Max-Planck-Institut
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On a mesoscopic many-body Hamiltonian describing elastic shears and dislocations

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by

Stephan Luckhaus, and Luca Mugnai

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ON A MESOSCOPIC MANY-BODY HAMILTONIAN DESCRIBING ELASTIC SHEARS AND DISLOCATIONS

STEPHAN LUCKHAUS AND LUCA MUGNAI

Abstract. We define a "reference-free" many-body Hamiltonian acting on finite systems of particles, and study some properties of "low-energy" states. More precisely we show that "low-energy" states are locally well described (on a mesoscale) by appropriate affine transformations of a ground state lattice. Moreover we use such (local) description to define an "holonomy representation map" and a consequent notion of topological defect.

1. Introduction

The purpose of this paper is to present a "mesoscopic" many-body interaction potential acting on finite systems of particles (a Hamiltonian in the language of statistical mechanics and of this paper) that is able to describe deformed crystals with defects. In principle such a Hamiltonian should be derived from the ground state energy of the electronic Schrödinger operator in the Born-Oppenheimer approximation. This is far too ambitious for this paper. Instead we start from the assumption that low-energy states are given by approximately linear deformations of a ground state lattice, and construct a Hamiltonian that, given a finite particle configuration, measures the shear and the deviations from the linearly sheared lattice in a mesoscopic interaction range.

In order to describe the construction of the Hamiltonian we need to introduce some notation. We assume that the ground state lattice is given by a simple Bravais lattice $\mathcal{L}_G := \{Gz : \ z \in \mathbb{Z}^d\}$, where G belongs to the space $GL^+(d,\mathbb{R})$ of the $d \times d$ matrices with positive determinant. With Ω we denote an open, connected, bounded, subset of $\mathbb{R}^d$ ($d \leq 3$), with $\mathcal{X} := \{x_i\}_{i\in I} \subset \Omega$ we denote a finite subset whose elements represent the positions of the particles of a given configuration and with $B(x, R)$ we denote the ball of center x and radius $R > 0$.

We define the Hamiltonian in two steps. In the first step we define an "energy density" which depends on the point $x \in \Omega$ (in the Eulerian space), an auxiliary variable represented by an affine deformation, and the particle configuration $\mathcal{X}$ in a finite (range) neighborhood of x of size $\lambda << L$ ($L > 0$ being the diameter of Ω). In the second step we minimize the "energy-density" with respect to the affine deformation, and integrate it over the Eulerian coordinate $x \in \Omega$. As a result we obtain a Hamiltonian which depends only on the particle configuration $\mathcal{X}$ and, in our case, is invariant with respect to rigid motions and permutations acting on $\mathcal{X}$.

Let us describe in more detail how the Hamiltonian is constructed. For a point $x \in \Omega$, an affine deformation $(A, \tau) \in GL^+(d,\mathbb{R}) \times \mathbb{R}^d$ and a finite particle configuration $\mathcal{X}$ in Ω, the value of our "energy-density" $h_\lambda(x,(A,\tau),\mathcal{X})$ is given by the sum of the "distance" of $\mathcal{X} \cap B(x, \lambda)$ from the Bravais lattice $\mathcal{L}_x(A, \tau) := \{A(z-\tau)+x : z \in \mathbb{Z}^d\}$, plus the (elastic) energy cost of a linear deformation transforming the ground state lattice $\mathcal{L}(G)$ into the lattice $\mathcal{L}(A) := \{Az : z \in \mathbb{Z}^d\}$. More precisely $h_\lambda(x,(A,\tau),\mathcal{X})$ is given by the sum of three terms:

(i) The first term is obtained assigning a value to the linearly deformed ground state lattice $\mathcal{L}(A)$;

(ii) The second term is obtained assigning an excess-energy for each individual particle $x_i \in \mathcal{X}$ through a periodic potential, which has the periodicity of the lattice $\mathcal{L}_x(A,\tau)$, and which can be thought of as a one-particle potential in an otherwise periodic lattice, multiplied with a cut-off function of finite mass to ensure a finite interaction range;

(iii) The third and last term penalizes the presence in $\mathcal{X} \cap B(x,\lambda)$ of (suitably defined) "vacancies" with respect to $\mathcal{L}_x(A,\tau)$ by measuring the difference between the determinant of the inverse of A and the empirical density of $\mathcal{X}$ in x.

The sum of the second and third term measures the "distance" of $\mathcal{L}_x(A,\tau)$ from $\mathcal{X} \cap B(x,\lambda)$. In fact, roughly speaking, term (ii) measures the "mean" deviation of the $x_i \in \mathcal{X} \cap B(x,\lambda)$ from the lattice sites of $\mathcal{L}_x(A,\tau)$. However this term alone is not sufficient to estimate how "near" $\mathcal{L}_x(A,\tau)$ is to $\mathcal{X} \cap B(x,\lambda)$. Indeed term (ii) assumes a small value also on those lattices $\mathcal{L}_x(A,\tau)$ such that the points of $\mathcal{L}_x(A,\tau) \cap B(x,\lambda)$ are many more than the elements of $\mathcal{X} \cap B(x,\lambda)$, but these sit very near to $\mathcal{L}_x(A,\tau)$. For this reason we also have to add term (iii), which approximately measures the difference between the number of points of $\mathcal{L}_x(A,\tau) \cap B(x,\lambda)$ divided by the volume of $B(x,\lambda)$ and the "empirical density of $\mathcal{X}$ in the point x", that is the number of elements of $\mathcal{X} \cap B(x,\lambda)$ divided by the volume of $B(x,\lambda)$.

We now come to the second step of our construction and define the Hamiltonian

$$H_\lambda(\mathcal{X},\Omega) := \int_\Omega \Big[\inf_{\mathcal{A} \in GL^+(d,\mathbb{R}) \times \mathbb{R}^d} h_\lambda(x,\mathcal{A},\mathcal{X}) \Big]\, dx.$$

In view of the above description of $h_\lambda(x,(A,\tau),\mathcal{X})$, we can say that minimization of $h_\lambda(x,\mathcal{A},\mathcal{X})$ with respect to $\mathcal{A}$ is approximately the same as identifying the simple Bravais lattice optimally fitted with $\mathcal{X} \cap B(x,\lambda)$, and then calculating its elastic energy plus the cost of the deviation of $\mathcal{X} \cap B(x,\lambda)$ from this lattice. We can thus expect that a simple Bravais lattice (nearly) optimally fitted with $\mathcal{X} \cap B(x,\lambda)$ represents a good (local) description of $\mathcal{X}$ only when the value of the "energy-density" is small. That is, only for "low-energy states" we can expect the Hamiltonian to give a realistic picture.

In order to discuss the relation between measurable quantities and the Hamiltonian $H_\lambda(\mathcal{X},\Omega)$, we need to introduce the mathematical definition of the terms involved in its construction. The analytical expression of term (i) is given by a function $F \in C^2(GL^+(d,\mathbb{R}))$ such that

- $F(A) \geq 0$ for every $A \in GL^+(d,\mathbb{R})$;
- F is frame-indifferent, that is $F(RA) = F(A)$ for every rotation R of $\mathbb{R}^d$;
- F is invaraint with respect to (positive) changes of the lattice-basis of $\mathcal{L}(A)$, that is $F(A) = F(AB)$ for every $B \in \mathbb{Z}^{d\times d}$ such that $\det B = 1$;
- the function F takes its minimum on the ground state lattice $\mathcal{L}_G$, more precisely we require that

$$F(M) = 0 \iff \mathcal{L}(M) = \mathcal{L}(G).$$

The analytical expression of the second term, the one described in (ii) above, is

$$\frac{1}{\lambda^d}\sum_{x_i\in I}\Big[W\big(x_i,\,\mathcal{L}_x(A,\tau)\big)-\vartheta_0\Big]\varphi_{\lambda,x}(x_i),$$

where: for fixed $x \in \Omega$ and $(A,\tau) \in GL^+(d,\mathbb{R}) \times \mathbb{R}^d$, the map $W(\cdot,\mathcal{L}_x(A,\tau)) \in C^0(\mathbb{R}^d)$ behaves similarly to the squared distance function from the lattice $\mathcal{L}_x(A,\tau)$; $\vartheta_0 > 0$ is a positive constant; and $\varphi_{\lambda,x}(\cdot) \in C^\infty(\mathbb{R}^d,[0,1])$ is a cut-off function supported in the ball of radius 2λ centered at x, with finite mass (independent of x). The last term, the one corresponding to (iii), is given by

$$\vartheta_1\left(\frac{1}{\det A}-\frac{1}{C_\varphi\,\lambda^d}\sum_{x_i\in X}\varphi_{\lambda,x}(x_i)\right),$$

where $\vartheta_1 > 0$ is a constant, and C_φ is a renormalizing factor depending on the mass of the cut-off function $\varphi_{\lambda,x}$.

Finally we can define the energy density at a point x, depending still on the auxiliary variable represented by the affine deformation $\mathcal{A} = (A,\tau) \in GL^+(d,\mathbb{R}) \times \mathbb{R}^d$, by

$$\begin{aligned}h_\lambda(x,\mathcal{A},X) :=&F(A)+\frac{1}{\lambda^d}\sum_{x_i\in I}\Big[W\big(x_i,\,\mathcal{L}_x(A,\tau)\big)-\vartheta_0\Big]\varphi_{\lambda,x}(x_i)\\&+\vartheta_1\left(\frac{1}{\det A}-\frac{1}{C_\varphi\,\lambda^d}\sum_{x_i\in X}\varphi_{\lambda,x}(x_i)\right).\end{aligned}$$

As we already said $W(\cdot,\mathcal{L}_x(A,\tau))$ has the period of the affinely deformed ground-state lattice $\mathcal{L}_x(A,\tau)$. We think of $D^2_{yy}W(0,\mathcal{L}_x(A,\tau))$ as the quadratic-form describing independent deviations of particles from the lattice position. The meaning of $-\vartheta_0$ is that of the energy per particle in the ground state, ϑ_1 is the cost of a vacancy, and $F(A)$ the energy-cost of a linear deformation of the ground state lattice. Note that the third term can be incorporated in the first two, but its meaning is that of measuring the presence in $X \cap B(x,\lambda)$ of vacancies with respect to $\mathcal{L}_x(A,\tau)$.

In this paper we consider low-energy configurations with an additional hard-core constraint. The result we are able to present says that such configurations are characterized by a large set of low energy-density whose connected components we call "grains". On each open, simply connected subset U of a grain we show the existence of a family of maps $\{\mathcal{A}_\mathcal{B}(\cdot)\}_\mathcal{B} = \{(A_\mathcal{B}(\cdot),\tau_\mathcal{B}(\cdot))\}_\mathcal{B} \in C^1(U, GL^+(d,\mathbb{R})\times\mathbb{R}^d)$, indexed by $\mathcal{B} \in GL^+(d,\mathbb{Z}) \times \mathbb{Z}^d$ (that is the set of affine maps mapping a simple Bravais lattice onto itself), with the following properties. For every $x \in U$ we have

$$\mathcal{L}_x(\mathcal{A}_\mathcal{B}(x)) = \mathcal{L}_x(\mathcal{A}_{\mathcal{B}'}(x)), \quad \forall \mathcal{B},\, \mathcal{B}' \in GL^+(d,\mathbb{Z}) \times \mathbb{Z}^d, \tag{1.1}$$

$$h_\lambda(x,\mathcal{A}_\mathcal{B}(x),X) = \inf_{\mathcal{A}\in GL^+(d,\mathbb{R})\times\mathbb{R}^d} h_\lambda(x,\mathcal{A},X), \tag{1.2}$$

that is $\mathcal{L}_x(\mathcal{A}_\mathcal{B}(x))$ is the unique simple Bravais lattice optimally fitted with $X \cap B(x,\lambda)$. Moreover for every $\mathcal{B},\mathcal{B}' \in GL^+(d,\mathbb{Z}) \times \mathbb{Z}^d$ we have

$$[\mathcal{A}_\mathcal{B}(\cdot)]^{-1} \circ \mathcal{A}_{\mathcal{B}'}(\cdot) = \widetilde{\mathcal{B}} \in GL^+(d,\mathbb{Z}) \times \mathbb{Z}^d \tag{1.3}$$

and

$$\lambda\|\nabla A_\mathcal{B}(\cdot)\|_{L^\infty(U)} + \|\nabla\tau_\mathcal{B}(\cdot) - A^{-1}_\mathcal{B}(\cdot)\|_{L^\infty(U)} \le \frac{C^\mathcal{B}_\nabla}{\lambda}, \tag{1.4}$$

where $C^{\mathcal{B}}_{\nabla} > 0$ is a constant which is proportional to the "small" value of the energy-density in U. We can think of the shift part of the affine deformation $\tau_{\mathcal{B}}$ as a transformation from Eulerian to Lagrangian coordinates, while we can think of its inverse as the (local) deformation which is defined only up to the period of the lattice (e.g. the flat torus). Moreover, by (1.4) we can think of $A_{\mathcal{B}}(\cdot)$ as an approximation of $\nabla\tau_{\mathcal{B}}^{-1}(\cdot)$, that is the gradient of the local deformation.

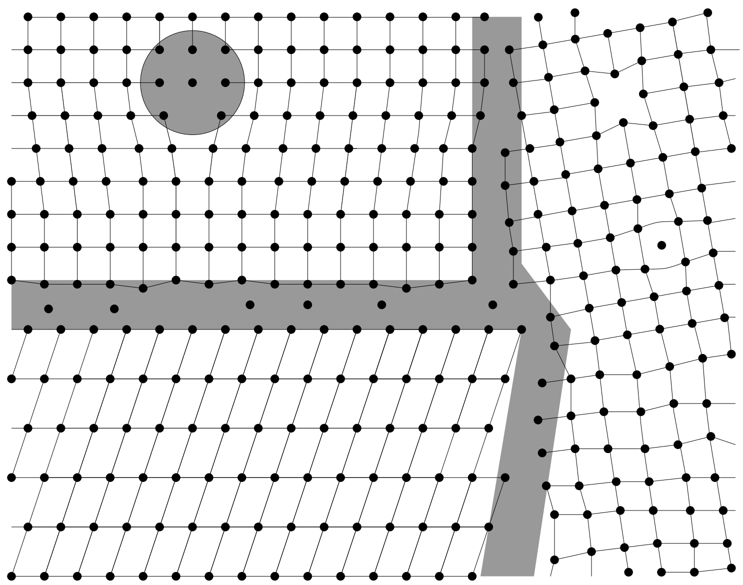

FIGURE 1. A schematic picture of a low-energy configuration. Three grains are separated by the shaded region, corresponding to the set where the energy density is "high". The particles in the grain on the bottom left are arranged to form a defect free, linearly sheared ground state lattice. The particles in the grain on the right correspond to a (non-linear) elastically deformed ground state lattice. Here two point-defects (a vacancy and an interstitial) are present. Finally the grain on the top left side is not simply-connected and contains a dislocation, whose core corresponds to the shaded disk in the grain.

