$$\iota_{\mathbb{Z}^2}:\mathbb{Z}^2\to\mathbb{R}^2, \qquad a\mapsto \iota(a)=a_*. \tag{4.6}$$

Proposition 4.6 (discrete charts become metric charts)**.** *There exists a constant $L\geq 1$ with the following properties. Let $\alpha\in[0,\alpha_0)$, with α_0 given by Lemma 3.5. Let (Φ,Λ) be a discrete $\mathcal{Z}_\boxtimes$-chart of $\mathcal{G}_\alpha$ and let $\mathscr{T}$ be a planar triangulation associated to (Φ,Λ). Assume that*

$$\overline{\Phi(\Lambda)} := \bigcup \left\{ \overline{\mathrm{Conv}(\{a^1_*,a^2_*,a^3_*\})} :\ \{a^1,a^2,a^3\} \text{ triangle in } \mathscr{T} \right\}.$$

Then, there exists a Lipschitz continuous map $u:\overline{\Phi(\Lambda)}\to\mathbb{R}^2$ which satisfies the following conditions:

1. *$u(\Phi(p))=X(p)$ for all $p\in\Lambda$;*
2. *u is piecewise affine on $\mathrm{Conv}(\{a^1_*,a^2_*,a^3_*\})$ for every triangle $\{a^1,a^2,a^3\}\in\mathscr{T}$;*
3. *u satisfies*

$$\sup_{x\in\overline{\Phi(\Lambda)}} \mathrm{dist}(Du(x),SO(2)) < L\alpha. \tag{4.7}$$

Note that in [48] the map u was going in the opposite direction than our map, but since u is bijective and Du is invertible, this actually makes not much difference.

Proof. For every $p\in\Lambda$ we set $u(\Phi(p)):=X(p)$ and we extend u affinely over each triangle in $\mathscr{T}$. Let $T^{-1}:=\{p^1,p^2,p^3\}\in\mathscr{T}^{-1}$ and set $a^i:=\Phi(p^i)$ for $i=1,2,3$; set moreover $T:=\{a^1_*,a^2_*,a^3_*\}$. By construction, $T\in\mathscr{T}$. By definition of $\mathcal{G}_\alpha$, the image $\{X(p^1),X(p^2),X(p^3)\}$ of $\{p^1,p^2,p^3\}$ through X equals, up to a rotation, to a small deformation of $\{z^1,z^2,z^3\}$ with $z^1=(0,0), z^2=(0,1), z^3=(1,0)$, in the sense that up to reassigning the labels p^1,p^2,p^3, we have

$$\frac{|X(p^1)-X(p^2)|}{|z^1-z^2|},\ \frac{|X(p^1)-X(p^3)|}{|z^1-z^3|},\ \frac{|X(p^2)-X(p^3)|}{|z^2-z^3|}\in E^1_\alpha.$$

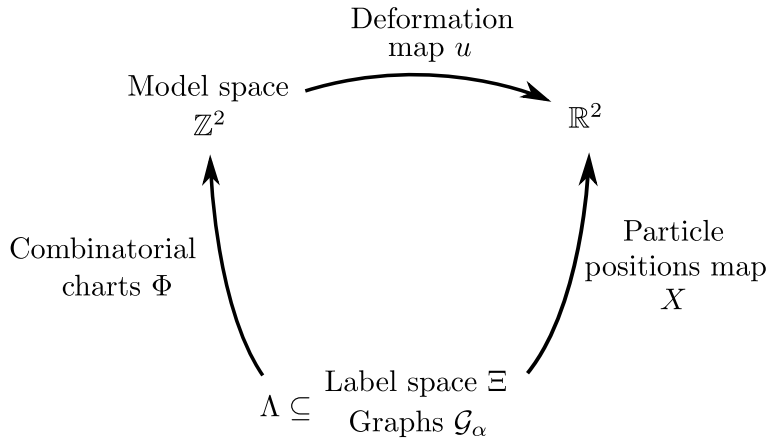


FIGURE 4. Summary of the different maps and spaces used in this section.

Then due to Proposition 4.3 and to Definition 4.4 of discrete $\mathcal{Z}_{\boxtimes}$-chart, Φ sends T^{-1} to a congruent copy of $\{z^1, z^2, z^3\}$. Therefore, we can define u over $\mathrm{Conv}(T)$ as the affine map with gradient $Du(x) =: F^T$, where

$$F^T(X(p^2) - X(p^1)) = (0,1), \quad \text{and} \quad F^T(X(p^3) - X(p^1)) = (1,0).$$

By using the cosine rule (with details left to the reader), it follows that for every $T \in \mathscr{T}$ there exist two vectors $v_1^T, v_2^T \in B_1$ such that

$$F^T \in \left(e_1 + \alpha v_1^T, e_2 + \alpha v_2^T\right) O(2),$$

thus for a value of L independent of α (and of T) it holds

$$\mathrm{dist}(F^T, O(2)) \le L\alpha \qquad \text{for all } T \in \mathscr{T}. \tag{4.8}$$

By the first bullet in the Definition 4.4, we can apply Lemma 3.5 to all $p \in \Lambda$, and we find that maps F corresponding to neighboring triangles either all preserve orientation or all reverse orientation. By the connectedness of $\Phi(\Lambda)$, which follows from the second point in Definition 4.4, we find inductively that this is also true for the collection of maps F corresponding to all triangles in $\mathscr{T}$. Thus $Du(x)$ stays $L\alpha$-close either to $SO(2)$ or to $\{M \in O(n) : \det(M) = -1\}$. In the latter case, we may compose the discrete chart Φ with the self-embedding of $\mathcal{Z}_{\boxtimes}$ given by the map $\Phi_-(a,b) := (-a,b)$, which has the effect of making all F orientation-preserving. Thus we have from (4.8) that

$$L\alpha \ge \mathrm{dist}(F^T, O(2)) = \mathrm{dist}(F^T, SO(2)) \qquad \text{for all } T \in \mathscr{T};$$

whence (4.7) follows. This completes the proof. □

We will use different distortion bounds for treating linear and quadratic deformations. The first one is [34, Lemma III] which was slightly extended by [48, Proposition 4.1], and gives the following result.

Lemma 4.7 (John distortion [34])**.** *For every $d \in \mathbb{N}$ there exists $\alpha_1 = \alpha_1(d) > 0$ such that for each $\alpha \in [0, \alpha_1)$ the following holds. Given $a, b \in \mathbb{R}^d$, if $u : \mathrm{Ell}_\alpha(a,b) \to \mathbb{R}^d$ is Lipschitz continuous and satisfies*

$$\sup_{x \in \mathrm{Ell}_\alpha(a,b)} \mathrm{dist}(Du(x), SO(d)) < \alpha, \tag{4.9}$$

then, with notation of Definition 3.4, we have

$$\delta_u(a,b) \leq \alpha. \tag{4.10}$$

The next result allows to obtain good enough bounds for quadratic distortions. Although it holds in general dimension, we prove it only in the special 2-dimensional case, because this is the version that we require in the remainder of the paper.

Proposition 4.8 (Quadratic distortion estimate)**.** *There exists a constant $C_6 > 0$ depending only on the dimension such that if $\alpha \in (0, \alpha_1)$, with α_1 as in Lemma 4.7, the following holds true. Let (Φ, Λ) is a discrete $\mathcal{Z}_{\boxtimes}$-chart of $\mathcal{G}_\alpha$ and let $u : \overline{\Phi(\Lambda)} \to \mathbb{R}^2$ be the map constructed in Propostion 4.6; then for every $r \in \mathcal{D}$ and for every $\{a,b\} \in \mathrm{Sides}(\mathcal{Q}_r) \cup \mathrm{Sides}(\mathcal{Q}_{\sqrt{2}r})$ it holds*

$$\delta^2_{u\circ\Phi}(a,b) := \delta^2_u(\Phi(a),\Phi(b)) \leq C_6\ r \sum_{\substack{\{p,q\}\in\mathcal{S}_\alpha \\ \mathrm{dist}(X(\{p,q\}),[X(a),X(b)])<4}} \delta^2_{u\circ\Phi}(p,q). \tag{4.11}$$

Proof. Throughout the proof all our constants are either explicit or they depend only on L, α_1 above, which in turn depend only on the dimension.

Let $\mathscr{T}$ be a triangulation associated to (Φ, Λ) according to the Definition 4.4.

By Definition 4.4, and more precisely by Definition 4.1, we have that $\{p,q\} \in \mathcal{S}_\alpha$ for every $p, q \in \Lambda$ with $|\Phi(p) - \Phi(q)| \in \{1, \sqrt{2}\}$. Moreover, again by Definition 4.4, the union of the triangles $T \in \mathscr{T}$ contains a neighborhood of the segment $[X(a), X(b)] = [u(\Phi(a)), u(\Phi(b))]$. Thus, all triangles $\tau = \{p_1, p_2, p_3\} \in \mathscr{T}^{-1}$ with $\mathrm{Conv}(X(\tau)) \cap [X(a), X(b)] \neq \emptyset$ satisfy $\mathrm{dist}(X(p_i), [X(a), X(b)]) < 2$ because $2 > \sqrt{2} + \alpha$ for α sufficiently small. Next note that, since u is affine, the maximum

$$\max_{x,y\in\mathrm{Conv}(X(\tau))} \delta_u(x,y)$$

is achieved at the vertices of the simplex $\mathrm{Conv}(X(\tau))$, i.e. for $x = X(p_i), y = X(p_j)$, for some $i, j \in \{1,2,3\}$ with $i \neq j$, i.e.,

$$\max_{x,y\in\mathrm{Conv}(X(\tau))} \delta_u(x,y) \leq \max_i \delta_{u\circ\Phi}(p_i, p_{i+1}) \leq \sum_{i=1}^3 \delta_{u\circ\Phi}(p_i, p_{i+1}), \tag{4.12}$$

in which the indices i are intended modulo 3. Let now $\mathscr{T}^{-1}_{a,b}$ denote the set of the triangles $\tau \in \mathscr{T}^{-1}$ with $\mathrm{Conv}(X(\tau)) \cap [X(a), X(b)] \neq \emptyset$ and let $[\xi^\tau, \eta^\tau] = \mathrm{Conv}(X(\tau)) \cap [X(a), X(b)]$ where ξ^τ and η^τ are not necessarily distinct. Then $\mathscr{T}^{-1}_{a,b} = \{\tau^m\}_{m\in M}$ for some $M \subset \mathbb{N}$, where the indices m are chosen in such a way that the subsegments $\sigma^m := [\xi^{\tau^m}, \eta^{\tau^m}]$ are concatenated.

By (4.12) and by triangular inequality, it follows that

$$\begin{aligned} |X(a) - X(b)| &= \sum_{m=1}^M |u(\sigma^m)| \geq \sum_{m=1}^M (|\sigma^m| - \delta_u(\sigma^m)) \geq |\Phi(a) - \Phi(b)| - \sum_{m=1}^M \delta_u(\sigma^m) \\ &\geq |\Phi(a) - \Phi(b)| - 2 \sum_{\substack{\{p,q\}\in\mathcal{S}_\alpha \\ \mathrm{dist}(X(\{p,q\}),[X(a),X(b)])<4}} \delta_{u\circ\Phi}(p,q), \end{aligned} \tag{4.13}$$

where in the last inequality we have used that each edge used can appear at most 2 times, i.e., at most one for each triangle of which it is an edge. Proceeding symmetrically and considering

segments $\widetilde{\sigma}^k$, $k = 1, \dots, K$, which are intersections of $[\Phi(a), \Phi(b)]$ with successive triangles of $\mathscr{T}$, and arguing as in (4.13) we get

$$\begin{aligned} |\Phi(a) - \Phi(b)| &= \sum_{k=1}^{K} |\widetilde{\sigma}^k| \geq \sum_{k=1}^{K} \Big(|u(\widetilde{\sigma}^k)| - \delta_u(\widetilde{\sigma}^k) \Big) \geq |X(a) - X(b)| - \sum_{k=1}^{K} \delta_u(\widetilde{\sigma}^k) \\ &\geq |X(a) - X(b)| - 3 \sum_{\substack{\{p,q\} \in \mathcal{S}_\alpha \\ \operatorname{dist}(X(\{p,q\}), [X(a), X(b)]) < 4}} \delta_{u \circ \Phi}(p, q). \end{aligned} \tag{4.14}$$

Combining (4.13) and (4.14) we find

$$\begin{aligned} \delta_{u \circ \Phi}(a, b) &= \big| |X(a) - X(b)| - |\Phi(a) - \Phi(b)| \big| \\ &\leq 3 \sum_{\substack{\{p,q\} \in \mathcal{S}_\alpha \\ \operatorname{dist}(X(\{p,q\}), [X(a), X(b)]) < 4}} \delta_{u \circ \Phi}(p, q). \end{aligned} \tag{4.15}$$

Using that $\min_{\{p,q\} \in \mathcal{S}_\alpha} |X(p) - X(q)| > 1 - \alpha > 1 - \alpha_1$ and a packing bound, we find that the number of terms of the sum in (4.15) is at most Cr, with C a constant depending only on L, α_1, and thus only on the dimension. Thus, we may apply the Cauchy-Schwarz inequality to (4.15) in order to obtain (4.11).

□

Remark 4.9. The content of Proposition 4.8 is similar in spirit to [48, Proposition 4.3] but it presents some differences. On the one hand, the result in [48] yields the scaling $\log(r)$ which is better than the scaling r we achieve. On the other hand, the proof of the upper bound in [48] relies on the rigidity estimate by Friesecke-James-Müller [26]. Here we preferred to include the "worse" upper bound in (4.11) - which however does not affect our final result - and to provide the more transparent proof above.

The last result of this subsection deals with the partitioning of the edge set of the complete graph generated by $\mathbb{Z}^2$ into edges coming from sides and diagonals of squares of sidelength r. We first need the following definition.

Definition 4.10 (Rescaled copies of $\mathcal{Z}_{\boxtimes}$)**.** Let $\mathcal{D}$ be defined as in (4.3). For every $r \in \mathcal{D}$ we define

$$\mathcal{L}_r := \{\text{sublattice } \Lambda \subset \mathbb{Z}^2 \text{ such that } \Lambda \simeq r\mathbb{Z}^2\}, \quad \mathcal{L} = \bigcup_{r \in \mathcal{D}} \mathcal{L}_r, \tag{4.16a}$$

$$m(r) := \sharp \mathcal{L}_r = \frac{1}{4} \sharp \left\{ x \in \mathbb{Z}^2 : \ |x| = r \right\}. \tag{4.16b}$$

Let $\mathcal{K}_{\mathbb{Z}^2}$ be the complete graph associated to $\mathbb{Z}^2$, i.e.

$$\mathcal{K}_{\mathbb{Z}^2} := (\mathbb{Z}^2, \{\{a, b\} : \ a \neq b \in \mathbb{Z}^2\}).$$

We note the following well-known number-theoretical result:

Lemma 4.11. *With the above definitions, for all $r \in \mathcal{D}$ we have $m(r) = m(\sqrt{2}r)$.*

Proof. This amounts to prove that for each integer $n > 1$ the number of ways to write n as a sum of two squares equals the number of ways to write $2n$ as the sum of two squares.