In order to detect the presence of dislocations in a grain we also define an "holonomy representation map" which depends on the topology of the grain and the behavior of $\{\mathcal{A}_{\mathcal{B}}(\cdot)\}_{\mathcal{B}}$ on the whole of the grain. In fact in general a grain needs not to be simply connected, and when this is the case it can happen that the maps $\{\mathcal{A}_{\mathcal{B}}(\cdot)\}_{\mathcal{B}}$ are not globally continuous on the whole of the grain. More precisely, let $\gamma \in C^0([0,1],\Omega)$ be a, simple, closed loop whose support (γ) lies in the interior of the grain, and it is nontrivial, that is γ is not homotopically equivalent (in the grain) to a constant. We can construct a simply connected subset U of the grain such that $U \supset [(\gamma) \setminus \{x_0\}]$ (where $x_0 := \gamma(0) = \gamma(1)$) removing a disc-like surface from a neighborhood of (γ). Hence, by the results discussed above we can prove that $\{\mathcal{A}_{\mathcal{B}}(\gamma(\cdot))\}_{\mathcal{B}} \subset C^0((0,1),\Omega)$, that is every $\mathcal{A}_{\mathcal{B}}(\cdot)$ is continuous on the support of the loop γ once the point x_0 is removed. Moreover we can also prove that, setting

$\mathcal{A}_{\mathcal{B}}^- = \lim_{s\to 0} \mathcal{A}_{\mathcal{B}}(\gamma(s))$, $\mathcal{A}_{\mathcal{B}}^+ = \lim_{s\to 1} \mathcal{A}_{\mathcal{B}}(\gamma(s))$, both $\mathcal{A}_{\mathcal{B}}^-$ and $\mathcal{A}_{\mathcal{B}}^+$ satisfy (1.1), (1.2) with $x = x_0$. Nevertheless we can have $\mathcal{A}_{\mathcal{B}}^- \neq \mathcal{A}_{\mathcal{B}}^+$. If this is the case, it follows from (1.3) and (1.1) that for every $\mathcal{B} \in GL^+(d,\mathbb{Z})\times\mathbb{Z}^d$ we can find a "transition element" $\widehat{\mathcal{B}}_{\mathcal{B}} \in GL^+(d,\mathbb{Z}) \times \mathbb{Z}^d$ such that $[\mathcal{A}_{\mathcal{B}}^-]^{-1} \circ \mathcal{A}_{\mathcal{B}}^+ = \widehat{\mathcal{B}}_{\mathcal{B}}$. When the matrix component of the transition element $\widehat{\mathcal{B}}_{\mathcal{B}}$ is the identity, the jump in the translation component between $\mathcal{A}_{\mathcal{B}}^-$ and $\mathcal{A}_{\mathcal{B}}^+$ defines a vector (independent of $\mathcal{B}$) in the lattice $\mathcal{L}_{x_0}(\mathcal{A}_{\mathcal{B}}^+)$. This we call the Burgers vector associated with a dislocation. If one wants to be more precise in algebraic terms in this theory a dislocation structure in a grain is a homeomorphism from the homothopy group of the grain into $GL^+(d,\mathbb{Z}) \times \mathbb{Z}^d$, only it turns out that a nontrivial component in $GL^+(d,Z)$ is much more costly in energy than one in $\mathbb{Z}^d$ (the Burgers vector).

Note that much of the final description is very similar to the one given in a rational mechanics context by Kondo [7] and Kröner [8] (see also [3, 4, 5] and references therein). The point of this paper is to make the connection with a Hamiltonian depending only on particle configurations. In the end this should be a starting point for a non-equilibrium statistical mechanics theory. But that is work for the future.

The plan of the paper is the following. In Section 2 we introduce some notation. In Section 3 we study the behavior of $H_\lambda(\mathcal{X}_L, \Omega_L)$, when Ω_L is a family of sets of diameter L invading $\mathbb{R}^d$ as $\lambda \to \infty$ ($L >> \lambda^2$), and $\mathcal{X}_L$ is obtained via a smooth deformation of a portion of the ground state. In Section 4 we collect the statements of our main results. In Section 5 we prove the preliminary lemmata and propositions we need in the proofs of the main results, which are presented in Sections 6-8. In Section 9 we define an holonomy representation map and discuss how such map can be used to describe dislocations in our setting. Finally in Appendix A we exihibit a function $W \in C^0(\mathbb{R}^d \times \mathbb{R}^{d\times d} \times \mathbb{R}^d)$ fulfilling the assumptions we make in the definition of our many-body Hamiltonian.

2. Notation

2.1. **General Notation.** Throughout the paper we adopt the following notation. By Ω we denote an open, bounded, connected subset of $\mathbb{R}^d$ ($d = 2, 3$) with Lipschitz boundary, and by $\mathcal{X} = \{x_i\}_{i\in I} \subset \{y \in \mathbb{R}^d : \ \mathrm{dist}(y,\Omega) \le 2\lambda\}$ a finite subset of points. However, with a small abuse of notation, we will often write $\mathcal{X} \subset \Omega$.
By $B(x,r)$ we denote the Euclidean ball of radius r centered in y. By $\mathbb{Z}^d$ we denote the set of points of $\mathbb{R}^d$ with integer coordinates. Given $z_k \in \mathbb{Z}^d$ we set

$$Q(z_k) := \{z_k + v : \ v \in [0,1)^d\}.$$

For every $y \in \mathbb{R}^d$ we define

$$[y]_{\mathbb{Z}^d} := z_k \in \mathbb{Z}^d \quad \text{such that } y \in Q(z_k),$$
$$\{y\}_{\mathbb{Z}^d} := y - [y]_{\mathbb{Z}^d} \in Q(0).$$

Throughout the paper we consider the following spaces and sets

$$GL^+(d,\mathbb{R}) := \left\{M \in \mathbb{R}^{d\times d} : \det M > 0\right\}, \quad \mathit{Aff}^+(\mathbb{R}^d) := \left\{\mathcal{M} = (M,\mu) \in GL^+(d,\mathbb{R}) \times \mathbb{R}^d\right\},$$
$$GL^+(d,\mathbb{Z}) := \left\{B \in \mathbb{Z}^{d\times d} : \det B = 1\right\}, \quad \mathit{Aff}^+(\mathbb{Z}^d) := \left\{\mathcal{B} = (B,b) \in GL^+(d,\mathbb{Z}) \times \mathbb{Z}^d\right\}.$$

Given $M = (m_{ij})_{1\le i,j\le d} \in \mathbb{R}^{d\times d}$ we define

$$|M| := \sqrt{\sum_{i=1}^{d}\sum_{j=1}^{d}(m_{ij})^2},$$
$$\|M\|_* := \sup\{|Mv| : v \in \mathbb{R}^d,\ |v| = 1\}.$$

We often equip the space $\mathit{Aff}^+(\mathbb{R}^d)$ with the norm $\|\cdot\|_\lambda$ defined by

$$\|\mathcal{M}\|_\lambda := \sqrt{\|M\|_*^2\lambda^2 + |\mu|^2}, \tag{2.1}$$

and we set

$$\mathfrak{B}_\lambda(\mathcal{M}, r) := \{\mathcal{N} \in \mathit{Aff}^+(\mathbb{R}^d) : \|\mathcal{N} - \mathcal{M}\|_\lambda < r\}, \quad r > 0. \tag{2.2}$$

Given $x \in \Omega$ we define

$$\mathit{Aff}^+_\triangleright(\mathbb{R}^d_x) := \{(A, x - A\tau) :\ A \in GL^+(d,\mathbb{R}),\ \tau \in \mathbb{R}^d\} \subset \mathit{Aff}^+(\mathbb{R}^d).$$

Let us remark that, for every fixed $x \in \Omega$, $\mathit{Aff}^+_\triangleright(\mathbb{R}^d_x)$ is isomorphic to the semidirect product $GL^+(d,\mathbb{R}) \triangleright \mathbb{R}^d$.
With a small abuse of notation, when no confusion may arise we denote by $\mathcal{A} = (A,\tau) \in \mathit{Aff}^+_\triangleright(\mathbb{R}^d_x)$ the element $(A, x - A\tau) \in \mathit{Aff}^+(\mathbb{R}^d)$ and by $\mathfrak{B}_\lambda(\mathcal{A}, r) \subset \mathit{Aff}^+_\triangleright(\mathbb{R}^d_x)$ we mean $\mathfrak{B}_\lambda\big((A, x - A\tau), r\big) \subset \mathit{Aff}^+(\mathbb{R}^d)$.

2.2. **Notation and Preliminaries on Simple Bravais Lattices.** In the present section we fix some notation and recall some terminology and results concerning simple Bravais lattices in $\mathbb{R}^d$ $(d = 2, 3)$.

Let $M \in GL^+(d,\mathbb{R})$. We define the Bravais lattice generated by M to be the discrete subset $\mathcal{L}(M)$ of $\mathbb{R}^d$ defined by

$$\mathcal{L}(M) := \{y \in \mathbb{R}^d : y = Mz_k \text{ for some } z_k \in \mathbb{Z}^d\}. \tag{2.3}$$

Notice that $\mathcal{L}(M) = \mathcal{L}(MB)$ for every $B \in GL(d,\mathbb{Z})$. Moreover if $\mathcal{L}(M') = \mathcal{L}(M)$ for some $M' \in GL^+(d,\mathbb{R})$, then we can find $B \in GL^+(d,\mathbb{Z})$ such that $MB = M'$.

Given $a_1, \dots, a_d \in \mathcal{L}(M)$, linearly independent vectors, we say that $a_1, \dots, a_d$ are a lattice basis for $\mathcal{L}(M)$ if and only if

$$\mathcal{L}(M) = \Big\{\sum_{j=1}^{d} \zeta_j a_j : \zeta_j \in \mathbb{Z}\Big\}.$$

In particular a basis for the lattice $\mathcal{L}(M)$ is given by the d raws of the matrix M.

Let $\{a_1, \dots, a_d\}$ and $\{a'_1, \dots, a'_d\}$ be two lattice bases of the same Bravais lattice. Denote by M (respectively M') the matrix whose raws are given by the $\underline{a}_j$ (respectively the $\underline{a}'_j$), and let $B \in GL(d,\mathbb{Z})$ be the unique matrix such that

$$M = M'B. \tag{2.4}$$

We say that the bases $a_1, \dots, a_d$ and $a'_1, \dots, a'_d$ have the *same orientation* if the matrix B satisfying (2.4) is such that $B \in GL^+(d,\mathbb{Z})$, that is $\det B = 1$. Moreover we say that a lattice basis $a_1, \dots, a_d$ is *positively oriented* if it has the same orientation as the lattice basis associated with the matrix M.

Next we recall a result concerning the existence of a particular basis for a given lattice $\mathcal{L}(M)$ (see [6, Theorem 4.2, Theorem 4.3]).

Theorem 2.1. *Let $\mathcal{L}(M)$ be a simple Bravais lattice in $\mathbb{R}^d$. The d shortest and linearly independent lattice vectors form a lattice basis.*

We call a lattice basis made of d shortest linearly independent vectors a *reduced lattice basis*. As a consequence of the results in [6, Section 4.2, Section 4.3], we can conclude the existence of a positively oriented reduced basis. More precisely we have the following

Proposition 2.2. *Let $\mathcal{L}(M)$ be a simple Bravais lattice in $\mathbb{R}^d$. There exists a positively oriented reduced lattice basis $a_1, \dots, a_d$ such that*

- *if $d = 2$ then*
$$2|\langle a_1, a_2\rangle| \le |a_1|^2 \le |a_2|^2. \tag{2.5}$$
- *if $d = 3$ then*
$$\begin{aligned} &|a_1|^2 \le |a_2|^2 \le |a_3|^2,\\ &2|\langle a_i, a_j\rangle| \le |a_i|^2, \quad \textit{for } 1 \le i < j \le 3. \end{aligned} \tag{2.6}$$

Remark 2.3. Since positively oriented lattice bases of $\mathcal{L}(M)$ are in one-to-one correspondence with the elements of $GL^+(d,\mathbb{Z})$, by Proposition 2.2 we obtain the existence of $B_M \in GL^+(d,\mathbb{Z})$ such that MB_M is the matrix associated with a reduced positively oriented lattice basis satisfying (2.5) if $d = 2$ (respectively (2.6) if $d = 3$). Moreover, since the elements of a reduced lattice basis are the d shortest linearly independent lattice vectors, we can conclude that
$$|MB_M| = \min\{|MB| : \, B \in GL^+(d,\mathbb{Z})\}. \tag{2.7}$$

Let $a_1, \dots, a_d$ be a reduced positively oriented lattice basis for the simple Bravais lattice $\mathcal{L}(M)$, and suppose $a_1, \dots, a_d$ satisfies (2.5) (respectively (2.6)) if $d = 2$ (respectively if $d = 3$). We define
$$\mathcal{m}_0(\mathcal{L}(M)) := |a_1|, \quad \mathcal{m}_1(\mathcal{L}(M)) := |a_d|. \tag{2.8}$$
By definition of reduced lattice basis we also have
$$\mathcal{m}_0(\mathcal{L}(M)) = \min\{|M(z_l)| : \, z_l \neq 0, \, z_l \in \mathbb{Z}^d\}.$$

As a further consequence of (2.5), (2.6),denoting by α_{ij} the angle between a_i and a_j, we have
$$|\langle a_i, a_j\rangle| = |a_i|\,|a_j||\cos(\alpha_{ij})| \le \frac{|a_i|^2}{2} \le \frac{|a_i|\,|a_j|}{2},$$
that is $\alpha_{ij} \in [-\arccos(1/2), \arccos(1/2)]$ for every $1 \le i \neq j \le d$. This fact implies the existence of a positive constant C_d depending only on the dimension such that, denoting by $B_M \in GL^+(d,\mathbb{Z})$ the matrix defined in Remark 2.3, we have
$$|MB_M e_1| \dots |MB_M e_d| = |a_1| \dots |a_d| \le C_d \det M, \tag{2.9}$$
where the e_i are the elements of the canonical basis of $\mathbb{R}^d$.