By a theorem of Euler, n is the sum of two squares if and only if all its prime factors equal to 3 modulo 4 occur to an even power. If this condition is met, then the ways of writing n as two squares are given (see [30], Thm. 278) by

$$4\prod_{j=1}^{s}(b_j+1), \quad \text{if} \quad n = 2^{a_0}\prod_{i=1}^{r} p_i^{2a_i}\prod_{j=1}^{s} q_j^{b_j},$$

where a_i, b_j are integers, q_j are distinct primes all equal to 1 modulo 4 and p_i are distinct primes equal to 3 modulo 4. In particular, the number of ways to write n as a sum of two squares does not depend on a_0, as desired. □

Now we can give the splitting result announced earlier, which will be useful for organizing the values of V taken on our configurations.

Lemma 4.12 (Covering of $\mathcal{K}_{\mathbb{Z}^2}$ by lattices and squares)**.** *There exists $\widetilde{\mathcal{D}} \subset \mathcal{D}$ such that*

$$\{\{0,a\} \,:\, a\in\mathbb{Z}^2\setminus\{0\}\} = \bigsqcup_{r\in\widetilde{\mathcal{D}}}\bigsqcup_{\Lambda\in\mathcal{L}_r}\Big\{\{0,x\} : x\in\Lambda,\ |x|\in\{r,\sqrt{2}r\}\Big\}, \tag{4.17}$$

where the symbol $\bigsqcup$ denotes the pairwise disjoint union. Moreover, we necessarily have $1\in\widetilde{\mathcal{D}}$ and

$$r\in\widetilde{\mathcal{D}}\setminus\{1\} \quad\Rightarrow\quad r\geq 2, \tag{4.18}$$

whereas for edge multiplicities we have

$$\sum_{\{a,b\}:\ a\neq b\in\mathbb{Z}^2}\delta_{\{a,b\}} = \frac{1}{2}\sum_{r\in\widetilde{\mathcal{D}}}\sum_{Q\in\mathcal{Q}'_r\cup\mathcal{Q}'_{\sqrt{2}r}}\ \sum_{\{a,b\}\in\mathrm{Sides}(Q)}\delta_{\{a,b\}}. \tag{4.19}$$

Proof. We already know that each $\Lambda\in\mathcal{L}$ is isomorphic to $\mathbb{Z}^2$. Let

$$Q_{++} := \{(a,b)\in\mathbb{Z}^2 :\ a>0, b\geq 0\}.$$

Let $B:\mathcal{L}\to Q_{++}$, $\Lambda\mapsto B(\Lambda):=v_\Lambda$, where $|v_\Lambda| = \min\{|v| \,:\, v\in\Lambda\cap Q_{++}\}$. By the very definition of Q_{++}, B is well-defined and bijective, so that we can write $\Lambda[v] := B^{-1}(v)$ for $v\in Q_{++}$.

Define then a map $F: Q_{++}\to Q_{++}$ by taking $F(v)=v'$ to be the shortest vector in $\Lambda[v]\cap(Q_{++}\setminus\{0,v\})$. Note that v' is one of the 4 vectors in $\Lambda[v]$ that have length $\sqrt{2}|v|$, and furthermore it forms an angle of 45° with v. We notice that

$$v' = F(v) \quad\Leftrightarrow\quad \Lambda[v'] = \begin{pmatrix} 1 & 1\\ -1 & 1\end{pmatrix}\Lambda[v],$$

which shows also that F is injective, as B is bijective and the above relation is one-to-one.

Now note that Q_{++} can be partitioned into maximal orbits of F, i.e., there exists a set $\mathcal{V}\subset\mathbb{Z}^2$ made of distinct vectors such that

$$Q_{++} := \bigcup_{v\in\mathcal{V}}\bigcup_{n\in\mathbb{N}} F^n(v),$$

where the vectors $v\in\mathcal{V}$ are such that $F(q)\neq v$ for every $q\in Q_{++}$. Indeed, any point in Q_{++} belongs to an orbit $\{F^n(v) : n\in\mathbb{N}\}$ for some $v\in\mathcal{V}$ and if two orbits meet at v then they coincide on all the "positive direction" $\{F^n(v) :\ n\in\mathbb{N}\}$, because F is well defined, and in the "negative direction", because F is injective.

Next, we can then split each maximal orbit

$$\{v, F(v), F^2(v), \ldots\} = \bigsqcup_{n\geq 0} \{F^{2n}(v), F^{2n+1}(v)\},$$

where we have set $F^0(v) := v$. Therefore, there exists $\tilde{V} \subset Q_{++}$ such that

$$Q_{++} = \bigsqcup_{v\in\widetilde{V}} \{v, F(v)\}, \quad \mathbb{Z}^2 \setminus \{0\} = \bigsqcup_{v\in\widetilde{V}} \left\{x \in \Lambda[v] :\ |x| \in \{|v|, \sqrt{2}|v|\}\right\}, \tag{4.20}$$

where the second equality follows by covering $\mathbb{Z}^2 \setminus \{0\}$ by four rotations of Q_{++} by $\pi/2$ and observing that (the restriction of) this operation on each $\Lambda[v]$ translates. We now define

$$\widetilde{\mathcal{D}} := \{|v| :\ v \in \widetilde{V}\}, \quad \text{so that } \sqrt{2}\widetilde{\mathcal{D}} = \{|F(v)| :\ v \in \widetilde{V}\}, \tag{4.21}$$

where $\sqrt{2}\widetilde{\mathcal{D}} := \{\sqrt{2}r :\ r \in \widetilde{\mathcal{D}}\}$. Directly from (4.21) we have

$$\bigsqcup_{r\in\widetilde{\mathcal{D}}} \mathcal{L}_r \supseteq \bigcup_{v\in\widetilde{V}} \Lambda[v] \quad \text{and} \quad \bigsqcup_{r\in\sqrt{2}\widetilde{\mathcal{D}}} \mathcal{L}_r \supseteq \bigcup_{v\in\widetilde{V}} \Lambda[F(v)]. \tag{4.22}$$

Due to the bijectivity of the map $Q_{++} \ni v \mapsto \Lambda[v] \in \mathcal{L}$ and to (4.20), we have

$$\mathcal{L} = \{\Lambda[v] :\ v \in \widetilde{V}\} \sqcup \{\Lambda[F(v)] :\ v \in \widetilde{V}\}. \tag{4.23}$$

Now consider the map $\Lambda[v] \mapsto \Lambda[F(v)]$, which as we saw is well defined over $\mathcal{L}$ and injective. By Lemma 4.11 we know $m(r) = m(\sqrt{2}r)$, and in particular for each $r \in \widetilde{\mathcal{D}}$ the above map restricts to a bijection $\mathcal{L}_r \to \mathcal{L}_{\sqrt{2}r}$, thus giving

$$\mathcal{D} = \widetilde{\mathcal{D}} \bigsqcup (\sqrt{2}\widetilde{\mathcal{D}}), \tag{4.24}$$

which in combination with (4.23) implies that the inclusions (4.22) are equalities. Therefore we can rewrite the second formula from (4.20) by taking the union over $\mathcal{L}_r, r \in \widetilde{\mathcal{D}}$ instead of $\widetilde{V}$, and we get (4.17).

Now note that $r = 1$ necessarily belongs to $\widetilde{\mathcal{D}}$, because $\Lambda = \mathbb{Z}^2$ is the only element of $\mathcal{L}$ that contains the edge $\{(0,0),(0,1)\}$. Then all edges of $\mathbb{Z}^2$ of length $\sqrt{2}$ from $\mathbb{Z}^2$ are covered by the choice $\Lambda = \mathbb{Z}^2$ in (4.17), and thus because the union in (4.17) must be disjoint, the next $r \in \widetilde{\mathcal{D}}$ must be $r \geq 2$, as claimed in (4.18).

For (4.19), note that each edge $\{a, b\}$ from the left hand side of (4.19) has length r for some $r \in \mathcal{D}$. Due to (4.24) two mutually excluding cases can happen:

- $r \in \widetilde{\mathcal{D}}$, in which case $\{a, b\}$ is the side of precisely two squares congruent to $\{0, r\}^2$, and is counted exactly twice in the sum from the right hand side of (4.19).
- $r \in \sqrt{2}\widetilde{\mathcal{D}}$, in which case $\{a, b\}$ is the side of precisely two squares congruent to $\{0, \sqrt{2}r'\}^2$ and $r' = r/\sqrt{2} \in \widetilde{\mathcal{D}}$. Thus again $\{a, b\}$ is counted exactly twice in the sum from the right hand side of (4.19).

In both cases multiplicities on the two sides of (4.19) coincide, and the equation is proved. □

We finally notice that, due to Proposition 4.3, we are able to pass the combinatorial structure (4.16) from $\mathbb{Z}^2$ to $\mathcal{G}_\alpha$ in a robust way in the presence of sufficiently extended charts as in Definition 4.4. Lemma 4.7 allows to add to this a metric structure. In particular, as a direct corollary of Lemma 4.7 and Proposition 4.6 we then obtain the following result.

Lemma 4.13. *With the constants $\alpha_1, L > 0$ as in Lemma 4.7 and Proposition 4.6 for all $\alpha \in [0, \alpha_1)$ and whenever Q_r is a square of scale r in $\mathcal{G}_\alpha$ and $r \in \mathcal{D}$, it holds*

$$X(Q_r) \sim_{L\alpha} \{0, r\}^2 \subset \mathbb{R}^2. \tag{4.25}$$

4.2. **Boundary error bounds.** We are going to write the energy of our configuration as the sum of contributions coming from sides (i.e. edges different than diagonals) of squares Q_r with $r \in \mathcal{D}$ and the remainder:

$$\begin{aligned}\mathcal{E}[V](X_N) =& \frac{1}{2}\sum_{r\in\mathcal{D}}\sum_{Q_r\in\mathcal{Q}_r}\sum_{\{a,b\}\in \mathrm{Sides}(Q_r)} V(|x_a - x_b|) \\ &+ \sum_{\{a,b\}\in\mathcal{N}\mathcal{Q}^{(2)}} V(|x_a - x_b|) + \frac{1}{2}\sum_{\{a,b\}\in\mathcal{N}\mathcal{Q}^{(1)}} V(|x_a - x_b|),\end{aligned} \tag{4.26}$$

where $\mathcal{N}\mathcal{Q}^{(j)}$ are the edges that are sides of $2-j$ squares, for $j = 1, 2$.

The first result of this subsection is Proposition 4.14 which allows to compare, for every $r \in \mathcal{D}$, the cardinality and the area of the squares at scales r and 1. We preliminarily introduce some notations.

If $P \subset \mathbb{R}^2$ is a polygon, i.e. a finite set of points $P = \{p_j : j \in \mathbb{Z}/n\mathbb{Z}\}$ ordered in cyclical order such that the associated polygonal line $\gamma(P) := \cup_j [p_j, p_{j+1}]$ does not self-intersect), then we denote as usual by

$$\mathrm{Area}(P) := \left|\left\{x : \ x \text{ belongs to the bounded connected component of } \mathbb{R}^2 \setminus \gamma(P)\right\}\right|.$$

If $Q \subset \mathbb{R}^2$ is a small deformation of a square then in order to define $\mathrm{Area}(Q)$, unless otherwise specified, we always consider it with the cyclic order along the perimeter of the square.
For every $r \in \mathcal{D}$ and for every $Q_1 \in \mathcal{Q}_1$ we set

$$\mathcal{Q}_r^b(Q_1) := \left\{ Q_r \in \mathcal{Q}_r : \bigcup_{\{p,q\}\subset Q_r} \{z \in \mathrm{Conv}(X(Q_1)) : \ \mathrm{dist}(z, [X(p), X(q)]) < 4\} \neq \emptyset, \ \ Q_r \supset Q_1 \right\}. \tag{4.27}$$

Finally, the symbol Δ denotes the symmetric difference between sets $A\Delta B := (A\setminus B)\cup(B\setminus A)$.

Proposition 4.14. *There exists $C_7 > 0$ such that, for all $\alpha \in (0, \min\{\alpha_0, \alpha_1\})$, where α_0 is as in Lemma 3.5 and α_1 is as in Lemma 4.7, the following holds. If X satisfies* (3.13)*, then for all $r \in \mathcal{D}$ we have:*

$$0 \ \leq \ m(r)\sharp\mathcal{Q}_1 - \sharp\mathcal{Q}_r \leq C_7 r^2 m(r)\sharp\partial\mathcal{G}_\alpha; \tag{4.28a}$$

$$0 \ \leq \ r^2 m(r)\sum_{Q_1\in\mathcal{Q}_1}\mathrm{Area}(X(Q_1)) - \sum_{Q_r\in\mathcal{Q}_r}\mathrm{Area}(X(Q_r)) \leq C_7 r^4 m(r)\sharp\partial\mathcal{G}_\alpha; \tag{4.28b}$$

$$\sharp\{\{p,q\} \in \mathrm{Sides}(\mathcal{Q}_1) : \ [X(p), X(q)]\cap[X(a), X(b)] \neq \emptyset\} \leq C_7 r \quad \forall \{a,b\} \in \mathrm{Sides}(\mathcal{Q}_r); \tag{4.28c}$$

$$\sharp\mathcal{Q}_r^b(Q_1) \leq C_7 r\ m(r) \qquad \textit{for all } Q_1 \in \mathcal{Q}_1; \tag{4.28d}$$

$$\sharp(\mathrm{Sides}(\mathcal{Q}_{\sqrt{2}r})\Delta\mathrm{Diag}(\mathcal{Q}_r)) \leq C_7 r^2 \sharp\partial\mathcal{G}_\alpha \qquad \textit{for all } r \in \widetilde{\mathcal{D}}. \tag{4.28e}$$

Proof. Note that below by abuse of notation we denote by C a constant that can possibly change at each step. For (4.28a) we proceed as in [48, Proposition 2.9], and start with a double count of

$$\{(x, Q_r) \,:\, Q_r \in \mathcal{Q}_r,\ x \in X(Q_r)\}.$$

On the one hand, setting $s(x,r) := \sharp\{Q_r \in \mathcal{Q}_r :\ x \in X(Q_r)\}$ for every $r \in \mathcal{D}$ and for every $x \in X(\Xi) =: X$, we get that

$$\sum_{x\in X} s(x,r) = 4\sharp\mathcal{Q}_r. \tag{4.29}$$

On the other hand, we will check that

$$s(x,r) \le m(r)s(x,1) \qquad \text{for every } x \in X,\ r \in \mathcal{D}, \tag{4.30}$$

which together with (4.29), and summing over $x \in X$, implies the first inequality in (4.28a). To prove (4.30), we preliminarily note that if $s(x,r) \neq 0$ then for $p := X^{-1}(x)$ there holds $\mathcal{N}_\alpha(p) \cap \partial\mathcal{G}_\alpha = \emptyset$, by definition of $\mathcal{Q}_r$, thus $s(x,1) = 4$. Moreover, if $r > 1$ only two facts can happen: either $s(x,r) = 4m(r) = m(r)s(x,1)$, corresponding to the case that there are four squares at scale r having x as a vertex; or, $s(x,r) < 4m(r) = m(r)s(x,1)$, corresponding to the case that not all the four squares at scale r having x as a vertex are in the discrete $\mathcal{Z}_\boxtimes$-chart. This argument implies (4.30).
In order to get the second inequality in (4.28a), we notice that if $s(x,r) < 4m(r) = m(r)s(x,1)$, then there exists a point $y = X(q)$ with $q \in \partial\mathcal{G}_\alpha$ at distance at most Cr from x. Due to Lemma 3.1 and by a packing bound, this can happen for at most $Cr^2\sharp\partial\mathcal{G}_\alpha$ points x. By (4.29), summing over X, we get

$$4\sharp\mathcal{Q}_1 - 4\frac{\sharp\mathcal{Q}_r}{m(r)} = \sum_{x\in X}\left(s(x,1) - \frac{s(x,r)}{m(r)}\right) \le Cr^2\sharp\partial\mathcal{G}_\alpha,$$

namely the second inequality in (4.28a).