For a given $x \in \Omega$ and $\mathcal{A} = (A, \tau) \in \mathit{Aff}^+_{\triangleright}(\mathbb{R}^d_x)$, by $\mathcal{L}_x(\mathcal{A})$ we denote *the (simple) Bravais lattice generated by the affine map associated to $\mathcal{A}$*, that is
$$\mathcal{L}_x(\mathcal{A}) := \{y \in \mathbb{R}^d : \, y = A(z_k - \tau) + x \text{ for some } z_k \in \mathbb{Z}^d\}.$$
Hence $\mathcal{L}_x(\mathcal{A}) = \mathcal{L}(A) + (x - A\tau)$, where $\mathcal{L}(A)$ is the simple Bravais lattice generated by A. We define $0 < \mathcal{m}_0(\mathcal{L}_x(\mathcal{A})) := \mathcal{m}_0(\mathcal{L}(A)) \le \mathcal{m}_1(\mathcal{L}_x(\mathcal{A})) := \mathcal{m}_1(\mathcal{L}(A))$, where $\mathcal{m}_0(\mathcal{L}(A))$ and $\mathcal{m}_1(\mathcal{L}(A))$ are as in (2.8). Eventually we remark that $\mathcal{L}_x(\mathcal{A}) = \mathcal{L}_x(\widetilde{\mathcal{A}})$

if and only if there exists $\mathcal{B} := (B, b) \in \mathit{Aff}^+(\mathbb{Z}^d)$ such that $(\widetilde{A}, x - \widetilde{A}\widetilde{\tau}) = (AB, x - AB(B^{-1}\tau + b))$, and we define

$$[\![\mathcal{A}]\!]_{\mathit{Aff}^+(\mathbb{Z}^d)} := \{(AB, x - AB(B^{-1}\tau + b)) : (B, b) \in \mathit{Aff}^+(\mathbb{Z}^d)\} \subset \mathit{Aff}^+_{\triangleright}(\mathbb{R}^d_x).$$

Let $\mathcal{A} = (A, \tau) \in \mathit{Aff}^+_{\triangleright}(\mathbb{R}^d_x)$, $B \in \mathit{Aff}^+(\mathbb{Z}^d)$ and $\tau_0 \in \mathbb{R}^d$ be such that

(i) $A_0 := AB$ is associated with a reduced, positively oriented lattice basis of $\mathcal{L}(A)$ fulfilling Proposition 2.2;
(ii) $\tau_0 := \{B^{-1}\tau\}_{\mathbb{Z}^d}$ (so that $|\tau_0| < \sqrt{d}$).

Then

$$(A_0, x - A_0\tau_0) = (AB, x - AB(B^{-1}\tau - [B^{-1}\tau]_{\mathbb{Z}^d})) \in [\![\mathcal{A}]\!]_{\mathit{Aff}^+(\mathbb{Z}^d)},$$

and hence $\mathcal{L}_x(\mathcal{A}) = \mathcal{L}_x(\mathcal{A}_0)$. Whenever $\mathcal{A}_0 = (A_0, \tau_0) \in [\![\mathcal{A}]\!]_{\mathit{Aff}^+(\mathbb{Z}^d)}$ satisfies conditions (i)-(ii) above we call it a *canonical representation for* $\mathcal{L}_x(\mathcal{A})$. Let us notice that canonical representations are not unique.

2.3. **Further notation and definition of the Hamiltonian $H_\lambda(\mathcal{X}, \Omega)$.** Next we specify the notation we need to define our many-body Hamiltonian.

The ground state: We assume that a stress-, strain-, defect-free configuration is given by a ground state lattice, that we suppose to be a simple Bravais lattice $\mathcal{L}(G) \subset \mathbb{R}^d$, for some $G \in GL^+(d, \mathbb{R})$.

The cut-off function φ: We choose $\varphi \in C^\infty(\mathbb{R}, [0,1])$ such that $\varphi(s) \equiv 0$ if $s \geq 2$, $\varphi(s) \equiv 1$ if $s \leq 1$ and $\varphi' \leq 0$ on $\mathbb{R}$. We then define

$$\varphi_{\lambda,x}(y) := \varphi\left(\frac{|y - x|}{\lambda}\right), \forall x, y \in \Omega, \quad C_\varphi := \int_{\mathbb{R}^d} \varphi(|y|)\, dy. \tag{2.10}$$

The hard-core potential V: By $V : [0, +\infty) \to \{0, +\infty\}$ we denote the function

$$V(s) := \begin{cases} 0 & \text{if } s \in (s_0, +\infty) \\ +\infty & \text{if } s \in [0, s_0] \end{cases}, \tag{2.11}$$

where $\frac{s_0}{2} < \frac{m_0(\mathcal{L}(G))}{2}$.

The periodic potential W: By $W \in C^0(\mathbb{R}^d \times \mathit{Aff}^+(\mathbb{R}^d))$ we denote a function such that

(P1) there exist $0 < C_{W,0} \leq C_{W,1}$ such that, for every $y \in \mathbb{R}^d$ and $\mathcal{M} \in \mathit{Aff}^+(\mathbb{R}^d)$, we have

$$C_{W,0} \operatorname{dist}^2(y, \mathcal{L}(\mathcal{M})) \leq W(y, \mathcal{M}) \leq C_{W,1} \operatorname{dist}^2(y, \mathcal{L}(\mathcal{M})); \tag{2.12}$$

(P2) for every $v \in \mathbb{R}^d$ and $\mathcal{M} = (M, \mu) \in \mathit{Aff}^+(\mathbb{R}^d)$ we have

$$W(v, (M, \mu)) = W(v, (MB, \mu + Mb)), \quad \forall \mathcal{B} = (B, b) \in \mathit{Aff}^+(\mathbb{Z}^d); \tag{2.13}$$

$$W(v, (M, \mu)) = W(v - \mu, (M, 0)). \tag{2.14}$$

(P3) there exists $0 < \overline{m_0} < \overline{m_1}$ verifying

$$\frac{s_0}{2}, \frac{s_0^d(2C_\varphi - 1)}{2^{(d+1)}(\overline{m_1})^{(d-1)}} \in (\overline{m_0}, \overline{m_1}), \tag{2.15}$$

(s_0 being the hard-core threshold defined above) such that $W \in C^2(\mathbb{R}^d \times \mathcal{E})$, where

$$\mathcal{E} := \{\mathcal{M} \in \mathit{Aff}^+(\mathbb{R}^d) : \ \overline{m_0} < m_0(\mathcal{L}(\mathcal{M})) \leq m_1(\mathcal{L}(\mathcal{M})) < \overline{m_1}\},$$

and $[\![(G,0)]\!]_{\mathit{Aff}^+(\mathbb{Z}^d)} \subset \mathcal{E}$.

There exists $\beta_0 \in (0, s_0/2)$ such that for every $\mathcal{M} \in \mathcal{E}$ and $y \in \mathbb{R}^d$ verifying $\operatorname{dist}(v, \mathcal{L}(\mathcal{M})) < \beta_0$, we have

$$\left| D_{\mathcal{M}} W(y, \mathcal{M}) \right| \leq C_{W,1} D_{\mathcal{M}} \operatorname{dist}^2(y, \mathcal{M}),$$

$$\frac{C_{W,0}}{2} D^2_{\mathcal{M}\mathcal{M}} \left(\sum_{z_k \in \mathbb{Z}^d} |v - \mathcal{M}(z_k)|^2 \ \chi_{B(0,m_0)}(|v - \mathcal{M}(z_k)|) \right) \leq D^2_{\mathcal{M}\mathcal{M}} W(v, \mathcal{M}).$$

Notice that by (P1) we have $\{y \in \mathbb{R}^d : W(y, \mathcal{M}) = 0\} = \mathcal{L}(\mathcal{M})$. From now on, with a small abuse of notation, given $x \in \Omega$ and $\mathcal{A} \in \mathit{Aff}^+_{\triangleright}(\mathbb{R}^d_x)$, we will set

$$W(\cdot, \mathcal{L}_x(\mathcal{A})) := W(\cdot, (A, x - A\tau)) = W(\cdot - x, (A, -A\tau)).$$

Such an abuse of notation is justified by assumption (P2), from which follows that $W(\cdot, \mathcal{L}_x(\mathcal{A})) = W(\cdot, \mathcal{L}_x(\widetilde{\mathcal{A}}))$ whenever $\mathcal{A}, \ \widetilde{\mathcal{A}} \in \mathit{Aff}^+_{\triangleright}(\mathbb{R}^d_x)$ verify $\mathcal{L}_x(\widetilde{\mathcal{A}}) = \mathcal{L}_x(\mathcal{A})$. Moreover, again thanks to (P2), we have

$$0 < \mathcal{W} := \|W(\cdot,\cdot)\|_{C^2\left(\mathbb{R}^d \times (\mathcal{E} \cap \{\mathcal{M} \in \mathit{Aff}^+(\mathbb{R}^d) : \ |M| < \overline{m_1}\})\right)} < +\infty. \tag{2.16}$$

In Appendix A we exihibit an explicit example of a function $W(\cdot,\cdot)$ satisfying (P1)-(P3).

Remark 2.4. Condition (2.15) is nothing but a technical assumption that simplifies some of the statements and proofs.

The elastic potential F: By $F \in C^2\big(GL^+(d,\mathbb{R})\big)$ we denote a function such that the following relations hold for every $M \in GL^+(d,\mathbb{R})$

$$\begin{aligned} &F(M) \geq 0, \quad F(M) = 0 \Longleftrightarrow \mathcal{L}(M) = \mathcal{L}(G), \\ &F(RM) = F(M), \quad \forall R \in SO_d(\mathbb{R}), \\ &F(MB) = F(M), \quad \forall B \in GL^+(d,\mathbb{Z}). \end{aligned}$$

Moreover we assume the existence of $T_{\rm el}$, $C_{\rm el} > 0$ verifying

$$\{F(M) < T_{\rm el}\} \subset \{(\det M) < C_{\rm el}\}. \tag{2.17}$$

Let us remind the reader that we think of $F(M)$ as the excess energy associated with the linear shear MG^{-1} applied to $\mathcal{L}(G)$.

We are now in a position to define the energy density $h_\lambda(\cdot,\cdot)$.

Definition 2.5. *Given $X \subset \Omega$, $x \in \Omega$ and $\lambda \in \mathbb{R}^+$ we set*

$$\begin{aligned} &J_\lambda(x,\cdot,X) : \mathit{Aff}^+_{\triangleright}(\mathbb{R}^d_x) \to [0,+\infty[, \\ &\mathcal{A} = (A,\tau) \mapsto \lambda^{-d} \sum_{x_i \in X} \Big(W(x_i, \mathcal{L}_x(\mathcal{A})) - \theta_0 \Big) \varphi_{\lambda,x}(x_i) \end{aligned} \tag{2.18}$$

$$\begin{aligned} &\mathcal{V}_\lambda(x,\cdot,X) : \mathit{Aff}^+_{\triangleright}(\mathbb{R}^d_x) \to [0,+\infty[, \\ &\mathcal{A} = (A,\tau) \mapsto \vartheta_1 \left(\frac{1}{\det A} - \frac{1}{\lambda^d C_\varphi} \sum_{x_i \in X} \varphi_{\lambda,x}(x_i) \right), \end{aligned} \tag{2.19}$$

where C_φ *is as in* (2.10). *We define*

$$\begin{aligned} h_\lambda(x,\cdot,\mathcal{X}) : \mathcal{A}\!f\!f^+_{\triangleright}(\mathbb{R}^d_x) &\to [0,+\infty), \\ \mathcal{A} \mapsto\ & J_\lambda(x,\mathcal{A},\mathcal{X}) + \mathcal{V}_\lambda(x,A,\lambda) + F(A), \end{aligned} \tag{2.20}$$

and eventually

$$\begin{aligned} h_\lambda(\cdot,\mathcal{X}) &: \Omega \to \mathbb{R}, \\ h_\lambda(x,\mathcal{X}) &:= \inf_{\mathcal{A}\in \mathcal{A}\!f\!f^+(\mathbb{R}^d)} h_\lambda(x,\mathcal{A},\mathcal{X}). \end{aligned} \tag{2.21}$$

Remark 2.6. By the invariance assumptions made on $W(x,\cdot)$ and $F(\cdot)$ we obtain that $h_\lambda(x,\mathcal{A},\mathcal{X}) = h_\lambda(x,\mathcal{A}_{\mathcal{B}},\lambda)$ for every $\mathcal{A}\in \mathcal{A}\!f\!f^+_{\triangleright}(\mathbb{R}^d_x)$ and every $\mathcal{A}_{\mathcal{B}} \in [\![\mathcal{A}]\!]_{\mathcal{A}\!f\!f^+(\mathbb{Z}^d)}$.

Remark 2.7. Throughout the paper we assume that the hard-core threshold s_0 and the single vacancy cost constant ϑ_1 satisfy

$$C_{W,0}\frac{s_0^2}{4} - \frac{\vartheta_1}{C_\varphi} > 0, \tag{2.22}$$

where $C_{W,0}$ denotes the positive constant appearing in the definition of $W(\cdot,\cdot)$. Condition (2.22) is, roughly speaking, needed to ensure that, when $\mathcal{X}$ satisfies the hard-core constrain $\sum_{i,j\in I,\, i\neq j} V(|x_i-x_j|)=0$, "interstitials" of $\mathcal{X}$ with respect to $\mathcal{L}_x(\mathcal{A})$ have a positive cost in terms of $J_\lambda(x,\mathcal{A},\mathcal{X}) + \mathcal{V}_\lambda(x,\mathcal{A},\mathcal{X})$.

3. Behavior of H_λ with respect to an elastically deformed lattice

In the present section we analyze the behavior of

$$\lim_{\lambda,L\to+\infty} H_\lambda(\mathcal{X}_L,\Omega_L)$$

under two assumptions: first we assume that $\mathcal{X}_L \subset \Omega_L$ coincides with the image through a smooth (elastic) deformation Φ_L of some portion of the ground state $\mathcal{L}(G)$ (for ease of exposition throughout this section we choose $\mathcal{L}(G)=\mathbb{Z}^d$); second we assume that $L=\operatorname{diam}(\Omega_L)$ and $L/\lambda^2 \to +\infty$. (Relaxing the scaling ansatz $\lim_{L,\lambda\to\infty}\operatorname{diam}(\Omega_L)/\lambda^2=\infty$ to $\lim_{L,\lambda\to\infty}\operatorname{diam}(\Omega_L)/\lambda=\infty$ would produce in the limit a term that depends on the second and higher derivatives of Φ_L).