To prove (4.28b), we first set

$$\mu(Q_1, Q_r) := \left|\mathrm{Conv}(X(Q_1)) \cap \mathrm{Conv}(X(Q_r))\right|.$$

We note that for every $Q_1 \in \mathcal{Q}_1$

$$\sum_{\substack{Q_r\in\mathcal{Q}_r \\ \Phi(Q_1)\cap\mathrm{Conv}(\Phi(Q_r))\neq\emptyset}} \mu(Q_1,Q_r) \le r^2 m(r)\mathrm{Area}(X(Q_1)), \tag{4.31}$$

from which, summing over $Q_r \in \mathcal{Q}_r$ we deduce

$$\begin{aligned}\sum_{Q_r\in\mathcal{Q}_r}\mathrm{Area}(X(Q_r)) &= \sum_{Q_r\in\mathcal{Q}_r}\sum_{\substack{Q_1\in\mathcal{Q}_1 \\ \Phi(Q_1)\cap\mathrm{Conv}(\Phi(Q_r))\neq\emptyset}} \mu(Q_1,Q_r) \\ &= \sum_{Q_1\in\mathcal{Q}_1}\sum_{\substack{Q_r\in\mathcal{Q}_r \\ \Phi(Q_1)\cap\mathrm{Conv}(\Phi(Q_r))\neq\emptyset}} \mu(Q_1,Q_r) \le r^2m(r)\sum_{Q_1\in\mathcal{Q}_1} r^2m(r)\mathrm{Area}(X(Q_1)),\end{aligned}$$

thus yielding the first inequality in (4.28b). As for the second inequality in (4.28b), it is enough to notice that the inequality (4.31) is in fact an equality if $\mathrm{dist}(X(Q_1), X(\partial\mathcal{G}_\alpha)) > Cr$ for some universal constant $C > 0$.

We now show (4.28c). Since $\{a,b\} \in \mathrm{Sides}(\mathcal{Q}_r)$, the segment $[X(a),X(b)]$ is included in the image of a discrete chart, and then $\{p,q\} \in \mathcal{S}_\alpha$ for all $\{p,q\} \in \mathrm{Sides}(\mathcal{Q}_1)$.

A direct packing bound implies that the number of edges in this neighborhood is of order r. Since their length is of order 1 we get the desired upper bound (4.28c).

To prove (4.28d), first note that it suffices to bound the number of squares $Q_r \in \mathcal{Q}_r$ such that $[X(a),X(b)] \cap \mathrm{Conv}(X(Q_1))$ meets the convex hull of Q_1 (see proof of Proposition 4.8 for further details).

We further reduce the problem noting that to intersect the hull of Q_1 is equivalent to intersecting one of its sides, so it suffices to bound the number of squares of scale r one of whose edges meets an edge of scale 1. The desired bound (4.28d) then follows from (4.28c) via a double counting procedure similar to the proof of (4.28a). The details are left to the reader.

Finally, to prove (4.28e), we note that if $\{p,q\} \in \mathrm{Sides}(\mathcal{Q}_{\sqrt{2}r})\Delta\mathrm{Diag}(\mathcal{Q}_r)$, then there exists a point of $\partial\mathcal{G}_\alpha$ which is mapped to the $4r$-neighborhood of $\{p,q\}$. We then proceed by a packing argument as before, and we obtain (4.28e). □

4.3. **Control of large-scale deformation errors by short-scale deformations.** In this section we improve upon the finite-range result of Theorem 3.16. This is done by effectively controlling short-distance interactions via the nearest-neighbors interaction, and treating all the large-distance interactions effectively as perturbation terms.

The following result is the "square lattice version" of [48, Proposition 2.10]. It uses as the Euclidean geometry basic tool again Heron's formula, but the reasoning is different. Combinatorially, if $\boxtimes$ is the complete graph on 4 vertices $\{a,b,c,d\}$ there are 4 distinct triangles in this graph, and each edge is covered by 2 triangles. On the metric side, if $\widetilde{\boxtimes} = X(\{a,b,c,d\})$ is realized as a plane quadrilateral which is a small deformation of a square $\boxtimes$ congruent to $\{0,1\}^2 \subset \mathbb{R}^2$, then pairs of triangles which have in common only a diagonal make a decomposition of $\widetilde{\boxtimes}$. Then we compute the area by using Heron's formula on all triangles $\widetilde{\Delta} \subset \widetilde{\boxtimes}$, where $s_{\widetilde{\Delta}}$ is the semiperimeter of $\widetilde{\Delta}$:

$$\mathrm{Area}(\widetilde{\boxtimes}) = \frac{1}{2}\sum_{\widetilde{\Delta}\subset\widetilde{\boxtimes}} \mathrm{Area}(\widetilde{\Delta}) = \frac{1}{2}\sum_{\widetilde{\Delta}\subset\widetilde{\boxtimes}} \sqrt{s_{\widetilde{\Delta}}\prod_{\widetilde{e}\in\widetilde{\Delta}}(s_{\widetilde{\Delta}} - |\widetilde{e}|)}. \tag{4.32}$$

We apply Taylor expansion around the sidelengths $|e|$ corresponding to $\boxtimes \simeq \{0,1\}^2$ and call $|\widetilde{e}| = |e| + \delta_e$ the perturbed sidelengths. Then for Δ a triangle of sidelengths $1,1,\sqrt{2}$ we get $\frac{d}{d|e|}\mathrm{Area}(\widetilde{\Delta})\Big|_{\widetilde{\Delta}=\Delta}$ equal to 0 if $|e| = \sqrt{2}$ and equal to $\mathrm{Area}(\Delta)$ if $|e| = 1$, thus the diagonal contributions disappear (this is due to the fact that Δ has a right angle opposite to the sides of length $\sqrt{2}$). Thus Taylor expansion gives using (4.32), for a function $O(\cdot)$ which is bounded if $\alpha < \alpha_0$ with α_0 small enough,

$$\mathrm{Area}(\widetilde{\boxtimes}) = 1 + \sum_{e\in\boxtimes,|e|=1}\delta_e + O\left(\sum_{e\in\boxtimes}\delta_e^2\right).$$

Given $\alpha > 0$, introducing the scaling factor r, we denote by $r\widetilde{\boxtimes} =: \widetilde{Q}_r$ the deformations of the square with sidelength r, i.e., $\widetilde{Q}_r \sim_\alpha \{0,r\}^2 \subset \mathbb{R}^2$. Moreover, denoting by $\phi_r : \{0,r\}^2 \to \widetilde{Q}_r$ the α-deformation map given by Definition 3.4, whenever $\widetilde{Q}_r$ is clear from the context, we set

$\delta := \delta_{\phi_r}$ (with δ_{ϕ_r} given in Definition 3.4). Notice that, by construction, $\delta(x,y) = ||x-y|-r|$ for $\{x,y\}$ sides of $\widetilde{Q}_r$ and $\delta(x,y) = ||x-y| - \sqrt{2}r|$ for $\{x,y\}$ diagonals of $\widetilde{Q}_r$.

With this notation (for $\widetilde{Q}_r = X(Q_r)$), by Proposition 4.8 and by (4.28d), for every $r \in \mathcal{D}$, $Q_r \in \mathcal{Q}_r$, we have, writing $Q_1 := \widetilde{\boxtimes}$,

$$\sum_{\substack{x,y\in X(Q_r)\\ x\neq y}} \delta^2(x,y) \le \bar{C} m(r)\, r^2 \sum_{\substack{\{x,y\}\in X(Q_1)\\ x\neq y}} \delta^2(x,y), \tag{4.33}$$

for some universal constant $\bar{C} > 0$.

Then using the chain rule for derivatives like in Theil's [48, Proposition 2.10], one can easily get the following result.

Proposition 4.15. *There exist $C_8, \alpha_2 > 0$ such that for all $\alpha \in [0,\alpha_2)$ for $v \in C^2([0,\infty))$ and $\lambda > 0$, if $\widetilde{Q}_r \subset \mathbb{R}^2$ satisfies $\widetilde{Q}_r \sim_\alpha \{0,r\}^2 \subset \mathbb{R}^2$ then we have*

$$\begin{aligned} &\left| \frac{v'(r)}{r}\left(\mathrm{Area}(\widetilde{Q}_r) - r^2\right) + 4v(r) - \sum_{\substack{x,y\in\widetilde{Q}_r\\ \{x,y\}\sim_\alpha\{0,r\}}} v(|x-y|)\right| \\ &\le C_8\left(\frac{|v'(r)|}{r} + \|v''\|_{L^\infty(rE^1_\alpha)}\right) \sum_{\substack{x,y\in\widetilde{Q}_r\\ x\neq y}} \delta^2(x,y) := e(v,r) \sum_{\substack{x,y\in\widetilde{Q}_r\\ x\neq y}} \delta^2(x,y). \end{aligned} \tag{4.34}$$

In what follows, with an abuse of notation, we still write $e(v,r)$ for the error term as in (4.34), even if the constant C changes from line to line, as long as C remains independent of X.

We are now ready to state the long-range version of Theorem 3.16. We recall that the constant $\overline{\alpha}$ is given by Lemma 3.3, the constants $\alpha_0 > 0$, $C_3 > 1$ are provided by Lemma 3.5, and $\alpha_0' > 0$ is given by Lemma 3.8.
Given $\alpha, \alpha'', \epsilon > 0$, $p > 4$, we denote by $K = K(\alpha,\alpha'',p)$ the constant given by Lemma 3.1 for $r_{min} := 1-\alpha$, $C_2 := 1$, $C_1 := \epsilon$ and $r_0 := \sqrt{2} + \alpha''$.

Theorem 4.16 (crystallization for smooth one-well potentials)**.** *Let $\alpha, \alpha', \alpha'' > 0$ be such that $\alpha' < \alpha < \frac{1}{C_3}\alpha'' < \frac{1}{C_3}\min\{(2-\sqrt{2})/4, \overline{\alpha}, \alpha_0, \alpha_0'\}$ and let $p > 4$.*
Set $r_{min} := 1-\alpha$, $C_1 := \epsilon$, $r_0 := \sqrt{2}+\alpha''$, $C_2 := 1$ and let $K > 0$ be as in Lemma 3.1. There exist two constants $\overline{c}, \overline{\epsilon} > 0$ such that for every $c', c'' \in (0,\overline{c}]$ and $\epsilon \in (0,\overline{\epsilon}]$ the following result holds true: If $V, W \in C^2_{pw}((0,\infty))$ are related by (3.19) and satisfy

(0) $\min_{s>0} W(s) = -1$,
(1) *V is convex in $E_{\alpha''}$ and V satisfies* $\inf_{r\in E_{\alpha''}\setminus[1,\sqrt{2}]} V''_\pm(r) \ge c$,
(2) *W satisfies* (3.27) *and* (3.28) *with constant c'*,
(3) $\sup_{r\in E_{\alpha'}} V(r) < -\frac{15}{16} - c''$,
(4) $V(r) > -\frac{1}{2}$ *if* $r \notin (1-\alpha, \sqrt{2}+\alpha)$,
(5) $V(r) \ge K$ *if* $r \le 1-\alpha$,
(6') $V(r) \le 0$ *for every* $r \ge 1$ *and* $|V(r)|$, $r|V'(r)|$, $r^2|V''(r)| < \epsilon r^{-p}$ *for* $r \ge \sqrt{2}+\alpha''$,

then

$$N\overline{\mathcal{E}}_{\mathrm{sq}}[V] \le \mathcal{E}[V](N) \le N\overline{\mathcal{E}}_{\mathrm{sq}}[V] + O(N^{1/2}) \qquad \text{as } N \to +\infty. \tag{4.35}$$

Before the proof we connect $\overline{\mathcal{E}}_{\rm sq}[V]$ to an $\mathcal{E}_4$-minimization problem, in a self-contained result.

We first introduce some notations. Recalling the decomposition (4.17), for every $t>0$ we set

$$\widetilde{W}(t^2) := \sum_{r\in\widetilde{\mathcal{D}}\setminus\{1\}} m(r)W(t^2r^2), \quad W_*(t^2) := \sum_{r\in\widetilde{\mathcal{D}}} m(r)W(t^2r^2) = W(t^2)+\widetilde{W}(t^2), \tag{4.36a}$$

and, as above,

$$\widetilde{V}(t) := \widetilde{W}(t^2), \quad V_*(t) := W_*(t^2) \quad \text{for all } t>0. \tag{4.36b}$$

Finally, for every $\Lambda\in\mathcal{L}$ with $0\in\Lambda$, we denote by $\mu(\Lambda)$ the set of shortest vectors in $\Lambda\setminus\{0\}$, i.e.,

$$\mu(\Lambda) := \{z\in\Lambda\setminus\{0\} \,:\, |z|\le|w| \qquad \text{for all } w\in\Lambda\setminus\{0\}\}.$$

Proposition 4.17. *Let $\alpha'',\epsilon>0$ and $p>4$. Let $V\in C^2_{pw}((0,\infty))$ satisfy assumption (6') of Theorem 4.16. Assume that the minimum $\min\mathcal{E}_4[V_*]$ is achieved at a square $\overline{\boxtimes}$. Then we have*

$$\mathcal{E}_4[V_*](\overline{\boxtimes}) = \overline{\mathcal{E}}_{\rm sq}[V]. \tag{4.37}$$

Proof. Let $\underline{t}>0$ be the value at which the minimum in the definition (1.4) is achieved. Up to scaling, we may, and will, assume that $\underline{t}=1$. Let $W\in C^2_{pw}((0,\infty))$ be defined by (3.19). By (4.17) of Lemma 4.12 and by Lemma 4.11, we have

$$\begin{aligned}\sum_{z\in\mathbb{Z}^2\setminus\{0\}} W(|z|^2) &= \sum_{\substack{\Lambda\in\mathcal{L}\\0\in\Lambda}}\sum_{z\in\mu(\Lambda)} (W(|z|^2)+W(2|z|^2))\\ &= 4\sum_{r\in\widetilde{\mathcal{D}}}(m(r)W(r^2)+m(\sqrt{2}r)W(2r^2)) = 4(W_*(1)+W_*(2)).\end{aligned} \tag{4.38}$$

For every $R>0$, by (4.38) we have

$$\begin{aligned}&\sum_{x\in\mathbb{Z}^2\cap B_R}\sum_{y\in(\mathbb{Z}^2\cap B_R)\setminus\{x\}} W(|x-y|^2)\\ =&\sum_{x\in\mathbb{Z}^2\cap B_R}\sum_{y\in\mathbb{Z}^2\setminus\{x\}} W(|x-y|^2) - \sum_{x\in\mathbb{Z}^2\cap B_R}\sum_{y\in\mathbb{Z}^2\setminus B_R} W(|x-y|^2)\\ =&4\sharp(\mathbb{Z}^2\cap B_R)(W_*(1)+W_*(2)) - S,\end{aligned} \tag{4.39}$$

where we have set

$$S := \sum_{x\in\mathbb{Z}^2\cap B_R}\sum_{y\in\mathbb{Z}^2\setminus B_R} W(|x-y|^2).$$

By assumption (6') we have that the series $\sum_{z\in\mathbb{Z}^2\setminus\{0\}}|W(|z|^2)|$ converges so that

$$\frac{|S|}{\sharp(\mathbb{Z}^2\cap B_R)} \le \sum_{z\in\mathbb{Z}^2\setminus B_R}|V(|z|)| \le \omega_R,$$

where $\omega_R \to 0$ as $R \to +\infty$. Thus from (4.39) we find

$$\begin{aligned}\overline{\mathcal{E}}_{\rm sq}[V] =& \lim_{R\to\infty} \frac{1}{\sharp(\mathbb{Z}^2\cap B_R)} \sum_{\substack{x,y\in\mathbb{Z}^2\cap B_R\\ x\neq y}} V(|x-y|)\\ =&\frac{1}{2}\lim_{R\to\infty} \frac{1}{\sharp(\mathbb{Z}^2\cap B_R)} \sum_{x\in\mathbb{Z}^2\cap B_R}\sum_{y\in(\mathbb{Z}^2\cap B_R)\setminus\{x\}} V(|x-y|)\\ =&2(V_*(1)+V_*(\sqrt{2})) = \mathcal{E}_4[V_*](\boxtimes) \geq \mathcal{E}_4[V_*](\overline{\boxtimes}),\end{aligned} \tag{4.40}$$

where $\boxtimes$ is a unit square configuration, which shows the inequality "$\leq$" in (4.37).

On the other hand, using the assumption that $\mathcal{E}_4[V_*]$ achieves its minimum at a square, say it achieves the minimum at $\{0,\tilde{t}\}^2 = \overline{\boxtimes}$. Then we renormalize $\tilde{t} = 1$ and we can repeat the above computations verbatim, getting the inequality "$\geq$" in (4.37), thus concluding the proof. □

4.4. **Proof of Theorem 4.16.** Let $X_N := X(\Xi_N)$ be a minimizer of $\mathcal{E}[V]$ in $\mathcal{X}_N(\mathbb{R}^2)$. To ease the notations, we set $x_a := X(a)$ for every $a \in \Xi_N$. Here and in the whole section an *edge* $\{a,b\}$ is any pair of distinct points $a,b \in \Xi_N$. We denote by

$$\overline{\mathcal{S}} = \overline{\mathcal{S}}(\Xi_N) := \{\{a,b\} :\ a \neq b \in \Xi_N\},$$

the set of all the edges associated to Ξ_N. In what follows, for every square $Q_r := \{\xi_1,\xi_2,\xi_3,\xi_4 := \xi_0\}$ at scale r (also called r-square), the *sides* of Q_r are $\{\xi_{i-1},\xi_i\}$ for $i = 1,\dots,4$, whereas the edges of Q_r are given by the sides plus the diagonals $\{\xi_1,\xi_3\}$ and $\{\xi_2,\xi_4\}$.

With a little abuse of notations the (universal) constants appearing in the estimates may change from line to line.

Step 1: Decomposition of $\mathcal{E}[V]$ into contributions of type $\mathcal{E}_4[V]$

Using assumption (6') and Lemma 3.1, we find that the minimal distance between points in $X(\Xi_N)$ is strictly larger than $1-\alpha$. This and the fact that $V(r)$ is negative for $r \geq 1$ gives that, via (4.26), and denoting by $\mathcal{NQ} := \mathcal{NQ}^{(1)} \cup \mathcal{NQ}^{(2)}$ with notation as in (4.26), there holds:

$$\begin{aligned}\sum_{\{a,b\}\in\mathcal{S}} V(|x_a-x_b|) \ \geq\ & \frac{1}{2}\sum_{r\in\widetilde{\mathcal{D}}\setminus\{1\}}\ \sum_{Q\in\mathcal{Q}_r\cup\mathcal{Q}_{\sqrt{2}r}}\ \sum_{\{a,b\}\in{\rm Sides}(Q)} V(|x_a-x_b|)\\ &+\sum_{Q_1\in\mathcal{Q}_1}\mathcal{E}_4[V](X(Q_1)) \ +\sum_{\{a,b\}\in\mathcal{NQ}} V(|x_a-x_b|).\end{aligned} \tag{4.41}$$

To justify the above inequality, note that (i) as a consequence of Lemma 4.12, all possible scales from $\mathcal{D}$ are partitioned into pairs $\{r,\sqrt{2}r\}$ for $r \in \widetilde{\mathcal{D}}$, (ii) each edge can be covered by at most 2 squares, (iii) diagonals of 1-squares include all sides of $\sqrt{2}$-squares. Then we can treat separately the multiplicity of edges which are either (a) the side of two r-squares with $r \geq 2$, (b) the side of exactly one r-square with $r \geq 2$, (c) the side of two $\sqrt{2}$-squares, (d) the side of exactly one $\sqrt{2}$-square, (e) the diagonal of one 1-square but not the side of any $\sqrt{2}$-square, (f) the side of two 1-squares (g) the side of precisely one 1-square, (h) not the side or diagonal of any r-square for $r \in \mathcal{D}$. The two sides of (4.41) account for multiplicity 1 precisely, except for cases (d) and (e), in which we have multiplicity 2. But in these cases, V takes a negative sign for the corresponding edge lengths, and we get the desired inequality.

We now treat the first sum on the right hand side of (4.41) for $r \geq 2$. Recalling the notations introduced before Proposition 4.15, applying Proposition 4.15 with $\widetilde{Q}_r = X(Q_r)$ and $v = V$, we get

$$\begin{aligned}
&\sum_{Q_r\in\mathcal{Q}_r}\sum_{\{a,b\}\in\mathrm{Sides}(Q_r)} V(|x_a-x_b|)\\
&\geq \sum_{Q_r\in\mathcal{Q}_r}\left(4V(r)+\frac{V'(r)}{r}\left(\mathrm{Area}(X(Q_r))-r^2\right)-e(V,r)\sum_{\substack{x,y\in X(Q_r)\\ x\neq y}}\delta^2(x,y)\right),
\end{aligned}$$

which together with (4.28a) and (4.28b) of Proposition 4.14, implies

$$\begin{aligned}
\sum_{Q_r\in\mathcal{Q}_r}\sum_{\{a,b\}\in\mathrm{Sides}(Q_r)} V(|x_a-x_b|) &\geq m(r)\sum_{Q_1\in\mathcal{Q}_1}\left(4V(r)+\frac{V'(r)}{r}\left(r^2\mathrm{Area}(X(Q_1))-r^2\right)\right)\\
-C\left(|V(r)|+r|V'(r)|\right)m(r)r^2\sharp\partial\mathcal{G}_\alpha \quad &- \quad e(V,r)\sum_{Q_r\in\mathcal{Q}_r}\sum_{\substack{x,y\in X(Q_r)\\ x\neq y}}\delta^2(x,y).
\end{aligned}$$

Using again Proposition 4.15 with $r=1$, $\widetilde{Q}_1 = X(Q_1)$, and $v(x) = V_r(x) := V(rx)$, together with the 2-homogeneity $r^2\mathrm{Area}(X(Q_1)) = \mathrm{Area}(rX(Q_1))$, we get

$$\begin{aligned}
\sum_{Q_r\in\mathcal{Q}_r}\sum_{\{a,b\}\in\mathrm{Sides}(Q_r)} V(|x_a-x_b|) &\geq m(r)\sum_{\{a,b\}\in\mathrm{Sides}(\mathcal{Q}_1)} V\left(r|x_a-x_b|\right)\\
&\quad - m(r)e(V_r,1)\sum_{Q_1\in\mathcal{Q}_1}\sum_{\substack{x,y\in X(Q_1)\\ x\neq y}}\delta^2(rx,ry)\\
-C\left(|V(r)|+r|V'(r)|\right)m(r)r^2\sharp\partial\mathcal{G}_\alpha \quad &- \quad e(V,r)\sum_{Q_r\in\mathcal{Q}_r}\sum_{\substack{x,y\in X(Q_r)\\ x\neq y}}\delta^2(x,y).
\end{aligned}\tag{4.42}$$

In view of (4.33) the error terms from the last sum in (4.42) can also be re-interpreted as a scale-1 error term, i.e.,

$$\sum_{Q_r\in\mathcal{Q}_r}\sum_{\substack{x,y\in X(Q_r)\\ x\neq y}}\delta^2(x,y) \leq \bar{C}m(r)r^2\sum_{Q_1\in\mathcal{Q}_1}\sum_{\substack{x,y\in X(Q_1)\\ x\neq y}}\delta^2(x,y).\tag{4.43}$$

Therefore, noting that $\delta^2(rx,ry) = r^2\delta^2(x,y)$, and setting

$$\begin{aligned}
\mathrm{err}_1(r,V) &:= C\left(|V(r)|+r|V'(r)|\right)m(r)r^2,\\
\mathrm{err}_2(r,V) &:= m(r)r^2\left(e(V_r,1)+\bar{C}e(V,r)\right),
\end{aligned}\tag{4.44}$$

we can reorder terms in (4.42), and the final inequality we get is

$$\begin{aligned}
\sum_{Q_r\in\mathcal{Q}_r}\sum_{\{a,b\}\in\mathrm{Sides}(Q_r)} V(|x_a-x_b|) &\geq m(r)\sum_{\{a,b\}\in\mathrm{Sides}(\mathcal{Q}_1)} V\left(r|x_a-x_b|\right)\\
&\quad - \mathrm{err}_1(r,V)\sharp\partial\mathcal{G}_\alpha - \mathrm{err}_2(r,V)\sum_{Q_1\in\mathcal{Q}_1}\sum_{\substack{x,y\in X(Q_1)\\ x\neq y}}\delta^2(x,y).
\end{aligned}\tag{4.45}$$

Similarly, for $\sqrt{2}r$-square contributions in (4.41), we get

$$\sum_{Q_{\sqrt{2}r}\in\mathcal{Q}_{\sqrt{2}r}}\sum_{\{a,b\}\in\mathrm{Sides}(Q_{\sqrt{2}r})} V(|x_a-x_b|) \geq m(\sqrt{2}r)\sum_{\{a,b\}\in\mathrm{Sides}(\mathcal{Q}_{\sqrt{2}})} V\left(r|x_a-x_b|\right) - \mathrm{err}_1(\sqrt{2}r,V)\sharp\partial\mathcal{G}_\alpha - \mathrm{err}_2(\sqrt{2}r,V)\sum_{Q_{\sqrt{2}}\in\mathcal{Q}_{\sqrt{2}}}\sum_{\substack{x,y\in X(Q_{\sqrt{2}})\\ x\neq y}}\delta^2(x,y). \tag{4.46}$$

We now estimate the above error terms.