More precisely we consider the following setting. Let $\{L_n\}_{n\in\mathbb{N}}$, $\{\lambda_n\}_{n\in\mathbb{N}} \subset \mathbb{R}^+$ be two sequences such that

$$\lim_{n\to\infty} L_n = \lim_{n\to\infty}\lambda_n = \lim_{n\to\infty}\frac{L_n}{\lambda_n^2} = +\infty.$$

Let $E\subset\mathbb{R}^d$ be open, bounded connected and with smooth boundary. Let $\Phi\in C^2(\overline{E},\mathbb{R}^d)$ be a diffeomorphism of $\overline{E}$ onto $\overline{\Omega_1}\subset\mathbb{R}^d$. For every $n\in\mathbb{N}$ we define

$$\Phi_{L_n} : E_{L_n} := L_nE \to \mathbb{R}^d, \qquad y\mapsto L_n\Phi\left(\frac{y}{L_n}\right),$$

and we consider

$$\begin{aligned} \mathcal{X}_n &:= \{x_i = \Phi_{L_n}(z_i) :\ z_i\in\mathbb{Z}^d\cap E_{L_n}\}, \\ \Omega_{L_n} &:= \{y\in\Phi_{L_n}(E_{L_n}) :\ \operatorname{dist}(y,\partial\Phi_{L_n}(E_{L_n}))\le 2\lambda\}. \end{aligned} \tag{3.1}$$

In the following we prove that, assuming $\sum_{x_i,x_j\in\mathcal{X}_n,\, x_i\neq x_j} V(|x_i-x_j|)=0$ for every n large enough and $\|F(\nabla\Phi)\|_{L^\infty(E)}$ sufficiently small, we have

$$\lim_{n\to\infty}\frac{1}{L_n^d}H_{\lambda_n}(\mathcal{X}_n,\Omega_{L_n}) = \int_E F(\nabla\Phi(y))\det(\nabla\Phi(y))\,dy - C_\varphi\vartheta_0|E|. \tag{3.2}$$

Remark 3.1. Let us notice that the assumption $\sum_{x_i,x_j\in\mathcal{X}_n,\, x_i\neq x_j} V(|x_i-x_j|)=0$ for n large ensures the existence of $\sigma_0 := \sigma_0(d,s_0)>0$ such that $\det\big(\nabla\Phi\big)>\sigma_0$ everywhere on E.

Let $y_{x,n} := \Phi_{L_n}^{-1}(x)$, and define $\mathcal{A}_n(x) := (\nabla\Phi_{L_n}(y_{x,n}), y_{x,n}) \in \mathit{Aff}^{+}_{\triangleright}(\mathbb{R}^d_x)$. As a first step in order to get (3.2) we prove that

$$\begin{aligned}\limsup_{n\to\infty}\frac{1}{L_n^d}H_{\lambda_n}(\mathcal{X}_n,\Omega_{L_n}) \le \lim_{n\to\infty}\frac{1}{L_n^d}\int_{\Omega_{L_n}} h_{\lambda_n}(x,\mathcal{L}(\mathcal{A}_n(x)),\mathcal{X}_n)\,dx \\ = \int_E F(\nabla\Phi(y))\,\det(\nabla\Phi(y)) - C_\varphi\vartheta_0\,dy.\end{aligned} \tag{3.3}$$

We begin showing that

$$\lim_{n\to\infty}\sup_{x\in\Omega_{L_n}}|\mathcal{V}_{\lambda_n}(x,\nabla\Phi_{L_n}(y_{x,n}),\mathcal{X}_n)| = 0. \tag{3.4}$$

Firstly we notice that

$$\begin{aligned}&\left|\sum_{z_k\in\mathbb{Z}^d}\varphi_{\lambda_n,x}(\Phi_{L_n}(z_k)) - \frac{\lambda_n^d}{\det\left(\nabla\Phi_{L_n}(y_{x,n})\right)}\int_{\mathbb{R}^d}\varphi(|w|)\,dw\right| \\ =&\left|\sum_{z_k\in\mathbb{Z}^d}\int_{Q(z_k)}\varphi_{\lambda_n,x}(\Phi_{L_n}(z_k)) - \varphi\left(\frac{|\nabla\Phi_{L_n}(y_{x,n})(v-y_{x,n})|}{\lambda_n}\right)\,dv\right|.\end{aligned} \tag{3.5}$$

As Φ is a smooth map, we have

$$\begin{aligned}&\left|\varphi\left(\frac{|\Phi_{L_n}(z_k)-x|}{\lambda_n}\right) - \varphi\left(\frac{|\nabla\Phi_{L_n}(y_{x,n})(v-y_{x,n})|}{\lambda_n}\right)\right| \\ \le&\frac{\|\varphi'\|_{L^\infty(\mathbb{R})}}{\lambda_n}\left(\|\nabla\Phi\|_{L^\infty(E)} + \frac{\|\nabla^2\Phi\|_{L^\infty(E)}}{L_n}\|\nabla\Phi^{-1}\|^2_{L^\infty(E)}\lambda_n^2\right).\end{aligned}$$

Hence, by (3.5) we get

$$\sup_{x\in\Omega_{L_n}}|\mathcal{V}_{\lambda_n}(x,\nabla\Phi_{L_n}(y_{x,n}),\mathcal{X}_n)| \simeq C\left(\frac{1}{\lambda_n}+\frac{\lambda_n}{L_n}\right),$$

and (3.4) follows.

Next we estimate the term $J_{\lambda_n}(x,\mathcal{A}_n(x),\mathcal{X}_n)$. By assumption (P1)-(P2) on W we have

$$\sum_{x_i\in\mathcal{X}_n} W(x_i,\mathcal{L}_x(\mathcal{A}_n(x)))\varphi_{\lambda_n,x}(x_i) \le C_{W,1}\sum_{z_k\in\mathbb{Z}^d}\mathrm{dist}^2(\Phi_{L_n}(z_k),\mathcal{L}_x(\mathcal{A}_n(x)))\varphi_{\lambda_n,x}(z_k).$$

We remark that

$$\begin{aligned}\Phi_{L_n}(z_k) =& x + \nabla\Phi_{L_n}(y_{x,n})(z_k-y_{x,n}) + (z_k-y_{x,n})^T\nabla^2\Phi_{L_n}(\xi_{x,k})(z_k-y_{x,n}) \\ =& \left[\mathcal{A}_n(x)\right](z_k) + (z_k-y_{x,n})^T\nabla^2\Phi_{L_n}(\xi_{x,k})(z_k-y_{x,n}),\end{aligned} \tag{3.6}$$

where $\xi_{x,k}$ belongs to the segment connecting $y_{x,n}$ and z_k. Hence, by

$$\nabla^2\Phi_{L_n}(\xi) = L_n^{-1}\nabla^2\Phi(\xi/L_n),$$

$$m_1(\mathcal{L}(\mathcal{A}_n(x)) \le \min_{B\in GL^+(d,\mathbb{Z})}\|\big[\nabla\Phi_{L_n}(x)\big]B\|_* \le \|\nabla\Phi\|_{L^\infty(E)},$$

and (3.6), we obtain that for $n \in \mathbb{N}$ large enough (uniform with respect to $x \in \Omega_{L_n}$) we have

$$\operatorname{dist}^2(\Phi_{L_n}(z_k), \mathcal{L}_x(\mathcal{A}_n(x))) = \min_{\zeta \in \mathcal{L}_x(\mathcal{A}_n(x))} |\Phi_{L_n}(z_k) - \zeta|^2$$

$$= \left|(z_k - y_{x,n})^T \nabla^2 \Phi_{L_n}(y_{x,n})(z_k - y_{x,n})\right|^2 \leq \frac{\lambda_n^4}{L_n^2} \|\nabla^2 \Phi\|_{L^\infty(E)} \|\nabla \Phi^{-1}\|_{L^\infty(E)}.$$

Hence, by (3.4), we conclude that

$$\lim_{n\to\infty} J_{\lambda_n}(x, \mathcal{A}_n(x), \mathcal{X}_n) = -\frac{\vartheta_0}{\det \nabla \Phi(0)}, \qquad \forall x \in \mathbb{R}^d, \tag{3.7}$$

and

$$\lim_{n\to\infty} \sup_{x \in \Omega_{L_n}} \left| J_{\lambda_n}(x, \mathcal{A}_n(x), \mathcal{X}_n) + \frac{\vartheta_0}{\det \nabla \Phi(y_{x,n})} \right| = 0. \tag{3.8}$$

Combining (3.4) and (3.8) we obtain (3.3).

We remark that in order to prove (3.3) we did not need any assumption on the smallness of $\|F(\nabla\Phi)\|_{L^\infty(E)}$. However, such an assumption is crucial in order to prove that

$$\liminf_{n\to\infty} \frac{1}{L_n^d} H_{L_n}(\mathcal{X}_n, \Omega_{L_n}) \geq \int_E \Big[F(\nabla\Phi(y)) \det(\nabla\Phi(y)) - C_\varphi \vartheta_0\Big]\, dy, \tag{3.9}$$

which is the missing step to conclude the proof of (3.2).

In order to get (3.9) we need the results stated in Proposition 3.2 and Proposition 3.3 (we postpone the proofs of these Propositions to end of the present section). Fixed $x \in \Omega$ and $\mathcal{A} \in \mathit{Aff}^{+}_{\triangleright}(\mathbb{R}^d_x)$, Proposition 3.2 provides us a (uniform with respect to $\mathcal{X}$) lower bound for $h_\lambda(x, \mathcal{A}, \mathcal{X})$ in terms of $m_1(\mathcal{L}_x(\mathcal{A}))$. Moreover, given $x \in \Omega$ and $\mathcal{X} \subset \Omega$, Proposition 3.3 provides us a bound on $m_1(\mathcal{L}_x(\mathcal{A}))$ in terms of the value of $J_\lambda(x, \mathcal{A}, \mathcal{X}) + \mathcal{V}_\lambda(x, A, \mathcal{X})$ and of the "empirical density" $\rho_\lambda(x, \mathcal{X}) = \frac{1}{C_\varphi \lambda^d} \sum_{x_i \in \mathcal{X}} \varphi_{\lambda,x}(x_i)$ of $\mathcal{X} \cap B(x, 2\lambda)$ with respect to x.

Proposition 3.2. *Let $x \in \Omega$. Let $\mathcal{A} = (A, \tau) \in \mathit{Aff}^{+}_{\triangleright}(\mathbb{R}^d_x)$. Then*

$$\min_{\mathcal{X} \subset \Omega} \left[\frac{1}{\lambda^d} \sum_{x_i \in \mathcal{X}} \left(W(x_i, \mathcal{L}_x(\mathcal{A})) - \frac{\vartheta_1}{C_\varphi}\right) \varphi_{\lambda,x}(x_i) + \frac{\vartheta_1}{\det A}\right]$$
$$\geq -\frac{d\vartheta_1\, m_1(\mathcal{L}_x(\mathcal{A})) + \sqrt{\vartheta_1/(C_{W,0} C_\varphi)}}{\lambda}.$$

Proposition 3.3. *Let $x \in \Omega$ be such that* $\operatorname{dist}(x, \partial\Omega) > \lambda$. *Suppose $\mathcal{X} \subset \Omega$ satisfies*

$$\rho \lambda^d \leq \sum_{\substack{i,j \in I \\ i \neq j}} V(|x_i - x_j|) + \sum_{x_i \in \mathcal{X}} \varphi_{\lambda,x}(x_i) < +\infty, \tag{3.10}$$

for some $\rho > 0$, and let $\eta > 0$ be such that

$$\Big(\frac{C_{W,0}\, s_0^2}{4} - \frac{\vartheta_1}{C_\varphi}\Big) \rho > \eta. \tag{3.11}$$

Then we can find $\widehat{C} := \widehat{C}(d, V, W, \vartheta_1, \rho, \eta)$ and $\lambda_{m_1} := \lambda_{m_1}(d, V, W, \vartheta_1, \rho, \eta)$ such that, if $\lambda > \lambda_{m_1}$, for every $\mathcal{A} = (A, \tau) \in \mathit{Aff}^{+}_{\triangleright}(\mathbb{R}^d_x)$ satisfying

$$\frac{C_{W,0}}{\lambda^d} \sum_{x_i \in \mathcal{X}} \operatorname{dist}^2(x_i, \mathcal{L}_x(\mathcal{A})) \varphi_{\lambda,x}(x_i) + \mathcal{V}_\lambda(x, A, \mathcal{X}) < \eta, \tag{3.12}$$

we have $m_1(\mathcal{L}_x(\mathcal{A})) < \widehat{C}$.

Let us show how to prove (3.9) by means of Proposition 3.2 and Proposition 3.3. By (3.4) we deduce that, fixed $n \in \mathbb{N}$ large enough, we have

$$\rho\lambda^d < \frac{2\lambda^d}{\det \nabla\Phi_{L_n}(x)} \leq \sum_{x_i \in X_n} \varphi_{\lambda_n,x}(x_i), \quad \forall x \in \Omega_{L_n},$$

where $0 < \rho := \|\det \nabla\Phi\|_{L^\infty(\Omega)}$. Hence (3.10) holds for every $n \in \mathbb{N}$.

Now, fixed $n \in \mathbb{N}$ large and $x \in \Omega_{L_n}$, we choose $\{\widetilde{\mathcal{A}}_{n,m}(x)\}_m \in \mathit{Aff}^+(\mathbb{R}^d_x)$ such that

$$\lim_{m\to\infty} h_{\lambda_n}(x, \widetilde{\mathcal{A}}_{n,m}(x), X_n) = \inf_{\mathcal{A}\in \mathit{Aff}^+(\mathbb{R}^d)} h_\lambda(x, \mathcal{L}_x(\mathcal{A}), X) = h_{\lambda_n}(x, X_n),$$

and such that $\widetilde{\mathcal{A}}_{n,m}(x)$ is a canonical representation for $\mathcal{L}_x(\widetilde{\mathcal{A}}_{n,m}(x))$. Again by (3.4) and (3.3) we obtain that for large enough $m \in \mathbb{N}$ we have

$$\begin{aligned}&\frac{C_{W,0}}{\lambda_n^d} \sum_{x_i\in X_n} \operatorname{dist}^2(x_i, \mathcal{L}_x(\widetilde{\mathcal{A}}_{n,m}(x)))\varphi_{\lambda_n,x}(x_i) + \mathcal{V}_{\lambda_n}(x, \widetilde{A}_{n,m}(x), X_n)\\ &\leq h_{\lambda_n}(x, \widetilde{\mathcal{A}}_{n,m}(x), X_n) + \frac{\vartheta_0}{\lambda^d} \sum_{x_i\in X} \varphi_{\lambda,x}(x_i) \leq 2F(\nabla\Phi(x/L_n)) + \frac{c}{\lambda_n},\end{aligned}$$

so that, if $\|F(\nabla\Phi)\|_{L^\infty(E)}$ is small enough, (3.12) holds. By Proposition 3.3 and the choice of $\widetilde{\mathcal{A}}_{n,m}(x)$ in $[\![\widetilde{\mathcal{A}}_{n,m}(x)]\!]_{\mathit{Aff}^+(\mathbb{Z}^d)}$, we can conclude that, up to the selection of a subsequence, we have $\lim_{m\to\infty} \widetilde{\mathcal{A}}_{n,m}(x) = \widetilde{\mathcal{A}}_n(x) \in \mathit{Aff}^+_\triangleright(\mathbb{R}^d_x)$. Moreover, again by Proposition 3.2 and Proposition 3.3, we obtain the existence of $c > 0$, independent of $n \in \mathbb{N}$, such that

$$J_{\lambda_n}(x, \widetilde{\mathcal{A}}_n(x), X_n) + \mathcal{V}_{\lambda_n}(x, \widetilde{A}_n(x), X_n) + \frac{\vartheta_0}{\det(\nabla\Phi(x/L_n))} \geq -\frac{c}{\lambda_n}.$$

This estimate, together with (3.4) and (3.8), shows that the sequence $\mathcal{A}_n(x) = (\nabla\Phi_{L_n}(y_{x,n}), y_{x,n}) \in \mathit{Aff}^+_\triangleright(\mathbb{R}^d_x)$, which is the same sequence we constructed to prove (3.3), approaches the minimum of $J_{\lambda_n}(x,\cdot,X_n)+\mathcal{V}_{\lambda_n}(x,\cdot,X_n)$ as $n \to \infty$. However, if we fix $y \in E$, set $x_n := L_n y \in \Omega_{L_n}$, and suppose that $\operatorname{dist}(\widetilde{\mathcal{A}}_n(x_n), [\![\mathcal{A}_n(x_n)]\!]_{\mathit{Aff}^+(\mathbb{Z}^d)})$ does not go to zero as $n \to \infty$, by the periodicity of $W(\cdot,\cdot)$ and since $\det\big(\nabla\Phi(y)\big) > \sigma_0$ on E, we obtain

$$J_{\lambda_n}(x_n, \widetilde{\mathcal{A}}_n(x), X_n) + \mathcal{V}_{\lambda_n}(x_n, \widetilde{A}_n(x), X_n) + \frac{\vartheta_0}{\det(\nabla\Phi(y))} \geq C - O\Big(\frac{\lambda_n^2}{L_n}\Big) - O\Big(\frac{1}{\lambda_n}\Big),$$

where $C > 0$ depends only on W, s_0, d, ϑ_1. Hence, assuming $\|F(\nabla\Phi)\|_{L^\infty(E)}$ smaller than C, we obtain that (3.9) holds.