Let $\rho\geq 2$. Using that $m(\rho)\leq C\rho$ and assumption (6'), we get that there exist two constants $C, C_{\mathrm{pot}}>0$ (depending only on the dimension) such that

$$\mathrm{err}_1(\rho,V) \leq C\epsilon\rho^{3-p} \tag{4.47a}$$

$$\mathrm{err}_2(\rho,V) \leq C_{\mathrm{pot}}\epsilon\rho^{3-p}. \tag{4.47b}$$

Now (4.45) and (4.46), together with (4.47), give that for every $r\in\mathcal{D}$ with $r\geq 2$

$$\begin{aligned}
&\sum_{Q_r\in\mathcal{Q}_r}\sum_{\{a,b\}\in\mathrm{Sides}(Q_r)} V(|x_a-x_b|) + \sum_{Q_{\sqrt{2}r}\in\mathcal{Q}_{\sqrt{2}r}}\sum_{\{a,b\}\in\mathrm{Sides}(Q_{\sqrt{2}r})} V(|x_a-x_b|)\\
&\geq m(r)\sum_{\{p,q\}\in\mathrm{Sides}(\mathcal{Q}_1)} V\left(r|x_p-x_q|\right) + m(\sqrt{2}r)\sum_{\{p,q\}\in\mathrm{Sides}(\mathcal{Q}_{\sqrt{2}})} V\left(r|x_p-x_q|\right) \qquad (4.48a)\\
&-C_{\mathrm{pot}}\epsilon r^{3-p}\left[\sum_{Q_1\in\mathcal{Q}_1}\sum_{\substack{x,y\in X(Q_1)\\ x\neq y}}\delta^2(x,y) + \sum_{Q_{\sqrt{2}}\in\mathcal{Q}_{\sqrt{2}}}\sum_{\substack{x,y\in X(Q_{\sqrt{2}})\\ x\neq y}}\delta^2(x,y)\right] \qquad (4.48b)\\
&-C\epsilon r^{3-p}\sharp\partial\mathcal{G}_\alpha.
\end{aligned}$$

As for the term in (4.48a), since $m(\sqrt{2}r)=m(r)$, for every $r\in\mathcal{D}$ with $r\geq 2$ we have that

$$\begin{aligned}
&m(r)\sum_{\{p,q\}\in\mathrm{Sides}(\mathcal{Q}_1)} V\left(r|x_p-x_q|\right) + m(\sqrt{2}r)\sum_{\{p,q\}\in\mathrm{Sides}(\mathcal{Q}_{\sqrt{2}})} V\left(r|x_p-x_q|\right)\\
=&m(r)\left[\sum_{\{p,q\}\in\mathrm{Sides}(\mathcal{Q}_1)} V\left(r|x_p-x_q|\right) + \sum_{\{p,q\}\in\mathrm{Sides}(\mathcal{Q}_{\sqrt{2}})} V\left(r|x_p-x_q|\right)\right]\\
=&2m(r)\sum_{Q_1\in\mathcal{Q}_1}\mathcal{E}_4[V_r](X(Q_1)) - 2m(r)\sum_{\{p,q\}\in\mathrm{Diag}(\mathcal{Q}_1)} V_r(|x_p-x_q|)\\
&+ m(r)\sum_{\{p,q\}\in\mathrm{Sides}(\mathcal{Q}_{\sqrt{2}})} V_r(|x_p-x_q|) \qquad (4.49)\\
\geq&2m(r)\sum_{Q_1\in\mathcal{Q}_1}\mathcal{E}_4[V_r](X(Q_1)) - m(r)\sum_{\{p,q\}\in\mathrm{Diag}(\mathcal{Q}_1)} V_r(|x_p-x_q|)\\
&+ m(r)\sum_{\{p,q\}\in\mathrm{Sides}(\mathcal{Q}_{\sqrt{2}})} V_r(|x_p-x_q|)\\
:=&2m(r)\sum_{Q_1\in\mathcal{Q}_1}\mathcal{E}_4[V_r](X(Q_1)) + \mathrm{err}_3(r,V),
\end{aligned}$$

where the inequality is a consequence of assumption (6') – in particular the fact that $V(r) \leq 0$ for $r \geq 1$ – and the last line is a definition of $\mathrm{err}_3(r, V)$.

To justify the second equality in (4.49) note that, by definition (3.20), $\mathcal{E}_4[V_r](Q)$ has coefficient $1/2$ for terms coming from the sides of Q, and coefficient 1 in front of diagonal terms.

By using (4.28e), the bound $m(r) \leq Cr$, the fact that $r \geq 2$, and again assumption (6'), we have

$$|\mathrm{err}_3(1, V_r)| \leq C\epsilon r^{3-p} \sharp \partial \mathcal{G}_\alpha. \tag{4.50}$$

We finally pass to the estimate of the two sums in (4.48b). By applying (4.33) with $r = \sqrt{2}$ we have

$$\sum_{Q_{\sqrt{2}} \in \mathcal{Q}_{\sqrt{2}}} \sum_{\substack{x,y \in X(Q_{\sqrt{2}}) \\ x \neq y}} \delta^2(x,y) \leq \sum_{Q_1 \in \mathcal{Q}_1} \sum_{\substack{x,y \in X(Q_1) \\ x \neq y}} \delta^2(x,y) \leq 2 \sum_{Q_1 \in \mathcal{Q}_1} \mathcal{E}_4[\overline{\delta^2}](X(Q_1)), \tag{4.51}$$

where $\overline{\delta^2} : E_\alpha \to [0, \infty)$ is defined by $\overline{\delta^2}(t) = (1-t)^2$ for $t \in E^1_\alpha$ and $\overline{\delta^2}(t) = (\sqrt{2} - t)^2$ for $t \in E^2_\alpha$.

By (4.48), (4.49), (4.50), and (4.51) we can conclude that for every $r \in \widetilde{\mathcal{D}}$ with $r \geq 2$ we have

$$\begin{aligned} &\sum_{Q_r \in \mathcal{Q}_r} \sum_{\{a,b\} \in \mathrm{Sides}(Q_r)} V(|x_a - x_b|) + \sum_{Q_{\sqrt{2}r} \in \mathcal{Q}_{\sqrt{2}r}} \sum_{\{a,b\} \in \mathrm{Sides}(Q_{\sqrt{2}r})} V(|x_a - x_b|) \\ &\geq 2m(r) \sum_{Q_1 \in \mathcal{Q}_1} \mathcal{E}_4[V_r](X(Q_1)) - C_{\mathrm{pot}} \epsilon r^{3-p} \sum_{Q_1 \in \mathcal{Q}_1} \mathcal{E}_4[\overline{\delta^2}](X(Q_1)) - C\epsilon r^{3-p} \sharp \partial \mathcal{G}_\alpha. \end{aligned} \tag{4.52}$$

Step 2: The sum over scales.

By summing (4.52) over all the scales $r \in \widetilde{\mathcal{D}} \setminus \{1\}$ and using the linearity of $\mathcal{E}_4[V]$ with respect to V, we get

$$\begin{aligned} \frac{1}{2} \sum_{r \in \widetilde{\mathcal{D}} \setminus \{1\}} \left[\sum_{Q_r \in \mathcal{Q}_r} \sum_{\{a,b\} \in \mathrm{Sides}(Q_r)} V(|x_a - x_b|) + \sum_{Q_{\sqrt{2}r} \in \mathcal{Q}_{\sqrt{2}r}} \sum_{\{a,b\} \in \mathrm{Sides}(Q_{\sqrt{2}r})} V(|x_a - x_b|) \right] \\ \geq \sum_{Q_1 \in \mathcal{Q}_1} \mathcal{E}_4[\widetilde{V} - C_{\mathrm{pot}} \epsilon \overline{\delta^2}](X(Q_1)) - C\epsilon \sharp \partial \mathcal{G}_\alpha, \end{aligned} \tag{4.53}$$

where we have used also the very definition of $\widetilde{V}$ in (4.36) and the fact that $p > 4$. Therefore, by (4.41) and (4.36), using again the linearity of $\mathcal{E}_4$ with respect to V, we deduce

$$\frac{1}{2} \sum_{\{a,b\} \in \mathcal{S}} V(|x_a - x_b|) \geq \sum_{Q_1 \in \mathcal{Q}_1} \mathcal{E}_4[V_* - C_{\mathrm{pot}} \epsilon \overline{\delta^2}](X(Q_1)) - C\epsilon \sharp \partial \mathcal{G}_\alpha + \sum_{\{a,b\} \in \mathcal{NQ}} V(|x_a - x_b|). \tag{4.54}$$

Step 3: Existence of a minimizer for $\mathcal{E}_4[V_* - C_{\mathrm{pot}} \varepsilon \overline{\delta^2}]$.

Here we show that there exists a unique minimizer of $\mathcal{E}_4[V_* - C_{\mathrm{pot}} \varepsilon \overline{\delta^2}]$ in $\mathcal{X}_4(\mathbb{R}^2)/\mathrm{Isom}(\mathbb{R}^2)$ and that such a minimizer is a square. To this purpose, we notice that the assumptions (0)-(4)

and (6') allow us to profit of the results in Subsection 3.4, and in particular of Proposition 3.15. Indeed, by (4.36) and assumption (6'), choosing $\epsilon > 0$ small enough we have

$$\|V - V_*\|_{C^2(1-\alpha,\infty)} = \|\widetilde{V}\|_{C^2(1-\alpha,\infty)} = \left\| \sum_{r \in \widetilde{\mathcal{D}} \setminus \{1\}} m(r) W(r^2 \cdot) \right\|_{C^2(1-\alpha,\infty)} \leq \bar{C}\epsilon < c''', \tag{4.55}$$

where c''' is the constant in Proposition 3.15.
By the second part of the statement of Proposition 3.15 we get that there exists a unique minimizer of $\mathcal{E}_4[V_*]$ in $\mathcal{X}_4(\mathbb{R}^2)/\mathrm{Isom}(\mathbb{R}^2)$ that is a square with sidelengths in $(1-\alpha, +\infty)$.
On the other hand, by a direct calculation one can easily check that $\overline{\delta^2}$ satisfies the assumptions of Lemma 3.11 and Lemma 3.12 so that $\boxtimes$ is the unique global minimizer of $\mathcal{E}_4[\overline{\delta^2}]$ in $\overline{\mathscr{S}}_\alpha$. Moreover, again by a direct calculation (or using Lemma 3.11), it easily follows that $\mathcal{E}_4[\overline{\delta^2}](\boxtimes) = 0$ and $\nabla \mathcal{E}_4[\overline{\delta^2}](\boxtimes) = 0$, and thus $\mathcal{E}_4[\overline{\delta^2}](\widetilde{\boxtimes}) = O(|\boxtimes - \widetilde{\boxtimes}|^2)$ for a small perturbation $\widetilde{\boxtimes}$ of $\boxtimes$.
This implies that for $\epsilon > 0$ small enough the function $\mathcal{E}_4[V_* - C_{\mathrm{pot}}\epsilon\overline{\delta^2}]$ still has a strict minimum at $\overline{\boxtimes}$. By Proposition 3.15, which can then be applied to V_* and $V_* - C_{\mathrm{pot}}\epsilon\overline{\delta^2}$ up to diminishing ϵ, we find that $\overline{\boxtimes}$ is also the unique minimum of $\mathcal{E}_4[V_* - C_{\mathrm{pot}}\epsilon\overline{\delta^2}]$.

Step 4: Estimate of the last term in (4.54)**.**

Now we bound the terms from the last sum in (4.54), i.e. the contributions not attributable to squares. Setting $\mathcal{NQ}_{\alpha''} := \mathcal{NQ} \cap \mathcal{S}_{\alpha''}$, we have

$$\begin{aligned} &\sum_{\{a,b\} \in \mathcal{NQ}} V(|x_a - x_b|) \\ &\quad = \sum_{\{a,b\} \in \mathcal{NQ}_{\alpha''}} V(|x_a - x_b|) + \sum_{d \in \sqrt{2}+\alpha''+\frac{1}{2}+\mathbb{N}} \sum_{\substack{\{a,b\} \in \mathcal{NQ} \\ |x_a - x_b| \in \left[d-\frac{1}{2}, d+\frac{1}{2}\right]}} V(|x_a - x_b|) \\ &\quad =: I + \mathrm{err}_4(V, X). \end{aligned} \tag{4.56}$$

As for $\mathrm{err}_4(V,X)$, since X is a minimizer, by the separation result of Lemma 3.1 and a packing bound, there exists $C > 0$ depending only on the dimension and on $\alpha_0 > 0$ such that the r-neighborhood of X contains at most Cr^2 points from X. This implies that

$$\sharp \left\{ \{a,b\} \in \mathcal{NQ} : \ |x_a - x_b| \in \left[d - \frac{1}{2}, d + \frac{1}{2} \right] \right\} \leq C d^3 \sharp \partial \mathcal{G}_\alpha. \tag{4.57}$$

The consequence of (4.56) and (4.57) is the following bound, valid under hypothesis (6′) with $p > 4$:

$$\begin{aligned} \mathrm{err}_4(V,X) &\geq \sum_{d \in \sqrt{2}+\alpha+\frac{1}{2}+\mathbb{N}} \sharp \left\{ \{a,b\} \in \mathcal{NQ} : \ ||x_a - x_b| - d| \leq \frac{1}{2} \right\} \min_{r : |r-d| \leq \frac{1}{2}} V(r) \\ &\geq C \sharp \partial \mathcal{G}_\alpha \sum_{d \in \sqrt{2}+\alpha+\frac{1}{2}+\mathbb{N}} d^3 \min_{r \in \left[d-\frac{1}{2}, d+\frac{1}{2}\right]} V(r) \geq -C\epsilon \sharp \partial \mathcal{G}_\alpha. \end{aligned} \tag{4.58}$$

Step 5: End of proof, following the strategy of Theorem 3.16

By (4.54), (4.56) and (4.58), we have

$$\mathcal{E}[V](X_N) \;\geq\; \sum_{Q_1\in\mathcal{Q}_1} \mathcal{E}_4[V_* - C_{\rm pot}\epsilon\overline{\delta^2}](X(Q_1)) + I - C\epsilon\sharp\partial\mathcal{G}_\alpha, \tag{4.59}$$

where both the constants do only depend on p and on the dimension. Now, in order to continue precisely along the strategy used for Theorem 3.16, we re-express the sum (4.59) via a potential which vanishes at distance larger that $\sqrt{2}+\alpha''$. We define

$$V_{**}(r) := (V_*(r) - C_{\rm pot}\epsilon\overline{\delta^2}(r))\mathbb{1}_{r<\sqrt{2}+\alpha''}(r). \tag{4.60}$$

For estimating I from (4.56) we apply a similar setup as in (3.45) from the proof of Theorem 3.16. Indeed, a similar decomposition as in (3.45) can be used also in this case.

Then (4.59) can be rewritten in a form very similar to (3.45):

$$\mathcal{E}[V](X_N) \;\geq\; \sum_{Q_1\in\mathcal{Q}_1} \mathcal{E}_4[V_{**}](X(Q_1)) + \sum_{\{a,b\}\in\mathcal{NQ}_{\alpha''}} V(|x_a-x_b|) - C\epsilon\sharp\partial\mathcal{G}_\alpha. \tag{4.61}$$

Then we have, directly from the Step 3 of the proof, that $\min\mathcal{E}_4[V_*] = \min\mathcal{E}_4[V_{**}]$, and moreover we have from Proposition 4.17 that

$$\mathcal{E}_4[V_{**}](\overline{\boxtimes}) = \min\mathcal{E}_4[V_{**}] = \overline{\mathcal{E}}_{\rm sq}[V]. \tag{4.62}$$

We next proceed exactly as in the proof of Theorem 3.16 with V replaced by V_{**}. We define the energy contribution of each point

$$\mathcal{E}^p[V_{**}](X_N) := \frac{1}{2}\sum_{q:q\neq p} V_{**}(|x_p-x_q|) = \frac{1}{2}\sum_{q\in\mathcal{N}_{\alpha''}(p)\setminus\{p\}} V(|x_p-x_q|),$$

and after enriching the graph $\mathcal{G}_\alpha$ by adding long edges and missing edges, we obtain a graph still denoted by $\overline{\mathcal{G}}$ and we reach the following version of (3.49a), in which we use the same notation $\overline{\mathcal{N}}(p)$ as for (3.49a):

$$\mathcal{E}^p[V_{**}](X_N) \geq \mathcal{E}_4[V_{**}](\overline{\boxtimes}) + \sum_{q\in\overline{\mathcal{N}}(p)\setminus\{p\}} \overline{\overline{w}}(\{p,q\}), \tag{4.63}$$

where we have the following substitute for the bounds (3.49b):

$$\overline{\overline{w}}(\{p,q\}) := \begin{cases} 0 & \text{if } \{p,q\}\in\mathcal{S}_\alpha\setminus\mathcal{NQ}, \\ -\frac{\mathcal{E}_4[V_{**}](\overline{\boxtimes})}{2} - \frac{1}{2} & \text{if } \{p,q\}\in\mathcal{NQ}\cap\mathcal{S}_\alpha, \\ -\frac{\mathcal{E}_4[V_{**}](\overline{\boxtimes})}{2} - \frac{1}{4} & \text{if } \{p,q\}\in\mathcal{S}_{\alpha'',\alpha}, \\ -\frac{\mathcal{E}_4[V_{**}](\overline{\boxtimes})}{2} & \text{if } \{p,q\} \text{ missing edge.} \end{cases} \tag{4.64}$$

Now with the notation for $m_{\alpha',V}, m_{\alpha',V_{**}}$ as in (3.47), we get instead of (3.50) the bound

$$-\frac{\mathcal{E}_4[V_{**}](\overline{\boxtimes})}{2} - \frac{1}{2} \geq -\frac{m_{\alpha',V_{**}}}{2} - \frac{1}{2} \geq -\frac{m_{\alpha',V}}{2} - \frac{1}{2} - \widetilde{C}\epsilon, \tag{4.65}$$

where the first inequality uses again assumption (3) and the definition of $m_{\alpha',V_{**}}$, and for the last bound we can use the fact that $V_{**}=V_*$ over $E_{\alpha'}$, and then the bound in (4.55) for $\widetilde{V}=V_*-V$.