We conclude the present section with the proofs of Proposition 3.2 and Proposition 3.3.

In order to prove Proposition 3.2 we need to estimate the deviation of the "discrete density" of the Bravais lattice $\mathcal{L}_x(\mathcal{A})$ n $B(x,\lambda)$ from $1/\det A$. This is the purpose of the following

Lemma 3.4. *Let $x \in \Omega$ and $\mathcal{A} := (A, \tau) \in \mathit{Aff}^+_{\triangleright}(\mathbb{R}^d_x)$. For every $R > 0$, the following hold*

$$\frac{\omega_d(R - d m_1(\mathcal{L}_x(\mathcal{A})))^d}{\det A} \le \sharp\{\mathcal{L}_x(\mathcal{A}) \cap B(x,R)\} \le \frac{\omega_d(R + d m_1(\mathcal{L}_x(\mathcal{A})))^d}{\det A}, \tag{3.13}$$

$$\Big| \sum_{z_k \in \mathbb{Z}^d} \varphi_{R,x}(\mathcal{A}(z_k)) - \frac{C_\varphi R^d}{\det A} \Big| \le \frac{m_1(\mathcal{L}_x(\mathcal{A}))C_1}{\det A} \omega_d R^{d-1}, \tag{3.14}$$

where $C_1 := 3^d d\omega_d \|\varphi'\|_{L^\infty(\mathbb{R})} > 0$.

Proof. We begin noticing that neither (3.13), nor (3.14), depend on the element in $[\![\mathcal{A}]\!]_{\mathit{Aff}^+(\mathbb{Z}^d)}$ chosen to represent $\mathcal{L}_x(\mathcal{A})$. Therefore we will from now on assume that the matrix A is associated with a reduced, positively oriented lattice basis of $\mathcal{L}(A)$.

We start proving (3.13). Let

$$\Delta^{\mathcal{A}}_- := \{z_k \in \mathbb{Z}^d : Q(z_k) \subset \mathcal{A}^{-1}(B(x,R))\}, \qquad Q(\Delta^{\mathcal{A}}_-) := \cup\{Q(z_k) : z_k \in \Delta^{\mathcal{A}}_-\},$$
$$\Delta^{\mathcal{A}}_+ := \{z_k \in \mathbb{Z}^d : Q(z_k) \cap \mathcal{A}^{-1}(B(x,R)) \neq \emptyset\}, \qquad Q(\Delta^{\mathcal{A}}_+) := \cup\{Q(z_k) : z_k \in \Delta^{\mathcal{A}}_+\}.$$

Then we have

$$B(x, R - \|A\|_*) \subset \mathcal{A}(Q(\Delta^{\mathcal{A}}_-)) \subset B(x,R) \subset \mathcal{A}(Q(\Delta^{\mathcal{A}}_+)) \subset B(x, R + \|A\|_*).$$

Equation (3.13) is a consequence of the following

$$\sharp\mathcal{L}_x(\mathcal{A}) \cap B(x,R) \ge \sharp\{\mathcal{A}(z_k) : z_k \in \Delta^{\mathcal{A}}_-\} = \sum_{z_k \in \Delta^{\mathcal{A}}_-} m(Q(z_k)) = \int_{Q(\Delta^{\mathcal{A}}_-)} dv$$
$$= \int_{\mathcal{A}(Q(\Delta^{\mathcal{A}}_-))} (\det A)^{-1}\, dy \ge (\det A)^{-1} \int_{B(x, R - \|A\|_*)} dy = \frac{(R - \|A\|_*)^d \omega_d}{\det A}.$$

Since A is associated with a positively oriented reduced lattice basis of $\mathcal{L}_x(\mathcal{A})$, we obtain the first inequality in (3.13). A similar argument produces a proof of the second inequality in (3.13).

We remark that, as a consequence of (3.13), we can conclude that the following holds for every $0 < R_0 < R_1$

$$\begin{aligned} &\sharp[\mathcal{L}_x(\mathcal{A}^{-1}) \cap (B(x,R_1) \setminus B(x,R_0))] \\ &\le \frac{(R_1 + d m_1(\mathcal{L}_x(\mathcal{A})))^d - (R_0 - d m_1(\mathcal{L}_x(\mathcal{A})))^d}{\det A} \omega_d. \end{aligned} \tag{3.15}$$

Next we prove (3.14). By

$$\frac{C_\varphi R^d}{\det A} = \int_{\mathbb{R}^d} (\det A)^{-1} \varphi\left(\frac{|y-x|}{R}\right) dy = \int_{\mathbb{R}^d} \varphi\left(\frac{|\mathcal{A}(v) - x|}{R}\right) dv$$

we deduce that

$$\begin{aligned} I :=& \Big| \sum_{z_k \in \mathbb{Z}^d} \varphi_{R,x}(\mathcal{A}(z_k)) - \frac{C_\varphi R^d}{\det A} \Big| \\ =& \left| \sum_{z_k \in \mathbb{Z}^d} \int_{Q(z_k)} [\varphi_{R,x}(\mathcal{A}(z_k)) - \varphi_{R,x}(\mathcal{A}(v))]\, dv \right|. \end{aligned} \tag{3.16}$$

Expanding up to the first order $\varphi_{R,x}(\mathcal{A}(\cdot))$ in v around z_k, we have

$$\begin{aligned}\varphi_{R,x}(\mathcal{A}(v)) &= \varphi_{R,x}(\mathcal{A}(z_k)) + \langle \nabla_v \varphi\left(\frac{|\mathcal{A}(\xi)|}{R}\right), (v-z_k)\rangle \\ &=\varphi_{R,x}(\mathcal{A}(z_k)) + \frac{1}{R}\varphi'\left(\frac{|\mathcal{A}(\xi)|}{R}\right)\langle \frac{\mathcal{A}(\xi)}{|\mathcal{A}(\xi)|}, A(v-z_k)\rangle,\end{aligned} \tag{3.17}$$

where $\xi := \xi(v, z_k)$ belongs to the line connecting v and z_k. Hence, by (3.16), (3.15),

$$\begin{aligned} I &\le \sum_{z_k\in\mathbb{Z}^d}\int_{Q(z_k)\cap\mathcal{A}(B(x,2R))}\left|\langle \nabla_v\varphi\left(\frac{|\mathcal{A}(\xi(v,z_k))|}{R}\right), (v-z_k)\rangle\right| dv \\ &\le \frac{\|\varphi'\|_{L^\infty(\mathbb{R})}\|A\|_*}{R}\sharp\Big(\mathcal{L}_x(\mathcal{A})\cap\Big(B(x,2R+\|A\|_*)\setminus B(x,R-\|A\|_*)\Big)\Big) \\ &\le \frac{\|\varphi'\|_{L^\infty(\mathbb{R})}\|A\|_*}{R}\omega_d\frac{(3R)^d}{\det A},\end{aligned} \tag{3.18}$$

and the thesis follows. □

We are now in a position to prove Proposition 3.2, Proposition 3.3.

Proof of Proposition 3.2. Let $\mathcal{X}\subset\Omega$. By the assumptions (P1)-(P2) on W we have

$$\begin{aligned}&\frac{1}{\lambda^d}\sum_{x_i\in\mathcal{X}}\left(W(x_i,\mathcal{L}_x(\mathcal{A}))-\frac{\vartheta_1}{C_\varphi}\right)\varphi_{\lambda,x}(x_i)+\frac{\vartheta_1}{\det A} \\ \ge\ &\frac{1}{\lambda^d}\sum_{x_i\in\mathcal{X}}\left(C_{W,0}\operatorname{dist}^2(x_i,\mathcal{L}_x(\mathcal{A}))-\frac{\vartheta_1}{C_\varphi}\right)\varphi_{\lambda,x}(x_i)+\frac{\vartheta_1}{\det A}\end{aligned}$$

Moreover, setting

$$\begin{gathered}\mathcal{X}^+ := \{x_i\in\mathcal{X}:\ \operatorname{dist}(x_i,\mathcal{L}_x(\mathcal{A}))>\sqrt{\vartheta_1/(C_{W,0}C_\varphi)}=:\widetilde{\beta}\},\quad \mathcal{X}^-:=\mathcal{X}\setminus\mathcal{X}^+,\\ \mathcal{L}^- := \{z_k\in\mathbb{Z}^d:\ \operatorname{dist}(\mathcal{A}(z_k),\mathcal{X})>\widetilde{\beta}\},\end{gathered}$$

by (3.14) we have

$$\begin{aligned}&\frac{1}{\lambda^d}\sum_{x_i\in\mathcal{X}}\left(C_{W,0}\operatorname{dist}^2(x_i,\mathcal{L}_x(\mathcal{A}))-\frac{\vartheta_1}{C_\varphi}\right)\varphi_{\lambda,x}(x_i)+\frac{\vartheta_1}{\det A}\\ =\ &\frac{1}{\lambda^d}\sum_{x_i\in\mathcal{X}^-}C_{W,0}\operatorname{dist}^2(x_i,\mathcal{L}_x(\mathcal{A}))\varphi_{\lambda,x}(x_i)+\frac{1}{\lambda^d}\sum_{x_i\in\mathcal{X}^+}\left(C_{W,0}\operatorname{dist}^2(x_i,\mathcal{L}_x(\mathcal{A}))-\frac{\vartheta_1}{C_\varphi}\right)\varphi_{\lambda,x}(x_i)\\ &+\vartheta_1\left(\frac{1}{\det A}-\frac{1}{C_\varphi\lambda^d}\sum_{x_i\in\mathcal{X}^-}\varphi_{\lambda,x}(x_i)\right)\\ \ge\ &\vartheta_1\Big(\frac{1}{\det A}-\frac{1}{C_\varphi\lambda^d}\Big(\sum_{x_i\in\mathcal{X}^-}\varphi_{\lambda,x}(x_i)+\sum_{z_k\in\mathcal{L}^-}\varphi_{\lambda,x}(\mathcal{A}(z_k))\Big)\Big)\\ \ge\ &-\frac{3^d\omega_d\|\varphi'\|_{L^\infty(\mathbb{R})}(\vartheta_1\, m_1(\mathcal{L}_x(\mathcal{A}))+\widetilde{\beta})}{\lambda},\end{aligned}$$

which is our thesis. □

Proof of Proposition 3.3. Since (3.12) is invariant with respect to the change of lattice-bases, we can suppose without loss of generality that $\mathcal{A}$ is a canonical representation for $\mathcal{L}_x(\mathcal{A})$ and $m_1(\mathcal{L}_x(\mathcal{A})) = |Ae_d|$. Let Π be the unique hyperplane containing $A(e_m)$ for every $1 \leq m < d$, and let ν be a unit vector orthogonal to Π. By Remark 2.3 we can find $C := C(s_0, d) > 0$ such that if $m_1(\mathcal{L}_x(\mathcal{A})) > C$

$$\{y \in B(x, 2\lambda) : \operatorname{dist}(y, \mathcal{L}_x(\mathcal{A})) < s_0/4\} \subset \mathcal{G},$$

where

$$\mathcal{G} := \bigcup_{\{l \in \mathbb{Z} :\, |lAe_d - A\tau| < 2\lambda\}} \Big(\Big[\Pi \times (-\frac{s_0}{4}, \frac{s_0}{4})\nu\Big] + (x - A\tau) + lAe_d\Big),$$

and

$$\Big(\Big[\Pi \times (-\frac{s_0}{4}, \frac{s_0}{4})\nu\Big] + lAe_d\Big) \bigcap \Big(\Big[\Pi \times (-\frac{s_0}{4}, \frac{s_0}{4})\nu\Big] + mAe_d\Big)) = \emptyset,$$

for every $l \neq m$. However, using the assumption $|\tau| \leq \sqrt{d}$, we have

$$|lAe_d - A\tau| < 2\lambda \implies l \leq \frac{2\lambda}{m_1(\mathcal{L}_x(\mathcal{A}))} + d^2.$$

Hence, setting

$$\mathcal{X}^{+,s_0/2} := \{x_i \in \mathcal{X} \cap B(x, 2\lambda) : \operatorname{dist}(x_i, \mathcal{L}_x(\mathcal{A})) < s_0/2\},$$

by (3.10), we obtain

$$\sharp \mathcal{X}^{+,s_0/2} \leq \frac{|\mathcal{L}_x(\mathcal{A}) \cap \mathcal{G} \cap B(x, 2\lambda))|}{s_0^d} \leq \frac{(2\lambda)^{d-1}}{2s_0^{d-1}}\Big(\frac{2\lambda}{m_1(\mathcal{L}_x(\mathcal{A}))} + d^2\Big). \tag{3.19}$$

By (3.19), we conclude that

$$\eta > \frac{C_{W,0}}{\lambda^d} \sum_{x_i \in \mathcal{X}} \operatorname{dist}^2(x_i, \mathcal{L}_x(\mathcal{A}))\varphi_{\lambda,x}(x_i) + \mathcal{V}(x, A, \mathcal{X})$$

$$\geq \frac{1}{\lambda^d} \sum_{x_i \notin \mathcal{X}^{+,s_0/2}} \Big(C_{W,0} \operatorname{dist}^2(x_i, \mathcal{L}_x(\mathcal{A})) - \frac{\vartheta_1}{C_\varphi}\Big)\varphi_{\lambda,x}(x_i) + \vartheta_1\Big(\frac{1}{\det A} - \frac{1}{C_\varphi \lambda^d} \sum_{x_i \in \mathcal{X}^{+,s_0/2}} \varphi_{\lambda,x}(x_i)\Big)$$

$$\geq \Big(C_{W,0}\frac{s_0^2}{4} - \frac{\vartheta_1}{C_\varphi}\Big)\Big(\rho - \Big(\frac{1}{m_1(\mathcal{L}_x(\mathcal{A}))} + \frac{d}{2s_0^{d-1}\lambda}\Big)\Big) - \frac{\vartheta_1}{C_\varphi}\Big(\frac{1}{m_1(\mathcal{L}_x(\mathcal{A}))} + \frac{d^2}{2s_0^{d-1}\lambda}\Big)$$

$$= \Big(C_{W,0}\frac{s_0^2}{4} - \frac{\vartheta_1}{C_\varphi}\Big)\rho - \frac{C_{W,0}s_0^2}{4}\Big(\frac{1}{m_1(\mathcal{L}_x(\mathcal{A}))} + \frac{d^2}{2s_0^{d-1}\lambda}\Big),$$

and eventually, by (3.11) we deduce the existence of λ_{m_1} such that for $\lambda > \lambda_{m_1}$ we have

$$0 < \Big(C_{W,0}\frac{s_0^2}{4} - \frac{\vartheta_1}{C_\varphi}\Big)\rho - \eta - \frac{C_{W,0}s_0^2}{4}\frac{d^2}{2s_0^{d-1}\lambda} < \frac{C_{W,0}s_0^2}{4}\frac{1}{m_1(\mathcal{L}_x(\mathcal{A}))},$$

from which the thesis follows. □

Remark 3.5. If we replace (3.11) with

$$\Big(\frac{C_{W,0}s_0^2}{4} - \frac{\vartheta_1}{C_\varphi}\Big)\frac{\rho}{2} > \eta,$$

it follows from the proof of Proposition 3.3, that we can choose $\widehat{C}$ and λ_{m_1} independent of η.