Now we define the lost weight function exactly as in the proof of Theorem 3.16, namely $\mathrm{lw}(\{p,q\})$ is equal to $1/4$ for long edges and to $1/2$ for missing edges, and we obtain the bound (3.51). The cardinality of the set appearing on the right in (3.51) will be denoted by

$$N_1 := \sharp\left\{p:\ \mathcal{N}_\alpha(p)\cap\partial\mathcal{G}_\alpha\neq\emptyset \text{ or } \mathcal{N}_{\alpha''}(p)\setminus\mathcal{N}_\alpha(p)\neq\emptyset\right\}.$$

Now as in Theorem 3.16, we sum over p equation (4.63) in order to get all contributions $\mathcal{E}^p[V_{**}](X_N)$. We find from (4.61) the following analogue of (3.52) with further error terms coming from (4.65) and (4.61):

$$\begin{aligned}\mathcal{E}[V](X_N) &\geq N\mathcal{E}_4[V_{**}](\overline{\boxtimes}) - C\epsilon\,\sharp\partial\mathcal{G}_\alpha + N_1\left(-4m_{\alpha',V}-4+\frac{1}{16}-\widetilde{C}\epsilon\right)\\ &\geq N\mathcal{E}_4[V_{**}](\overline{\boxtimes}) + N_1\left(-4m_{\alpha',V}-4+\frac{1}{16}-(C+\widetilde{C})\epsilon\right) \qquad (4.66)\\ &\geq N\mathcal{E}_4[V_{**}](\overline{\boxtimes})\end{aligned}$$

where in the first passage we used the fact that $N_1\geq\sharp\partial\mathcal{G}_\alpha$ because N_1 measures the cardinality of a set containing $\partial\mathcal{G}_\alpha$, and in the last passage we used assumption (3) with $c''\geq(C+\widetilde{C})\epsilon$.

Now the property (4.62) and (4.66) conclude the proof of Theorem 4.16.

Appendix A. Proof of Lemmas 3.5 and 3.8

Since many constants are introduced throughout this section, for not confusing with the other constants above, we often replace α with ε. For every $\varepsilon>0$ and for every Ξ, $X:\Xi\to\mathbb{R}^2$, we recall that

$$\mathcal{S}_\varepsilon=\{\{p,q\}\ :\ p,q\in\Xi,\,|x_p-x_q|\in(1-\varepsilon,\sqrt{2}+\varepsilon)\},$$

where $x_p := X(p)$ for every $p\in\Xi$. We first prove two preliminary Lemmas that will be useful in the proof of Lemma 3.5.

Lemma A.1. *There exists $\varepsilon'>0$ such that for every $\varepsilon\in(0,\varepsilon')$ the following holds. Let X satisfy (3.2) with $r_{min}=1-\varepsilon$. Let $p_1,p_2,p_3\in\Xi$ and set $x_i:=X(p_i)$ for all $i\in\{1,2,3\}$. Then,*

(i) *if $\{p_1,p_2\}\in\mathcal{S}_\varepsilon$ and $\{p_1,p_3\}\in\mathcal{S}_\varepsilon$ but $\{p_2,p_3\}\notin\mathcal{S}_\varepsilon$, then in the triangle $\{x_1,x_2,x_3\}$, the interior angles satisfy $\hat{x}_1\geq 60^\circ$ and $\hat{x}_2,\hat{x}_3\leq\arccos\left(\frac{1}{2\sqrt{2}}\right)+O(\varepsilon)$;*

(ii) *if all pairs amongst p_1,p_2,p_3 are in $\mathcal{S}_\varepsilon$, then the interior angles of the triangle $\{x_1,x_2,x_3\}$ are in the interval*

$$\left[\arccos\left(\frac{3}{4}\right)-O(\varepsilon),\quad 90^\circ+O(\varepsilon)\right];$$

(iii) *if $\{p_1,p_2\},\{p_1,p_3\}\in\mathcal{S}_\varepsilon$, $|x_1-x_2|=1+O(\varepsilon)$ but $\{p_2,p_3\}\notin\mathcal{S}_\varepsilon$, then in the triangle $\{x_1,x_2,x_3\}$, we have $\hat{x}_1\geq\arccos\left(\frac{1}{2\sqrt{2}}\right)+O(\varepsilon)$;*

(iv) *if all pairs amongst p_1,p_2,p_3 are in $\mathcal{S}_\varepsilon$ and $|x_1-x_2|=1+O(\varepsilon)$, then*

$$\widehat{x_1x_2x_3},\widehat{x_3x_1x_2}\geq 45^\circ-O(\varepsilon). \qquad (A.1)$$

Proof. We set $a:=|x_1-x_2|$, $b:=|x_1-x_3|$, $c:=|x_2-x_3|$. We may assume, up to relabelling the points, that

$$1-\varepsilon<a\leq b<\sqrt{2}-\varepsilon. \qquad (A.2)$$

Proof of (i). The statement follows from the law of cosines, which states that

$$\cos(\hat{x}_1) = \frac{a^2+b^2-c^2}{2ab}. \tag{A.3}$$

If $\{p_2,p_3\} \notin \mathcal{S}_\varepsilon$, then due to (3.2) we need to have $c \geq \sqrt{2}+\varepsilon > b$, and from (A.3) and (A.2) we find $\cos(\hat{x}_1) < a/2b \leq 1/2$ and thus $\hat{x}_1 \geq 60^\circ$. For bounding $\hat{x}_2$, we observe that

$$\inf\left\{ \frac{a^2+c^2-b^2}{2ac} : \ a,b \in (1-\varepsilon, \sqrt{2}+\varepsilon),\ c \geq \sqrt{2}+\varepsilon \right\}$$

is reached as $(a,b,c) \to (1-\varepsilon, \sqrt{2}+\varepsilon, \sqrt{2}+\varepsilon)$, and equals the value of the expression $(a^2+c^2-b^2)/(2ac)$ in that limit, giving the desired bound on $\hat{x}_2$. The bound for $\hat{x}_3$ works similarly, with the roles of a,b interchanged.

Proof of (ii). If $\{p_2,p_3\} \in \mathcal{S}_\varepsilon$ then $c \in (1-\varepsilon, \sqrt{2}+\varepsilon)$. Moreover (A.2) holds. In such a range, the sup of the right hand side of (A.3) is realized by $c = 1-\varepsilon$, $a = b = \sqrt{2}+\varepsilon$, in which case

$$\hat{x}_1 = \arccos\left(\frac{3+(4\sqrt{2}+2)\varepsilon+\varepsilon^2}{2(\sqrt{2}+\varepsilon)^2} \right) = \arccos\left(\frac{3}{4} + O(\varepsilon) \right) = \arccos\left(\frac{3}{4}\right) + O(\varepsilon),$$

whereas the inf is reached for $a = b = 1-\varepsilon$, $c = \sqrt{2}+\varepsilon$, in which case

$$\hat{x}_1 = \arccos\left(\frac{-(4+2\sqrt{2})\varepsilon+\varepsilon^2}{2(1-\varepsilon)^2} \right) = \arccos(-O(\varepsilon)) = 90^\circ + O(\varepsilon).$$

Proof of (iii). By (A.3) and by the hypothesis we have

$$\cos(\hat{x}_1) = \frac{(1+O(\varepsilon))^2+b^2-c^2}{2(1+O(\varepsilon))b} \leq \frac{b^2-1-O(\varepsilon)}{2(1+O(\varepsilon))b}.$$

It is easy to see that the quantity on the right-hand-side is - for ε small enough - monotonically increasing with respect to b, so that it is maximized for $b = \sqrt{2}+\varepsilon$. From this, the claim follows.

Proof of (iv). Again by (A.3) and by the hypothesis we have

$$\cos(\hat{x}_1) \leq \frac{(1+O(\varepsilon))^2+c^2-b^2}{2(1-\varepsilon)c},$$

where the sup of the right-hand-side is reached for $|x_2-x_3| = \sqrt{2}+\varepsilon$ and $|x_1-x_3| = 1-\varepsilon$, thus yielding the claim. □

By applying verbatim the same reasoning of the proof of Lemma A.1(ii) one gets the following result.

Corollary A.2. *Let $X \subset \mathbb{R}^2$ and let $x,y,z \in X$ be such that $\{x,y\},\{y,z\} \in \mathcal{S}_0(X)$. Then $\widehat{xyz} \geq \arccos\left(\frac{3}{4}\right) \sim 41.4^\circ$.*

Lemma A.3. *There exists $\varepsilon'' \in (0,\varepsilon']$ (with ε' given by Lemma A.1) such that for every $\varepsilon \in (0,\varepsilon'')$ the following holds. Let Ξ be a set of labels and let $p_1,p_2,p_3,p_4 \in \Xi$ be such that $\{p_i,p_j\} \in \mathcal{S}_\varepsilon$ for all $i \neq j$ and set $x_i := X(p_i)$ for all $i = 1,\dots,4$; then, up to relabeling, for all $i \in \{1,2,3,4\}$ we have*

(i) $|x_i - x_{i+1}| = 1 + O(\varepsilon)$,
(ii) $x_i\widehat{x_{i+1}x_{i+2}} = 90^\circ + O(\varepsilon)$,
(iii) $|x_i - x_{i+2}| \leq \sqrt{2} + O(\varepsilon)$,

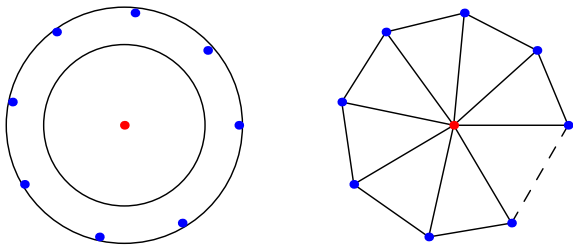


FIGURE 5. Illustration of Claim 1.

where $x_{i+4} = x_i$ for every $i = 1, \dots, 4$. If p_1, p_2, p_3, p_4 are such that $\{p_i, p_j\} \in \mathcal{S}_\varepsilon$ for all $i \neq j$, then the quadrilateral $\{p_1, p_2, p_3, p_4\}$ is called an ε-square.

Proof. Up to relabeling we may suppose that the points $x_1, \dots, x_4$ are in cyclic order along the boundary of the convex hull $\mathrm{Conv}(\{x_1, \dots, x_4\})$.
Proof of (i). Assume that $|x_1 - x_2| \geq |x_i - x_{i+1}|$ for every $i = 2, \dots, 4$. Then, under the constraints $|x_i - x_{i+1}| > 1 - \varepsilon$ and $|x_i - x_{i+2}| < \sqrt{2} + \varepsilon$, the sup of $|x_1 - x_2|$ is realized by $|x_2 - x_3| = |x_3 - x_4| = |x_4 - x_1| = 1 - \varepsilon$ and $|x_1 - x_3| = |x_2 - x_4| = \sqrt{2} + \varepsilon$, which gives the desired bound.
Proof of (ii). It follows directly by Lemma A.1.
Proof of (iii). By the law of cosines, (i) and (ii), we have

$$|x_i - x_{i+2}|^2 = 2(1 + O(\varepsilon))^2 - 2(1 + O(\varepsilon))^2 = 2 + O(\varepsilon),$$

which gives the claim. □

We are now in a position to prove Lemma 3.5.

Proof of Lemma 3.5. We assume that $p \in \Xi$ has the maximum number of 8 neighbors $\mathcal{G}_\varepsilon$. We write $x = X(p)$ and we set $x_i = X(p_i)$ for every $i = 1, \dots, 8$. Without loss of generality the x_i are ordered in counterclockwise order around x. We recall that $\arccos\left(\frac{1}{2\sqrt{2}}\right) \sim 69.2°$ and $\arccos\left(\frac{3}{4}\right) \sim 41.4°$. Let ε'' be the constant given in Lemma A.3.

Claim 1: There exists $\varepsilon_0 \in (0, \varepsilon'')$ such that for all $\varepsilon \in (0, \varepsilon_0)$ at least 7 indices $i = 1, \dots, 8$ are such that $\{p_i, p_{i+1}\} \in \mathcal{S}_\varepsilon$. We first note that if for more than two indices i there holds $|x_i - x_{i+1}| \geq \sqrt{2} + \varepsilon$ then by Lemma A.1, $\widehat{x_i x x_{i+1}} \geq 60°$, and thus at least one of the remaining 6 angles is smaller than $(360° - 120°)/6 = 40° < \arccos\left(\frac{3}{4}\right)$. As a consequence, there exists $\varepsilon_0 > 0$ such that for $\varepsilon \in [0, \varepsilon_0)$ we get a contradiction with Lemma A.1 and hence $|x_i - x_{i+1}| \geq \sqrt{2} + \varepsilon$ may hold for at most one index $i \in \mathbb{Z}/8\mathbb{Z}$.

Claim 2: For all $\varepsilon \in (0, \varepsilon_0)$, the configuration $X(\mathcal{N}_\varepsilon(p)) = \{x, x_1, \dots, x_8\}$ contains at least one ε-square as defined in Lemma A.3. Assume that this is not the case , namely that there exists $\varepsilon \in (0, \varepsilon_0)$ such that $X(\mathcal{N}_\varepsilon(p))$ does not contain any ε-square. Then, by Claim 1, each of the p_i's ($i = 1, \dots, 8$) has two or three neighbors in $\mathcal{N}_\varepsilon(p)$. Note also that the sum of internal angles of the octagon $\{x_1, \dots, x_8\}$ is $1080°$, thus at least one angle is larger than $1080°/8 = 135°$, say it is the angle at $\widehat{x_1 x_2 x_3}$. Since $\mathcal{N}_\varepsilon(p) \cap \partial\mathcal{G}_\varepsilon = \emptyset$, x_2 also has 8 neighbors. By considering the successive angles around x_2 formed with the 8 neighbors of p_2 in $\mathcal{G}_\varepsilon$, we have that 6 such angles are contained outside the sector spanned by the angle $\widehat{x_1 x_2 x_3}$, therefore at least one of these angles is smaller than or equal to $(360° - 135°)/6 = 37.5° <$

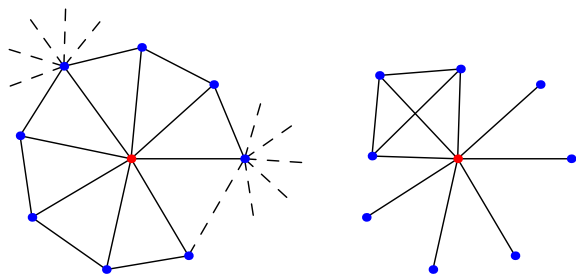


FIGURE 6. Hypothesis and final situation reached by Claim 2.

$\arccos\left(\frac{3}{4}\right)+O(\varepsilon)$ for $\varepsilon \in [0,\varepsilon_0)$ where ε_0 is the one given Claim 1. But this fact contradicts Lemma A.1, and hence we get the claim.

Claim 3: There exists $\varepsilon_1 \in (0,\varepsilon_0]$ such that for all $\varepsilon \in (0,\varepsilon_1)$, the configuration $X(\mathcal{N}_\varepsilon(p))$ contains at least two ε-squares. Assume that this is not the case , namely that there exists a sequence $\{\varepsilon_n\}_{n\in\mathbb{N}}$ with $\varepsilon_n \to 0^+$ as $n \to +\infty$ such that every $n \in \mathbb{N}$ there exists $q_n \in \Xi$ such that $\mathcal{N}_{\varepsilon_n}(q_n) \cap \partial\mathcal{G}_{\varepsilon_n} = \emptyset$ and $X(\mathcal{N}_{\varepsilon_n}(X(q_n)))$ does not contain two ε_n-squares. Fix $n \in \mathbb{N}$, and let $\varepsilon = \varepsilon_n$ and $p = q_n$ be as above. In view of Claim 2, this means that $X(\mathcal{N}_\varepsilon(p))$ contains only one ε-square. Let $\{x, x_1, x_2, x_3\}$ be such ε-square.

If $|x_1 - x_8| \geq \sqrt{2}+\varepsilon$ then by Lemma A.1(iii), $\widehat{x_8 x x_1} \geq 69^\circ$ for ε sufficiently small. But in this case, by Lemma A.3(ii) we conclude that

$$\sum_{i=4}^{8} \widehat{x_{i-1}xx_i} \leq 360^\circ - 69^\circ - 90^\circ + O(\varepsilon) = 201^\circ + O(\varepsilon),$$

which implies that the smallest angle between the $\widehat{x_{i-1}xx_i}$, for $4 \leq i \leq 8$, is smaller than $40.2^\circ < \arccos\left(\frac{3}{4}\right)$, thus contradicting Lemma A.1 for ε small enough.

This shows that for $\varepsilon_1 > 0$ sufficiently small we have $\{p_8, p_1\} \in \mathcal{S}_\varepsilon$. Similarly we find $\{p_3, p_4\} \in \mathcal{S}_\varepsilon$.

By Lemma A.1, we have $\widehat{xx_3x_4}, \widehat{xx_1x_8} \leq 90^\circ + O(\varepsilon)$, and as before, at least one of the 5 remaining internal angles of the octagon $\{x_1, \dots, x_8\}$ at vertices x_4, x_5, x_6, x_7, x_8 is larger than or equal to

$$\theta_\varepsilon := \frac{1}{5}\left(1080^\circ - 450^\circ - O(\varepsilon)\right) = 126^\circ - O(\varepsilon);$$

say that x_i is such a vertex. We are under the assumption that no ε-square at x contains x_i, thus by considering the possible allowed $\mathcal{S}_\varepsilon$-edges between vertices in $\mathcal{N}_\varepsilon(p)$ we find that $\sharp\left(\mathcal{N}_\varepsilon(p_i) \cap \mathcal{N}_\varepsilon(p) \setminus \{p_i\}\right) \leq 3$. On the other hand, we are also under the assumption that $\mathcal{N}_\varepsilon(p) \cap \partial\mathcal{G}_\varepsilon = \emptyset$, thus $\sharp(\mathcal{N}_\varepsilon(p_i) \setminus \{p_i\}) = 8$. Thus there are 6 angles at x_i formed by successive neighbors of x_i and not contained in $\widehat{x_{i-1}x_ix_{i+1}}$. At least one of these angles is smaller than or equal to

$$\beta_\varepsilon := (360^\circ - \theta_\varepsilon)/6 \leq 39^\circ + O(\varepsilon).$$

For ε_0 small enough we find $\beta_\varepsilon < \arccos(\frac{3}{4}) + O(\varepsilon)$, contrary to Lemma A.1, and our claim follows.

Claim 4: There exists $\varepsilon_2 \in (0,\varepsilon_1]$ such that for all $\varepsilon \in [0,\varepsilon_2)$ the configuration $X \cap B(x, \sqrt{2}+\varepsilon)$ cannot contain only two ε-squares with no common edges and two further successive edges

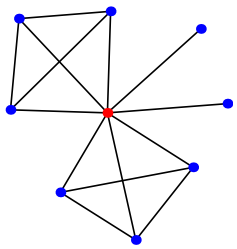


FIGURE 7. What Claim 4 proves impossible.

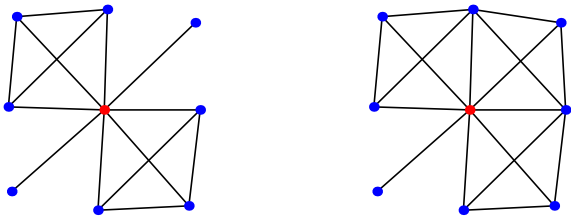


FIGURE 8. Hypothesis and end result of Claim 5.

from x. We will call "remaining vertices" the nearest neighbors of x that do not belong to an ε-square. From Claim 3, we know that there is at most 2 remaining vertices for $\varepsilon < \varepsilon_1$. Again we prove the claim by contradiction. Up to cyclic relabeling of the x_i the two ε-squares are $\{x, x_1, x_2, x_3\}$ and $\{x, x_4, x_5, x_6\}$. By Lemma A.3 and by the law of cosines we obtain

$$\widehat{x_3 x x_4} \geq \arccos\left(\frac{2(1+O(\varepsilon))^2 - (1-\varepsilon)^2}{2(1+O(\varepsilon))^2}\right) = \arccos\left(\frac{1}{2} + O(\varepsilon)\right) = 60^\circ + O(\varepsilon).$$

Moreover, by using again Lemma A.3, at least one of the angles $\widehat{x_i x x_{i+1}}, i = 6, 7, 8$ must be smaller than or equal to

$$\xi_\varepsilon := \frac{1}{3}(360^\circ - 2(90^\circ + O(\varepsilon)) - 60^\circ - O(\varepsilon)) = 40^\circ + O(\varepsilon) < \arccos\left(\frac{3}{4}\right) + O(\varepsilon),$$

for ε small enough. Therefore a contradiction to Lemma A.1 follows.

Claim 5: There exists $\varepsilon_3 \in (0, \varepsilon_2]$ *such that for all* $\varepsilon \in (0, \varepsilon_3)$ *the following holds: if the configuration* $X \cap B(x, \sqrt{2}+\varepsilon)$ *contains two* ε*-squares with no common edges and the two remaining vertices that are not successive, then it contains a further* ε*-square, sharing one edge with each given* ε*-squares.*

Up to cyclic relabeling of the x_i's, the two ε-squares are $\{x, x_1, x_2, x_3\}$ and $\{x, x_5, x_6, x_7\}$. We can assume without loss of generality $\beta_4 := \widehat{x_3 x x_5} \leq \widehat{x_7 x x_1} =: \beta_8$, $\beta_4^- := \widehat{x_3 x x_4} \leq \widehat{x_4 x x_5} =: \beta_4^+$, and $\beta_8^- := \widehat{x_7 x x_8} \leq \widehat{x_8 x x_1} =: \beta_8^+$. By Lemma A.3, it follows that $\beta_4 \leq 90^\circ - O(\varepsilon)$, $\beta_8 \geq 90^\circ - O(\varepsilon)$, and $\beta_4^- \leq 45^\circ - O(\varepsilon)$. By the assumption $|x_4 - x| \leq \sqrt{2} + \varepsilon$. By the law of cosines, we have

$$\begin{aligned}(1-\varepsilon)^2 \leq & |x_3 - x_4|^2 = |x_3 - x|^2 + |x_4 - x|^2 - 2|x_3 - x||x_4 - x| \cos \beta_4^- \\ \leq & (1+O(\varepsilon))^2 + |x_4 - x|^2 - 2(1+O(\varepsilon))|x_4 - x| \cos\left(45^\circ + O(\varepsilon)\right),\end{aligned} \tag{A.4}$$

whence, using

$$\cos\left(45^\circ + O(\varepsilon)\right) = \frac{\sqrt{2}}{2} + O(\varepsilon) \quad \text{and} \quad (1+O(\varepsilon))^2 - (1-\varepsilon)^2 = O(\varepsilon),$$

we deduce the following inequality

$$|x_4 - x|^2 - (\sqrt{2} + O(\varepsilon))|x_4 - x| + O(\varepsilon) \geq 0;$$

it follows that $|x_4 - x| = \sqrt{2} + O(\varepsilon)$.
Moreover, by (A.4), it follows also that, for ε small enough

$$\begin{aligned}\cos\beta_4^- =& \frac{|x_3 - x|^2 + |x_4 - x|^2 - |x_4 - x_3|^2}{2|x_3 - x||x_4 - x|} \\ \leq& \frac{(1+O(\varepsilon))^2 + (\sqrt{2}+O(\varepsilon))^2 - (1-\varepsilon)^2}{2(1-\varepsilon)(\sqrt{2}+O(\varepsilon))} = \frac{\sqrt{2}}{2} + O(\varepsilon),\end{aligned}$$

which together with the assumption on β_4^- implies that $\beta_4^- = 45^\circ + O(\varepsilon)$. Using again the law of cosines one can easily deduce that $|x_3 - x_4| = 1 + O(\varepsilon)$ and that $\widehat{xx_3x_4} = 90^\circ + O(\varepsilon)$. Analogously, one can see that $\beta_4^+ = 45^\circ + O(\varepsilon)$ and that $|x_4 - x_5| = 1 + O(\varepsilon)$. It follows that $|x_3 - x_5| = \sqrt{2} + O(\varepsilon)$. Finally, since p_3 has 8 neighbors, arguing by contradiction one can show that $|x_3 - x_5| \leq \sqrt{2} + \varepsilon$. In conclusion, $\{x, x_3, x_4, x_5\}$ is an ε-square and then the Claim follows.

Claim 6: There exists $\varepsilon_4 \in (0, \varepsilon_3]$ such that for all $\varepsilon \in (0, \varepsilon_4)$ the following holds: $X(\mathcal{N}(p))$ contains at least 3 adjacent ε-squares. In view of Claims 3 and 5, the Claim needs to be proven only in the case that there are two ε-squares sharing one edge. Let $\{x, x_1, x_2, x_3\}$ and $\{x, x_3, x_4, x_5\}$ be two ε-squares. By Lemma (A.3), we have that

$$\sum_{j=1}^{3} x_j\widehat{x_{j+1}x}_{j+2} \leq 360^\circ + O(\varepsilon)\,, \qquad \widehat{xx_1x_2} + \widehat{x_4x_5x} \leq 180^\circ + O(\varepsilon), \tag{A.5}$$

whereas by Lemma A.1 we obtain

$$\widehat{x_8x_1x} + \widehat{xx_5x_6} \leq 180^\circ + O(\varepsilon). \tag{A.6}$$

Then, using again that the sum of the internal angles of the octagon is 1080°, we have

$$\widehat{x_5x_6x_7} + \widehat{x_6x_7x_0} + \widehat{x_7x_0x_1} \geq 1080^\circ - 720^\circ - O(\varepsilon) = 360^\circ - O(\varepsilon)\,.$$

Therefore, one of the above three angles, say $x_{i-1}\widehat{x_ix_{i+1}}$ is larger than

$$\vartheta_\varepsilon = 120^\circ - O(\varepsilon).$$

Since p_i has eight neighbors in $\mathcal{G}_\varepsilon$ and since x_i does not belong to an ε-square, p_i has exactly three neighbors in $\mathcal{N}_\varepsilon(p)$ and their images through X cover an angle at x_i of at least ϑ_ε. Therefore amongst the remaining 6 angles at x_i spanned by successive neighbors of x_i, at least one is smaller than or equal to

$$\frac{360^\circ - \vartheta_\varepsilon}{6} = 40^\circ + O(\varepsilon),$$

contradicting Lemma A.1, and concluding the proof of Claim 6.

Claim 7: There exists $\varepsilon_5 \in (0, \varepsilon_4]$ such that for all $\varepsilon \in (0, \varepsilon_5)$ $X(\mathcal{N}_\varepsilon(p))$ contains four ε-squares.

By Claim 6, we can assume that there are three ε-squares. Up to relabeling such ε-squares are $\{x, x_1, x_2, x_3\}$, $\{x, x_3, x_4, x_5\}$, and $\{x_5, x_6, x_7, x\}$. By Lemma A.3 we have

$$\widehat{x_7 x x_1} = 90^\circ + O(\varepsilon), \tag{A.7}$$

and hence, by the law of cosines,

$$|x_7 - x_1| = \sqrt{2} + O(\varepsilon).$$

Moreover, again by the law of cosines the remaining angles $\widehat{x_7 x x_0}, \widehat{x_0 x x_1}$ also are $O(\varepsilon)$-close to 45°. By arguing as in Claim 5 one can easily get the claim.