Remark 3.6. We notice that when ρ takes value in a certain interval we can conclude that $\widehat{C} < \overline{m_1}$.

4. Main results and outline of the proofs

As already stated in the Introduction, the purpose of the present paper is that of deriving a qualitative description of "low energy" configurations fulfilling a hard-core constraint, that is finite systems of particles $\mathcal{X} \subset \Omega$ verifying

$$|\Omega|^{-1}(H_\lambda(\mathcal{X},\Omega) + \vartheta_0 \int_\Omega \rho_\lambda(x,\mathcal{X})\,dx + \sum_{\substack{i,j\in I\\ i\neq j}} V(|x_i - x_j|)) << 1,$$

where $\rho_\lambda(x,\mathcal{X}) = \lambda^{-d}\sum_{x_i\in\mathcal{X}}\varphi_{\lambda,x}(x_i)$ is the "empirical density" of $\mathcal{X}$ in $B(x,\lambda)$. The main result we obtain says that on a "large" subset of Ω a low-energy configuration $\mathcal{X}$ is (locally) similar to an elastically deformed ground state (that this a configuration like those considered in the previous section) plus, possibly, a small percentage of "point-defects". In fact, as already stated in the introduction, we show that for "low energy" configurations we can single out from Ω a subset $\widetilde{\Omega}_d$ such that:

- for every $x \in \widetilde{\Omega}_d$ there exists an unique Bravais lattice $\mathcal{L}_x(\mathcal{A}_{0,x})$ such that $h_\lambda(x,\mathcal{X}) = h_\lambda(x,\mathcal{A},\mathcal{X})$ if and only if $\mathcal{A} \in [\![\mathcal{A}_{0,x}]\!]_{\mathcal{A}ff^+(\mathbb{Z}^d)}$;
- $\mathcal{X}\cap B(x,2\lambda)$ is described "with good approximation" by $\mathcal{L}_x(\mathcal{A}_{0,x})\cap B(x,2\lambda)$;
- we can use the map $x \mapsto \mathcal{A}_{0,x}$ to define "approximated local Lagrangian coordinates" for $\mathcal{X}$;
- the measure of $\Omega\backslash\widetilde{\Omega}_d$ is proportional to $|\Omega|^{-1}(H_\lambda(\mathcal{X},\Omega)+\vartheta_0\int_\Omega \rho_\lambda(x,\mathcal{X})\,dx)$.

Let us remark that in general we expect $\mathcal{X}\cap B(x,\lambda)$ to deviate from the optimal fitted lattice $\mathcal{L}_x(\mathcal{A}_0(x))$. This is due to several reasons. A first reason is well exemplified by the case, studied in Section 3, of configurations obtained via a smooth elastic deformation of the ground state lattice. In fact in this case it turns out that, roughly speaking, $\mathcal{A}_{0,x}$ represents a first order approximation (on scale λ) of the elastic deformation. Hence it is reasonable to expect $\mathcal{X}\cap B(x,\lambda)$ to coincide with the Bravais lattice $\mathcal{L}(\mathcal{A}_{0,x})$ only up to errors due to second (and higher) derivatives of the deformation. However, even if $\mathcal{X}$ coincides with a simple Bravais lattice, that is $\mathcal{X} = \mathcal{L}(\overline{A})\cap\Omega$ for some $\overline{A}\in GL^+(d,\mathbb{R})$, in general minimizers of $h_\lambda(x,\cdot,\mathcal{X})$ fall in a $\|\cdot\|_\lambda$-ball of an element of $[\![(\overline{A},0)]\!]_{\mathcal{A}ff^+(\mathbb{Z}^d)}$, but do not belong to such set. This is due to the fact that the optimally fitted lattice $\mathcal{L}(\mathcal{A}_{0,x})$ is chosen only looking at $\mathcal{X}\cap B(x,\lambda)$. For example, if $\mathcal{A}_0 = (A_0,0)\in \mathcal{A}ff^+_\triangleright(\mathbb{R}^d_x)$ is such that $|A_0-\overline{A}| < \delta/\lambda$, it can happen that the error (of order $O(\delta^2)$) produced by the term involving the periodic potential $W(\cdot,\cdot)$, gets compensated by a gain in the term penalizing vacancies and in the term measuring the shear, so that

$$h_\lambda(x,\mathcal{A}_0,\mathcal{X}\cap\Omega) < h_\lambda(x,(\overline{A},0),\mathcal{X}\cap\Omega).$$

A last reason to expect a discrepancy between the optimally fitted lattice and $\mathcal{X}\cap B(x,\lambda)$ is due to the fact that $\mathcal{X}\cap B(x,2\lambda)$ may contain "point defects" even when $h_\lambda(x,\mathcal{X})$ is very small.

In order to state our main results we proceed as follows. We firstly introduce a subset $\widetilde{\Omega}_d$ of Ω (see Definition 4.1) for each element x of which there exists at least one $\mathcal{A}_x \in \mathcal{A}ff^+_\triangleright(\mathbb{R}^d_x)$ such that, roughly speaking, each of the three terms defining $h_\lambda(x,\mathcal{A}_x,\mathcal{X})$ is "small". We then state two of our main results in terms of the elements of $\widetilde{\Omega}_d$ (Theorem 4.4, Theorem 4.5). Eventually we show that if $\mathcal{X} \subset \Omega$ is a "low -energy" configuration such that $\rho_\lambda(x, \mathcal{X})$ is bounded from below by a positive constant independent of $x \in \Omega$, then $\widetilde{\Omega}_d$ contains a set of the form $\{x \in \Omega :\ h_\lambda(x, \mathcal{X}) + \vartheta_0 \rho_\lambda(x, \mathcal{X}) < \eta\}$, and we estimate the measure of $\Omega \setminus \{x \in \Omega :\ h_\lambda(x, \mathcal{X}) + \vartheta_0 \rho_\lambda(x, \mathcal{X}) < \eta\}$ in terms of the "low-energy" of the configuration (see Corollary 4.6).

Let us now give the following

Definition 4.1. *Let $K > 0$, $\varepsilon_v < 1/2$ and $\beta < s_0/2$ (where s_0 is defined in (2.11)). We define the set $\widetilde{\Omega}(K, \beta, \varepsilon_J, \varepsilon_v, \lambda) \subset \Omega \times \mathit{Aff}^+(\mathbb{R}^d)$ as the set of $(x, \mathcal{A} = (A, \tau)) \in \Omega \times \mathit{Aff}^+_\triangleright(\mathbb{R}^d_x)$ such that*

(O1) $m_1(\mathcal{L}_x(\mathcal{A})) < K$;
(O2) $\sum_{x_i \in \mathcal{X}} W(x_i, \mathcal{L}_x(\mathcal{A}))\varphi_{\lambda,x}(x_i) < \frac{\varepsilon_J \beta^2 \lambda^d}{\det A}$;
(O3) $\sum_{x_i \in \mathcal{X}} \varphi_{\lambda,x}(x_i) > \frac{(C_\varphi - \varepsilon_v)\lambda^d}{\det A}$;
(O4) $\sum_{i,j \in I, i \neq j} V(|x_i - x_j|)\varphi_{\lambda,x}(x_i)\varphi_{\lambda,x}(x_j) < +\infty$

From now on we will sometimes write $\widetilde{\Omega}$ as a shorthand for $\widetilde{\Omega}(K, \beta, \varepsilon_J, \varepsilon_v, \lambda)$, when no ambiguity may arise. Moreover

- we denote by $\widetilde{\Omega}_d$ the projection $\pi_d(\widetilde{\Omega})$ of $\widetilde{\Omega} \subset \Omega \times Aff(\mathbb{R}^d)$ on Ω;
- we denote by $\widetilde{\Omega}_x$ the set of $\mathcal{A} \in Aff(\mathbb{R}^d_x)$ such that $(x, \mathcal{A}) \in \widetilde{\Omega}$.

Let us briefly comment on the definition of the set $\widetilde{\Omega}(K, \beta, \varepsilon_J, \varepsilon, \lambda)$. Assumption (O4) prevents concentration of $\mathcal{X}$ in $B(x, 2\lambda)$, while assumption (O3), roughly speaking, says that the number of elements of $\mathcal{X} \cap B(x, 2\lambda)$ is larger than the number of elements of $\mathcal{L}_x(\mathcal{A})$ in $B(x, 2\lambda)$ minus ε_v, up to an error of order $1/\lambda$ (see Lemma 3.4). Eventually, by assumption (P1) on $W(\cdot, \cdot)$, we expect that (O2) implies that, up to an ε_J fraction of $\mathcal{X} \cap B(x, \lambda)$, "most" of the elements of $\mathcal{X}$ are in a β-neighborhood of $\mathcal{L}_x(\mathcal{A})$.

Remark 4.2. By the continuity of W, φ and the determinant, we can conclude that the set $\widetilde{\Omega}$ is an open subset of $\mathbb{R}^d \times \mathit{Aff}^+(\mathbb{R}^d)$. Moreover, by assumption (P2) on $W(\cdot, \cdot)$, if $\mathcal{A} \in \widetilde{\Omega}_x$ we have $[\![\mathcal{A}]\!]_{\mathit{Aff}^+(\mathbb{Z}^d)} \subset \widetilde{\Omega}_x$. Eventually we observe that $\widetilde{\Omega}(K, \beta, \varepsilon_J, \varepsilon_v, \lambda) \subseteq \widetilde{\Omega}(K', \beta', \varepsilon'_J, \varepsilon'_v, \lambda)$, whenever $K \le K'$, $\beta \le \beta'$, $\varepsilon'_J \le \varepsilon_J$, $\varepsilon'_v \le \varepsilon_v$, and that $\widetilde{\Omega}(K, \beta, s\varepsilon_J, \varepsilon_v, \lambda) = \widetilde{\Omega}(K, \sqrt{s}\beta, \varepsilon_J, \varepsilon_v, \lambda)$, for every $s > 0$.

Remark 4.3. Let $(x, \mathcal{A}) \in \widetilde{\Omega}_x(K, \beta, \varepsilon_J, \varepsilon_v, \lambda)$. By (O1) we can trivially conclude that

$$\det A < K^d.$$

Moreover, using only Definition 4.1- (O3), (O4) (and the assumption $\varepsilon_v \in (0, 1/2)$) we can deduce that

$$(\det A)^{-1} \le \frac{2^d}{s_0^d (C_\varphi - \varepsilon_v)} \le \frac{2^{d+1}}{s_0^d (2C_\varphi - 1)} := C_0. \tag{4.1}$$

Let $\mathcal{A}_0 = (A_0, \tau_0) \in \widetilde{\Omega}_x(K, \beta, \varepsilon_J, \varepsilon_v, \lambda)$ be a canonical representation for $\mathcal{L}_x(\mathcal{A}_0)$. By (4.1) and (O1), we obtain an upper bound for $\|A_0^{-1}\|_*$ and a lower bound for $m_0(\mathcal{L}_x(\mathcal{A}))$ in terms of K and ε_v only. More precisely we have

$$\|A_0^{-1}\|_* < C_0 K^{(d-1)}\sqrt{d}, \qquad \|A_0\|_* \ge C_0^{-1/d}, \quad m_0(\mathcal{L}_x(\mathcal{A})) \ge \frac{1}{C_0 K^{d-1}}. \tag{4.2}$$

In particular by (2.15) we have $\widetilde{\Omega}(K,\beta,\varepsilon_J,\varepsilon_v,\lambda)\subset\mathcal{E}$ for $K\in(\frac{1}{C_0^{1/d}},\overline{m_1})$, where $\overline{m_1}$ and $\mathcal{E}$ are as in the definition of the periodic potential W.
Finally we remark that if ε_v, $\varepsilon_J\beta^2$ are such that (3.10), (3.11) hold, thanks to Proposition 3.3, we can remove Definition 4.1-(O1).

Our first main result is the following

Theorem 4.4. *Let K, $K/2\in(\frac{1}{C_0^{1/d}},\overline{m_1})$ be given. We can find $\beta:=\beta(K)>0$ small, $\varepsilon_J,\varepsilon_v$ small (depending on (K,β)), such that if λ is bigger than $\overline{\lambda}:=\overline{\lambda}(K,\beta,\varepsilon_J,\varepsilon_v)$ the following hold.*

(A) *For every $(x_0,\mathcal{A})\in\widetilde{\Omega}(K,\beta,\varepsilon_J,\varepsilon_v,\lambda)$ we have*

$$\sum_{x_i\in\mathcal{X}}\varphi_{\lambda,x}(x_i)\le\left[C_\varphi+\frac{3^d\omega_d\|\varphi'\|_{L^\infty(\mathbb{R})}(K+\beta)}{\lambda}+\frac{\varepsilon_J}{C_{W,0}}\right]\frac{\lambda^d}{\det A},\tag{4.3}$$

$$\sum_{x_j\in\mathcal{R}^\beta_{\mathcal{A}}(x_0)}\varphi\left(\frac{|x_j-x_0|}{\lambda}\right)\ge\left[C_\varphi\omega_d-\left(\varepsilon_v+\frac{\varepsilon_J}{C_{W,0}}\right)\right]\frac{\lambda^d}{\det A},\tag{4.4}$$

where $\mathcal{R}^\beta_{\mathcal{A}}(x_0)=\{x_i\in\mathcal{X}:\sharp(B(x_i,\beta)\cap\mathcal{L}_{x_0}(\mathcal{A}))=1\}$.