Set $\alpha_0 := \varepsilon_5$. In view of Claim 7 and of the very definition of ε-square, (3.16) is satisfied for $\varepsilon \in [0, \alpha_0)$. We therefore define $\phi : \mathcal{N}_\varepsilon(p) \to \{-1, 0, 1\}^2$ as in (3.15) and by all the Claims above, it is easy to show that $\delta_\phi(x', x'') \le C_3 \alpha |x' - x''|$ for all $x', x'' \in \{x, x_1, ..., x_8\}$ for some constant $C_3 \in [1, \frac{1}{\alpha_0})$ (depending only on α_0). □

Notice that for $\varepsilon = 0$ the ε-squares are nothing but the unit squares. Therefore, by the same proof as for Lemma 3.5 with $\alpha = 0$ we obtain the following result.

Corollary A.4. *Let $X \in \mathcal{C}$ and let $x \in X$ have 8 neighbors in $\mathcal{G}_0(X)$, each of which has in turn 8 neighbors in $\mathcal{G}_0(X)$. Let $x_1, \dots, x_8, x_9 \equiv x_1$ be the neighbors of x ordered counterclockwise around x and let $|x_1 - x| = \min_{i=1,\dots,8} |x - x_i|$. Then, the quadrilaterals $\{x, x_1, x_2, x_3\}$, $\{x, x_3, x_4, x_5\}$, $\{x, x_5, x_6, x_7\}$, $\{x, x_7, x_8, x_9\}$ are all unit squares.*

We next pass to proving Lemma 3.8.

Proof of Lemma 3.8. Set $\alpha_0' := \varepsilon''$ where ε'' is the one given in Lemma A.3. Let $\alpha \in (0, \alpha_0']$ and let $\{p_1, p_2, p_3, p_4\}$ denote the set of vertices of $\mathcal{G}_\alpha$. By hypothesis, $\{p_i, p_j\} \in \mathcal{S}_\alpha$ for every $i, j = 1, \dots, 4$ with $i \neq j$. Then, the assumptions of Lemma A.3 are satisfied (with ε replaced by α), so that setting $x_i := X(p_i)$ for every $i = 1, \dots, 4$ and $x_{i+4} \equiv x_i$ for every $i \in \mathbb{Z}$, we deduce that, up to a relabeling, (i),(ii), and (iii) hold true. In particular, for every $\alpha \in [0, \alpha_0')$ we have

$$1 - \varepsilon \le |x_{i+1} - x_i| = 1 + O(\alpha), \qquad \sqrt{2} + O(\alpha) = |x_i - x_{i+2}| \le \sqrt{2} + \alpha. \tag{A.8}$$

Therefore, by (A.8), there exists a constant $C_3' \in [1, \frac{1}{\alpha_0'})$ (depending only on α_0') and a map $\phi : \{p_1, p_2, p_3, p_4\} \to \{0, 1\}^2$ with

$$\phi(p_1) = (0, 0), \quad \phi(p_2) = (1, 0), \quad \phi(p_3) = (1, 1), \quad \phi(p_4) = (0, 1),$$

such that $\delta_\phi(x', x'') \le C_3 \alpha |x' - x''|$ for all $x', x'' \in \{x_1, \dots, x_4\}$. As a consequence, (3.18) holds true. □

Appendix B. List of Notations

Below we produce a list of those notations used at several points in the paper which we feel would help the reader orient, together with the main equations in the paper in which those notations are introduced:

$\mathcal{E}[V](X_N)$	-	energy defined in (1.1)
$\overline{\mathcal{E}}_{\rm sq}[V]$	-	minimal energy per point of a square lattice, see (1.4)
$\mathcal{E}_4[V](x_1, x_2, x_3, x_4)$	-	energy as in (1.6) (see also Figure 1), and later also (3.20)
$E_\beta, E^1_\beta, E^2_\beta$	-	intervals of distances, see (1.7)
$W(s)$	-	(1.12), and later also (3.19)

$\mathcal{Z}_{\boxtimes}$ - combinatorial model-space from (3.10)
$\mathcal{S}_\alpha, \mathcal{G}_\alpha, \mathcal{N}_\alpha(p), \partial\mathcal{G}_\alpha$ - graph data from (3.11)
$X_1 \sim_\alpha X_2$ - α-deformation, see (3.14)
$\mathcal{X}_4(\mathbb{R}^2)/\mathrm{Isom}(\mathbb{R}^2)$ - space of 4-point configurations first appearing in (3.25)
$\mathscr{Q}_\alpha$ - small deformations of squares modulo isometry, see (3.29)
$\mathscr{S}_\alpha$ - small dilations of squares modulo isometry, see (3.30)
E_α^{sq} - square distances corresponding to E_α, and defined in (3.31)
$\mathcal{D}$ - set of distances from $\mathbb{Z}^2$, defined in (4.3)
$\mathrm{Ell}_\alpha(a,b)$ - ellipse defined in (4.2)
$\mathrm{Sides}(Q'_r), \mathrm{Sides}(\mathcal{Q}'_r), \mathrm{Diag}(Q'_r)\mathrm{Diag}(\mathcal{Q}'_r)$ - see (4.4)
$\mathrm{Sides}(Q_r), \mathrm{Sides}(\mathcal{Q}_r), \mathrm{Diag}(Q_r), \mathrm{Diag}(\mathcal{Q}_r)$ - see (4.5)
$\mathcal{L}_r$ - sublattices of $\mathbb{Z}^2$ of scale r, defined in (4.16a)
$m(r)$ - multiplicities of sublattices, defined in (4.16b)
$\widetilde{\mathcal{D}} \subset \mathcal{D}$ - the subset constructed in Lemma 4.12
$\mathcal{NQ}, \mathcal{NQ}^{(1)}, \mathcal{NQ}^{(2)}$ - sets defined in (4.26)
$\mathcal{Q}_r^b(Q_1)$ - squares of scale r intersecting Q_1, see (4.27)
$e(v,r)$ - error term as in (4.34)
$\widetilde{W}(t^2), W_*(t^2)$ - resummed interaction potentials defined in (4.36)
$\mathrm{err}_1(r,V), \mathrm{err}_2(r,V)$ - error terms from (4.44)
$\mathrm{err}_3(r,V)$ - error term from (4.49)
$\mathrm{err}_4(V,X)$ - error term from (4.56)
$V_{**}(r)$ - interaction potential defined in (4.60)

References

[1] A. Abrikosov: The Magnetic Properties of Superconducting Alloys, *Journal of Physics and Chemistry of Solids* **2** (1957), no. 3, 199–208.
[2] Y. Au Yeung, G. Friesecke, B. Schmidt: Minimizing atomic configurations of short-range pair potentials in two dimensions: crystallization in the Wulff shape, *Calc. Var. Partial Differ. Equ.* **44** (2012), no. 1-2, 81–100.
[3] L. Bétermin: Two-dimensional theta functions and crystallization among Bravais lattices, *SIAM Journal on Mathematical Analysis* **48** (2016), no. 5, 3236-3269.
[4] L. Bétermin: Local variational study of 2d lattice energies and application to Lennard-Jones type interactions, *Nonlinearity* **31** (2018), no. 9, 3973–4005.
[5] L. Bétermin: Minimizing lattice structures for Morse potential energy in two and three dimensions, *Journal of Mathematical Physics* **60** (2019), no. 10, 102901.
[6] L. Bétermin, M. Petrache: Optimal and non-optimal lattices for non-completely monotone interaction potentials, *Analysis and Mathematical Physics*, online first (2009) doi:10.1007/s13324-019-00299-6
[7] L. Bétermin, E. Sandier: Renormalized Energy and Asymptotic Expansion of Optimal Logarithmic Energy on the Sphere, *Constructive Approximation* **47** (2018), no. 1, p. 39–74.
[8] X. Blanc, C. Le Bris, A.B.H. Yedder: A numerical investigation of the 2-dimensional crystal problem, *Preprint du laboratoire J.-L. Lions, Universit de Paris 6* (2003)
[9] X. Blanc, M. Lewin: The crystallization conjecture: a review, *EMS Surv. Math. Sci.* **2** (2015), 255–306.
[10] D.P. Bourne, M.A. Peletier, F. Theil: Optimality of the triangular lattice for a particle system with Wasserstein interaction, *Comm. Math. Phys.* **329** (2014), no. 1, 117–140.
[11] C. R. Calladine: Buckminster Fuller's "Tensegrity" structures and Clerk Maxwell's rules for the construction of stiff frames, *Int. J. Solids Structures* **14** (1978), 161–172.
[12] H. Cohn, N. Elkies: New upper bounds on sphere packings. I, *Annals of Mathematics* **157** (2003), 689714.
[13] H. Cohn, A. Kumar: Universally optimal distribution of points on spheres, *Journal of the American Mathematical Society* **20** (2007), no. 1, 99–148.

[14] H. Cohn, A. Kumar, S. D. Miller, D. Radchenko, M. Viazovska: The sphere packing problem in dimension 24, *Annals of Mathematics* **185** (2017), no. 3, 1017–1033.
[15] H. Cohn, A. Kumar, S. D. Miller, D. Radchenko, M. Viazovska: Universal optimality of the E_8 and Leech lattices and interpolation formulas, *preprint* (2019) arXiv:1902:05438.
[16] E. Davoli, P. Piovano, U. Stefanelli: Sharp $N^{3/4}$ law for the minimizers of the edge-isoperimetric problem on the triangular lattice, *J. Nonlinear Sci.* **27** (2017), no. 2, 627–660.
[17] L. De Luca, G. Friesecke: Classification of particle numbers with unique Heitmann-Radin minimizer, *J. Stat. Phys.* **167** (2017), no. 6, 1586–1592.
[18] L. De Luca, G. Friesecke: Crystallization in two dimensions and a discrete Gauss-Bonnet theorem, *J. Nonlinear Sci.* **28** (2018), no. 1, 69–90.
[19] L. De Luca, M. Novaga, M. Ponsiglione: Γ-convergence of the Heitmann-Radin sticky disc energy to the crystalline perimeter, published online in *J. Nonlinear Sci.*.
[20] A.L. Dontchev, R.T. Rockafellar: *Implicit Functions and Solution Mappings*, second edition.
[21] W. E, D. Li,: On the Crystallization of 2D Hexagonal Lattices, *Communications in Mathematical Physics* **286** (2009), no. 3, 1099–1140.
[22] B. Farmer, S. Esedoglu, P. Smereka: Crystallization for a Brenner-like Potential, *Communications in Mathematical Physics* **349** (2017), no. 3, 1029–1061.
[23] L. Fejes Tóth,: Über die dichteste Kugellagerung, *Math. Z* **48** (1943), 676–684.
[24] L. Fejes Toth: Sur la representation d'une population infinie par un nombre fini d'elements, *Acta Math. Hungarica* **10** (1959), no. 3-4, 299–304.
[25] M. Friedrich, L. Kreutz: Finite crystallization and Wulff shape emergence for ionic compounds in the square lattice, arxiv.org/abs/1903.00331.
[26] G. Friesecke, R.D. James, S. Müller: A theorem on geometric rigidity and the deviation of nonlinear plate theory from three-dimensional elasticity, *Comm. Pure Appl. Math.* **55** (2002), 1461–1506.
[27] G. Friesecke, F. Theil: Validity and failure of the Cauchy-Born hypothesis in a two-dimensional mass-spring lattice, *J. Nonlinear Sci.* **12** (2002), 445-478.
[28] A. Hales 3d crystallization.
[29] H. Harborth: Lösung zu Problem 664A, *Elem. Math.* **29** (1974), 14–15.
[30] G. H. Hardy, E. M. Wright: An introduction to the theory of numbers. (1968) Oxford university press.
[31] R. C. Heitmann, C. Radin: The ground state for sticky disks, *J. Stat. Phys.* **22** (1980), no. 3, 281–287.
[32] P.M. Gruber: In many cases optimal configurations are almost regular hexagonal, *Rend. Mat. Palermo* **2** (2000), Suppl. 65, 121–145.
[33] I. Izmestiev:Statics and kinematics of frameworks in Euclidean and non-Euclidean geometry, arXiv preprint arXiv:1707.02172 (2017).
[34] F. John: Rotation and strain, *Comm. Pure Appl. Math.* **14** (1961), 391–413.
[35] R. Kershner: The number of circles covering a set. *Amer. J. Math.* **61** (1939), no. 3, 665–671.
[36] S. Luo, X. Ren, J. Wei: Non-hexagonal lattices from a two species interacting system, *preprint* (2019), arXiv:1902:09611.
[37] E. Mainini, P. Piovano, U. Stefanelli: Finite crystallization in the square lattice, *Nonlinearity* **27** (2014), no. 4, 717–737.
[38] É. Marcotte, F.H. Stillinger, S. Torquato: Unusual ground states via monotonic convex pair potentials, *The Journal of Chemical Physics* **134** (2011), 164105.
[39] J. C. Maxwell: L. on the calculation of the equilibrium and stiffness of frames, *The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science* **27** (1864) no. 182, 294–299.
[40] M. Petrache, S. Serfaty: Next-order asymptotics and renormalized energy for Riesz interactions, *Journ. Inst. Math. Jussieu* **16** (2017), no. 3, 501–569.
[41] M. Petrache, S. Serfaty: Crystallization for Coulomb and Riesz Interactions as a Consequence of the Cohn-Kumar Conjecture, arxiv.org/abs/1908.09714
[42] M. Petrache, to appear.
[43] C. Radin: The ground states for soft disks, *J. Stat. Phys.* **26** (1981), no. 2, 365–373.
[44] M.C. Rechtsman, F.H. Stillinger, S. Torquato: Self-assembly of the simple cubic lattice with an isotropic potential, *Physical Review E* **74** (2006), 021404.
[45] N. Rougerie, S. Serfaty: HigherDimensional Coulomb Gases and Renormalized Energy Functionals, *Communications on Pure and Applied Mathematics* **69** (2016), no. 3, 519–605

[46] E. Sandier, S. Serfaty: From the Ginzburg-Landau Model to Vortex Lattice Problems, *Communications in Mathematical Physics* **313** (2012), no. 3, 635–743.
[47] B. Schmidt: Ground states of the 2D sticky disk model: fine properties and $N^{3/4}$ law for the deviation from the asymptotic Wulff shape, *J. Stat. Phys.* **153** (2013), no. 4, 727–738.
[48] F. Theil: A proof of crystallization in two dimensions, *Comm. Math. Phys.* **262** (2006), no. 1, 209–236.
[49] M.S. Viazovska: The sphere packing problem in dimension 8, *Annals of Mathematics* **185** (2017), no. 3, 991–1015.

Faculty of Mathematics, University of Vienna, Oskar-Morgenstern-Platz 1, 1090 Vienna, Austria
Email address: laurent.betermin@univie.ac.at

Dipartimento di Matematica, Università di Pisa, Largo Bruno Pontecorvo 5, 56127 Pisa, Italy
Email address: lucia.deluca@unipi.it

PUC Chile, Facultad de Matemáticas, Av. Vicuna Mackenna 4860, 6904441, Santiago, Chile
Email address: decostruttivismo@gmail.com