(B) *If $\widetilde{\Omega}_{x_0}(\frac{K}{2},\beta,\frac{8}{9}\varepsilon_J,\frac{\varepsilon_v}{2},\lambda)$ is non-void, there exists an unique simple Bravais lattice $\mathcal{L}_{x_0}(\mathcal{A}_{0,x_0})$, with $\mathcal{A}_{0,x_0}\in\widetilde{\Omega}_{x_0}(\frac{2}{3}K,\beta,\frac{9}{10}\varepsilon_J,\frac{2}{3}\varepsilon_v,\lambda)$ a canonical representation for $\mathcal{L}_{x_0}(\mathcal{A}_{0,x_0})$, such that $[\![\mathcal{A}_{0,x_0}]\!]_{Aff^+(\mathbb{Z}^d)}$ are all the critical points of $h_\lambda(x_0,\cdot,\mathcal{X})$ in $\widetilde{\Omega}(K,\beta,\varepsilon_J,\varepsilon_v,\lambda)$, and these are all local minimizers.*

(C) *There exists $\delta_0>0$ such that if $\mathcal{A}\in\widetilde{\Omega}_{x_0}(K,\beta,\varepsilon_J,\varepsilon_v,\lambda)$, then we can find $\mathcal{A}_{\mathcal{B}}\in[\![\mathcal{A}]\!]_{Aff^+(\mathbb{Z}^d)}$ satisfying $\mathcal{A}_{\mathcal{B}}\in\mathfrak{B}_\lambda(\mathcal{A}_0,\delta_0)$, where $\mathcal{A}_{0,x_0}$ is as above.*

Theorem 4.4 says that, given $K>0$, we can tune the parameters β, ε_J, ε_v in such a way that, for large enough λ, we have: for every $\mathcal{A}\in\widetilde{\Omega}_{x_0}(K,\beta,\varepsilon_J,\varepsilon_v,\lambda)$ a large percentage of the elements of $\mathcal{X}\cap B(x_0,\lambda)$ are β-near to one and only one lattice site of the Bravais lattice $\mathcal{L}_{x_0}(\mathcal{A})$; there exists an unique simple Bravais lattice $\mathcal{L}_{x_0}(\mathcal{A}_{0,x_0})$ "best fitted" with $\mathcal{X}\cap B(x_0,\lambda)$; as λ grows if $\mathcal{A}\in\widetilde{\Omega}_{x_0}(K,\beta,\varepsilon_J,\varepsilon_v,\lambda)$ then $\min\{\mathrm{dist}(A,A_{0,x_0}B):\ B\in GL^+(d,\mathbb{Z})\}$ decays as $1/\lambda$.

In the statement of next theorem we assume that we tuned the parameters $(K,\beta,\varepsilon_J,\varepsilon_v,\lambda)$ in such a way that Theorem 4.4 holds.

Theorem 4.5. *Let $\mathrm{Argmin}_{\widetilde{\Omega}}:\widetilde{\Omega}_d(\frac{K}{2},\beta,\frac{8}{9}\varepsilon_J,\frac{\varepsilon_v}{2},\lambda)\to\widetilde{\Omega}(K,\beta,\varepsilon_J,\varepsilon_v,\lambda)$ be the multi-valued map defined by*

$$\mathrm{Argmin}_{\widetilde{\Omega}}(x):=\{(x,\mathcal{A}_{\mathcal{B}}):\ \mathcal{A}_{\mathcal{B}}\in[\![\mathcal{A}_{0,x}]\!]_{Aff^+(\mathbb{Z}^d)}\},\tag{4.5}$$

where $[\![\mathcal{A}_{0,x}]\!]_{Aff^+(\mathbb{Z}^d)}$ are the local minima of $h_\lambda(x,\cdot,\mathcal{X})$ in $\widetilde{\Omega}_x(K,\beta,\varepsilon_J,\varepsilon_v,\lambda)$. Fix $(x_0,\mathcal{A}_{\mathcal{B},x_0})\in\mathrm{Argmin}_{\widetilde{\Omega}}(x_0)$, and let $U\subset\subset\widetilde{\Omega}_d(\frac{K}{2},\beta,\frac{8}{9}\varepsilon_J,\frac{\varepsilon_v}{2},\lambda)\subset\Omega$ be an open, simply connected neighborhood of x_0. There exists an open neighborhood $V\subset\cup_{x\in U}\widetilde{\Omega}_x(K,\beta,\varepsilon_J,\varepsilon_v,\lambda)$ of $\mathcal{A}_{\mathcal{B},x_0}$ and a (single-valued) map $\mathcal{A}_{\mathcal{B}}(\cdot)\in C^1(U,V)$ such that

$$\mathcal{A}_{\mathcal{B}}(x_0)=\mathcal{A}_{\mathcal{B},x_0},\quad(x,\mathcal{A}_{\mathcal{B}}(x))\in\mathrm{Argmin}_{\widetilde{\Omega}}(x),\forall x\in U.\tag{4.6}$$

Moreover, there exists $C^{\mathcal{B}}_\nabla:=C^{\mathcal{B}}_\nabla(s_0,W,\varphi,K,\beta,\varepsilon_J)>0$ such that

$$\lambda\|\nabla A_{\mathcal{B}}(\cdot)\|_{L^\infty(U)}+\|\nabla\tau_{\mathcal{B}}(\cdot)-A^{-1}_{\mathcal{B}}(\cdot)\|_{L^\infty(U)}\le\frac{C^{\mathcal{B}}_\nabla}{\lambda},\tag{4.7}$$

and $C^{\mathcal{B}}_{\nabla} \to 0$, *as* $\varepsilon_J\beta^2 \to 0$.
Eventually, letting $(x_0, \mathcal{A}_{\widehat{\mathcal{B}},x_0}) \in \mathrm{Argmin}_{\widetilde{\Omega}}(x_0)$, *and denoting by* $\mathcal{A}_{\widehat{\mathcal{B}}}(\cdot) \in C^2(\widehat{U}, \widehat{V})$ *the smooth map satisfying* (4.6) *obtained starting from* $(x_0, \mathcal{A}_{\widehat{\mathcal{B}},x_0})$ *and* $\widehat{U}$, *for every* $U' \subset\subset U \cap \widehat{U}$ *connected, we have*

$$[\mathcal{A}_{\mathcal{B}}(x)]^{-1} \circ \mathcal{A}_{\widehat{\mathcal{B}}}(x) = [\mathcal{A}_{\mathcal{B},x_0}]^{-1} \circ \mathcal{A}_{\widehat{\mathcal{B}},x_0} = \Big((B^{-1}\widehat{B}),\, B^{-1}(b - \widehat{b})\Big) \in \mathit{Aff}^{+}(\mathbb{Z}^d), \quad (4.8)$$

for every $x \in U'$.

Let U and $\Phi_{\mathcal{B}}(\cdot) := \tau_{\mathcal{B}}^{-1}(\cdot)$ be as in Theorem 4.5. For fixed (big enough) λ, we can think of $\Phi_{\mathcal{B}}(\cdot)$ as local approximate Lagrangian coordinates for $\mathcal{X} \cap U$. In fact from (4.7) (4.4) and (4.3) follows that for most of the $z_k \in \mathbb{Z}^d$ we have $\Phi_{\mathcal{B}}(z_k) \in B(x_{i(k)}, C\beta)$ for an unique $x_{i(k)} \in \mathcal{X}$ and a constant $C > 0$ depending on $\overline{m_1}$, $\overline{m_0}$. Moreover, we can think of (4.8) as the relation describing the change of local coordinates in terms of an element of the isotropy group of $\mathcal{L}(G)$. We also notice that we can cover the set $\widetilde{\Omega}_d(\frac{K}{2}, \beta, \frac{8}{9}\varepsilon_J, \frac{\varepsilon_v}{2}, \lambda)$ with a one parameter family of open simply connected subsets $\{U_\alpha\}_{\alpha \in \mathfrak{A}}$ and think of $\{(U_\alpha, \tau_{\mathcal{B}_\alpha})\}_{\alpha\in\mathfrak{A}}$ as a *meso-scale* system of (approximate) local inverse deformations in the sense of [3].

The last main result of the paper is stated in Corollary 4.6, where we show the existence of a positive threshold $\eta > 0$, which depends on the empirical density of $\rho_\lambda(x, \mathcal{X}) := \lambda^{-d}\sum_{x_i\in\mathcal{X}} \varphi_{\lambda,x}(x_i)$, such that $\{h_\lambda(\cdot, \mathcal{X}) + \vartheta_0\rho_\lambda(x, \mathcal{X}) < \eta\} \subset \widetilde{\Omega}_d(K, \beta, \varepsilon_J, \varepsilon_v, \lambda)$ and the infimum defining $h_\lambda(x_0, \mathcal{X})$ is achieved by the lattice $\mathcal{L}_x(\mathcal{A}_{x_0,0})$ ($\mathcal{A}_{0,x_0} \in \widetilde{\Omega}_x(K, \beta, \varepsilon_J, \varepsilon_v, \lambda)$) obtained in Theorem 4.4-(B) . Eventually, assuming that $\mathcal{X} \subset \Omega$ satisfies an uniform lower bound on the "discrete density" and has "small energy", we produce a (rough) estimate of the measure of $\widetilde{\Omega}_d(K, \beta, \varepsilon_J, \varepsilon_v, \lambda) \subseteq \Omega$.

Corollary 4.6. *Let* $x_0 \in \Omega$. *Suppose* $\mathcal{X} \subset \Omega$ *verifies* (3.10) *for some* $\rho > 0$. *We can find* $\eta := \eta(d, V, W, \rho) > 0$ *such that, for* λ *large enough (depending on* d, V, W, ρ, η*), from* $h_\lambda(x_0, \mathcal{X}) < \eta$ *we can deduce the existence of* $\overline{K}, \beta, \varepsilon_J, \varepsilon_v$ *such that* $\widetilde{\Omega}_{x_0}(\frac{\overline{K}}{2}, \beta, \frac{8}{9}\varepsilon_J, \frac{\varepsilon_v}{2}, \lambda) \neq \emptyset$ *and* $(\overline{K}, \beta, \varepsilon_J, \varepsilon_v, \lambda)$ *verify the hypotheses of Theorem 4.4. Moreover (keeping the notation of Theorem 4.4) we have*

$$h_\lambda(x_0, \mathcal{X}) = h_\lambda(x_0, \mathcal{A}_{0,x_0}, \mathcal{X}). \quad (4.9)$$

Finally, if there exists $\rho > 0$ *such that* $\mathcal{X}$ *satisfies* (3.10) *for every* $x \in \Omega$, *and*

$$|\Omega|^{-1}\left[H_\lambda(\mathcal{X}, \Omega) + \int_\Omega \vartheta_0\rho_\lambda(x, \mathcal{X})\,dx\right] < \eta', \quad (4.10)$$

for some $\eta' \in (0, \eta)$ *(*η *being as above), we have*

$$\frac{|\Omega \setminus \widetilde{\Omega}_d|}{|\Omega|} \leq \frac{\eta'}{\eta} + \frac{d\vartheta_1\widehat{C} + \sqrt{\vartheta_1/(C_{W,0}c_\varphi)}}{\lambda\eta}.$$

4.1. **Outline of the Proofs.** We begin introducing the following notion of *generalized interstitial* and *generalized vacancy*: Fixed $\beta > 0$ small and $\mathcal{A} \in \mathit{Aff}^{+}_{\triangleright}(\mathbb{R}^d_x)$, we say that $x_i \in \mathcal{X} \cap B(x, \lambda)$ is a generalized interstitial (with respect to β and $\mathcal{A}$) if $\sharp(B(x_i, \beta) \cap \mathcal{L}_x(\mathcal{A})) = \emptyset$. In a similar way we call generalized vacancies those $\mathcal{A}(z) \in \mathcal{L}_x(\mathcal{A}) \cap B(x, 2\lambda)$ such that $B(\mathcal{A}(z), \beta) \cap \mathcal{X} = \emptyset$. In other words, we look at a generalized lattice $\mathcal{L}_x(\mathcal{A}, \beta)$ obtained replacing $\mathcal{A}(z)$ with $B(\mathcal{A}(z), \beta)$ ($z \in \mathbb{Z}^d$), and define interstitials and vacancies with respect to $\mathcal{L}_x(\mathcal{A}, \beta)$. The purpose of generalized interstitials and vacancies is that of furnishing a way to identify point-defects, once we assumed that second (and higher) derivatives of the local deformation produce on $x_i \in \mathcal{X} \cap B(x, 2\lambda)$ a deviation of order at most β from the sites of $\mathcal{L}_x(\mathcal{A})$.

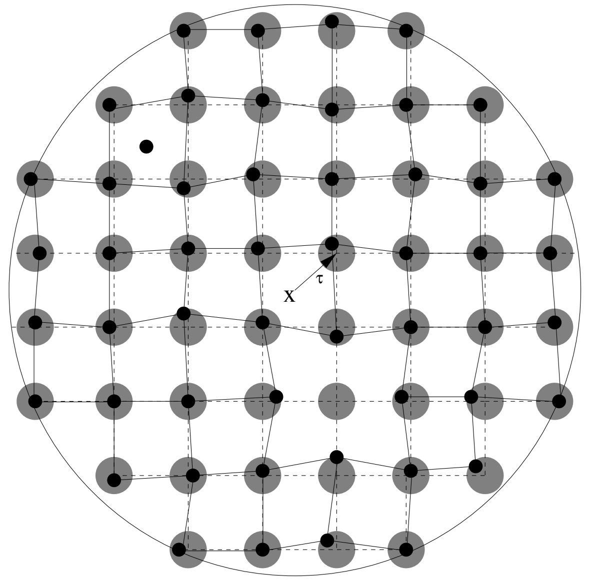

FIGURE 2. The black dots in the picture represent the elements of $\mathcal{X} \cap B(x, \lambda)$, where $\mathcal{X}$ is a low-energy configuration obtained adding two point defects (an interstitial and a vacancy) to an elastically deformed ground state lattice. The grey balls have radius β and are centered on the sites of a squared lattice $\mathcal{L}_x((Id, \tau))$ (nearly optimally fitted with $\mathcal{X} \cap B(x, \lambda)$). Particles falling in grey balls are β-regular points with respect to $\mathcal{L}_x((Id, \tau))$. The particle in the complementary of $\mathcal{L}_x((Id, \tau), \beta)$ represents a β-interstitial with respect to $\mathcal{L}_x((Id, \tau))$, while the empty grey ball corresponds to a β-vacancy with respect to $\mathcal{L}_x((Id, \tau))$.

Given $\mathcal{A} \in \widetilde{\Omega}_x(K, \beta, \varepsilon_J, \varepsilon_v, \lambda)$ we produce estimates on the number of regular points, generalized interstials and vacancies in terms of the values of $J_\lambda(x, \mathcal{A}, \mathcal{X}) + \vartheta_0 \rho_\lambda(x, \mathcal{X})$ and $\mathcal{V}_\lambda(x, \mathcal{A}, \mathcal{X})$ (see Proposition 5.6). Using such estimates, we find, for a given $K > 0$, thresholds for β, ε_J, ε_v such that for every $\mathcal{A}_1, \mathcal{A}_2 \in \widetilde{\Omega}_x(K, \beta, \varepsilon_J, \varepsilon_v, \lambda)$ the maps $\mathcal{A}_1 \mathcal{A}_2^{-1}$ and $\mathcal{A}_2 \mathcal{A}_1^{-1}$ transform most of the elements of $\mathbb{Z}^d \cap B(0, \lambda)$ in points belonging to a β-neighborhood of $\mathbb{Z}^d$. This enables us to find an unique element $\mathcal{B} = (B, b) \in \mathit{Aff}^+(\mathbb{Z}^d)$ such that $\mathcal{A}_{1,\mathcal{B}} := (A_1 B, x - AB^{-1}(B\tau + b))$ belongs to a $\| \cdot \|_\lambda$-ball of radius proportional to β centered in $\mathcal{A}_2$. This step is achieved in Lemma 5.12.

In Section 5.3 we compute the second derivatives $D^2_{\mathcal{A}\mathcal{A}} h_\lambda(x, \mathcal{A}, \mathcal{X})$ of $h_\lambda(x, \mathcal{A}, \mathcal{X})$ with respect to $\mathcal{A}$, and show that, for an appropriate choice of the parameters $\beta, \varepsilon_J, \varepsilon_v, \lambda$, we have $D^2_{\mathcal{A}\mathcal{A}} h_\lambda(x, \mathcal{A}, \mathcal{X}) > 0$ for every $\mathcal{A} \in \widetilde{\Omega}_x(K, \beta, \varepsilon_J, \varepsilon_v, \lambda)$. To obtain this result we use again the estimates on generalized point-defects and the uniform convexity of $W(\cdot, (A, x - A\tau))$ in $\{y \in \mathbb{R}^d : \mathrm{dist}(y, \mathcal{L}_x(\mathcal{A})) \le \beta\}$ when $\beta < \beta_0$.

The proof of Theorem 4.4 is then concluded as follows. Fixed $\mathcal{A}_0 \in \widetilde{\Omega}_x(K, \beta, \varepsilon_J, \varepsilon_v, \lambda)$ the continuity of $h_\lambda(x, \cdot, \mathcal{X})$ ensures the existence of $\delta > 0$ such that for every $\mathcal{A} \in \mathfrak{B}_\lambda(\mathcal{A}_0, \delta)$ we have $D^2_{\mathcal{A}\mathcal{A}} h_\lambda(x, \mathcal{A}, \mathcal{X}) > 0$; for every $\mathcal{A}_1, \mathcal{A}_2 \in \mathfrak{B}_\lambda(\mathcal{A}_0, \delta)$ Lemma 5.12 holds; there exists $\mathcal{A}_x \in \overline{\mathfrak{B}_\lambda(\mathcal{A}_0, \delta)}$ such that

$$h_\lambda(x, \mathcal{A}_x, \mathcal{X}) = \min_{\mathcal{A} \in \overline{\mathfrak{B}_\lambda(\mathcal{A}_0, \delta)}} h_\lambda(x, \mathcal{A}, \mathcal{X}).$$

We then show that we can choose our parameters in such way that if the minimizer A_x would belong to $\partial \mathfrak{B}_\lambda(\mathcal{A}_0, \delta)$ we would get a contradiction by Lemma 5.12. Finally we obtain the uniqueness of the minimum in $\mathfrak{B}_\lambda(\mathcal{A}_0, \delta)$ as a consequence of the strict convexity of $h_\lambda(x, \cdot, \mathcal{X})$ in $\mathfrak{B}_\lambda(\mathcal{A}_0, \delta)$

Again by the strict convexity of $h_\lambda(\cdot, \cdot, \mathcal{X})$ on $\widetilde{\Omega}(K, \beta, \varepsilon_J, \varepsilon_v, \lambda)$ and Theorem 4.4, we can apply the Implicit Function Theorem to the 0-level set of $D_{\mathcal{A}} h_\lambda(\cdot, \cdot, \mathcal{X})$ and obtain the existence of the map $\mathcal{A}(\cdot) \in C^1(U, V)$ satisfying (4.6) and (4.8). By a careful estimate, again based on the Implicit Function Theorem, we obtain (4.7), and this concludes the proof of Theorem 4.5.

Eventually the proof of Corollary 4.6 is obtained by the combination of the previous results and Proposition 3.3.

5. Preliminary Lemmata

5.1. **Generalized β-point-defects.** In the present section, given $x \in \Omega$, $\mathcal{X} \subset \Omega$, $\mathcal{A} \in Aff^+_{\triangleright}(\mathbb{R}^d_x)$ and $\beta \in [0, s_0/2)$, we define the β-*interstitials* and β-*vacancies* of $\mathcal{X}$ with respect to the lattice $\mathcal{L}_x(\mathcal{A})$ (see Figure 2). Such definitions depend on the parameter β and coincide with the usual notion of self-interstial and vacancy for the lattice $\mathcal{L}_x(\mathcal{A})$ when $\beta = 0$. This section's main result is Proposition 5.6 where, for $\mathcal{A} \in \widetilde{\Omega}_x(K, \beta, \varepsilon_J, \varepsilon_v, \lambda)$, we estimate the number of β-point defects of $\mathcal{X}$ in $B(x, 2\lambda)$ with respect to $\mathcal{L}_x(\mathcal{A})$ in terms of the parameters $K, \beta, \varepsilon_J, \varepsilon_v, \lambda$, and we derive an estimate from above on the cardinality of $\mathcal{X} \cap B(x, 2\lambda)$ by means of the number of lattice points of $\mathcal{L}_x(\mathcal{A})$ in $B(x, 2\lambda)$ and the number of β-interstitials (with respect $\mathcal{L}_x(\mathcal{A})$).

Definition 5.1. *Let $\beta \in [0, s_0/2)$. Let $x_j \in \mathcal{X}$ and $\mathcal{A} \in Aff^+_{\triangleright}(\mathbb{R}^d_x)$. We say that x_j belongs to the set of the β-regular points of $\mathcal{X}$ with respect to $\mathcal{L}_x(\mathcal{A})$, denoted by $\mathcal{R}^\beta_{\mathcal{A}}(x)$, if there exists $z_{k(j)} \in \mathbb{Z}^d$ such that*

$$\{x_j\} = B(\mathcal{A}(z_{k(j)}), \beta) \cap \mathcal{X}.$$

Moreover if $x_j \in \mathcal{X} \setminus \mathcal{R}^\beta_{\mathcal{A}}(x)$ we say that x_j belongs to the set $\mathcal{I}^\beta_{\mathcal{A}}(x)$ of the β-interstitials of $\mathcal{X}$ with respect to $\mathcal{L}_x(\mathcal{A})$.

Definition 5.2. *Let $\beta \in [0, \frac{s_0}{2})$ and $\mathcal{A} \in Aff^+_{\triangleright}(\mathbb{R}^d_x)$. We define the set of the β-vacancies of $\mathcal{X}$ with respect to $\mathcal{L}_x(\mathcal{A})$ as*

$$\mathcal{V}^\beta_{\mathcal{A}}(x) := \{\mathcal{A}(z_l) \in \mathcal{L}_x(\mathcal{A}) : B(\mathcal{A}(z_l), \beta) \cap \mathcal{X} = \emptyset\} \tag{5.1}$$

We notice that, for a given $\mathcal{X}$, the sets $\mathcal{R}^\beta_{\mathcal{A}}(x), \mathcal{I}^\beta_{\mathcal{A}}(x), \mathcal{V}^\beta_{\mathcal{A}}(x)$ depend only on $\mathcal{L}_x(\mathcal{A})$. That is if $\mathcal{L}_x(\mathcal{A}) = \mathcal{L}_x(\widehat{\mathcal{A}})$ the corresponding sets of β-regular points, -interstitials, -vacancies of $\mathcal{X}$ are the same.

Remark 5.3. If $2\beta < C_0^{-1} K^{1-d}$ (C_0 being as in (4.1)) and $\mathcal{A} \in \widetilde{\Omega}_x(K, \beta, \varepsilon_J, \varepsilon_v, \lambda)$, (4.2) we have

$$|\mathcal{A}(z_k) - \mathcal{A}(z_h)| \geq m_0(\mathcal{L}_x(\mathcal{A})) > 2\beta,$$

for every $z_k \neq z_h,\ z_k, z_h \in \mathcal{A}^{-1}(B(x, 2\lambda))$. Therefore, by Definition 4.1-(O4), for every $x_i \in \mathcal{X}$ such that $\operatorname{dist}(x_i, \mathcal{A}(\mathbb{Z}^d)) \leq \beta$ there exists a unique $z_{k(i)} \in \mathbb{Z}^d$ such that $x_i \in B(\mathcal{A}(z_{k(i)}), \beta)$, so that

$$\mathcal{R}^\beta_{\mathcal{A}}(x) = \{x_i \in \mathcal{X} : \sharp\big(B(x_i, \beta) \cap \mathcal{L}_x(\mathcal{A})\big) = 1\}.$$

Remark 5.4. By Definition 5.1 we have $\mathcal{I}^\beta_{\mathcal{A}}(x) = \mathcal{D}^\beta_{\mathcal{A}}(x) \cup \mathcal{S}^\beta_{\mathcal{A}}(x)$, where

$$\mathcal{D}^\beta_{\mathcal{A}}(x) := \left\{x_j \in \mathcal{X} : \operatorname{dist}(x_j, \mathcal{A}(\mathbb{Z}^d)) \geq \beta\right\}, \tag{5.2}$$

$$\mathcal{S}^\beta_{\mathcal{A}}(x) := \left\{x_j \in \mathcal{X} : \exists\, z_{l(j)} \in \mathbb{Z}^d \text{ such that } \sharp\left(B(\mathcal{A}(z_{l(j)}), \beta) \cap \mathcal{X}\right) \geq 2\right\}. \tag{5.3}$$

However, since $\beta < \frac{s_0}{2}$, whenever $\mathcal{A} \in \widetilde{\Omega}(K, \beta, \varepsilon_J, \varepsilon_v, \lambda)$ we have $\mathcal{S}^\beta_{\mathcal{A}} = \emptyset$ by Definition 4.1-(O4).

Remark 5.5. As a direct consequence of (5.1) we have

$$\begin{aligned} \sharp\mathcal{V}^\beta_{\mathcal{A}}(x) =& \sharp\mathcal{L}_x(\mathcal{A}) \setminus \{z_k \in \mathbb{Z}^d : \operatorname{dist}(\mathcal{A}(z_k), \mathcal{X}) \leq \beta\} \\ \leq& \sharp\mathcal{L}_x(\mathcal{A}) \setminus \mathcal{R}^\beta_{\mathcal{A}}(x) \\ =& \sharp\mathcal{L}_x(\mathcal{A}) \setminus (\mathcal{X} \setminus \mathcal{I}^\beta_{\mathcal{A}}(x)) \end{aligned}$$

We are now in a position to prove the following

Proposition 5.6. *Let* $(x, \mathcal{A}) = \Big(x, (A, \tau)\Big) \in \widetilde{\Omega}(K, \beta, \varepsilon_J, \varepsilon_v, \lambda)$. *Then*

$$\sum_{x_i \in \mathcal{I}^\beta_{\mathcal{A}}(x)} \varphi_{\lambda,x}(x_i) \leq \frac{\varepsilon_J}{C_{W,0}} \frac{\lambda^d}{\det A}, \tag{5.4}$$

$$\sum_{x_j \in \mathcal{R}^\beta_{\mathcal{A}}(x)} \varphi_{\lambda,x}(x_j) \geq \left[(C_\varphi \omega_d - \varepsilon_v) - \frac{\varepsilon_J}{C_{W,0}}\right] \frac{\lambda^d}{\det A}, \tag{5.5}$$

$$\sum_{z_k \in \mathcal{V}^\beta_{\mathcal{A}}(x)} \varphi_{\lambda,x}(\mathcal{A}(z_k)) \leq \left(\frac{(m_1(\mathcal{L}_x(\mathcal{A})) + \beta)C_1}{\lambda} + \varepsilon_v + \frac{\varepsilon_J}{C_{W,0}}\right) \frac{\lambda^d}{\det A}, \tag{5.6}$$

$$\sum_{x_i \in \mathcal{X}} \varphi_{\lambda,x}(x_i) \leq \left[C_\varphi + \frac{(m_1(\mathcal{L}(\mathcal{A})) + \beta)C_1}{\lambda} + \frac{\varepsilon_J}{C_{W,0}}\right] \frac{\lambda^d}{\det A}. \tag{5.7}$$

Proof. By Definition 4.1-(O2) we obtain

$$\begin{aligned} &C_{W,0}\, \beta^2 \sum_{x_i \in \{x_j \in \mathcal{X} :\, \operatorname{dist}(x_j, \mathcal{L}_x(\mathcal{A})) > \beta\}} \varphi_{\lambda,x}(x_i) \leq C_{W,0} \sum_{x_i \in \mathcal{X}} \operatorname{dist}^2(x_i, \mathcal{L}_x(\mathcal{A})) \varphi_{\lambda,x}(x_i) \\ &\leq \sum_{x_i \in \mathcal{X}} W(x_i, \mathcal{L}_x(\mathcal{A})) \varphi_{\lambda,x}(x_i) \leq \varepsilon_J \beta^2 \frac{\lambda^d}{\det A}, \end{aligned}$$

hence (5.4) holds. By Definition 5.1 and Definition 4.1-(O3) we deduce

$$\sum_{x_j \in \mathcal{R}^\beta_{\mathcal{A}}(x)} \varphi_{\lambda,x}(x_j) \geq \left[(C_\varphi - \varepsilon_v) - \frac{\varepsilon_J}{C_{W,0}}\right] \frac{\lambda^d}{\det A},$$

which is (5.5).

Given $x_j \in \mathcal{R}^\beta_{\mathcal{A}}(x)$ we denote by $z_{k(j)}$ an element of $\mathbb{Z}^d$ satisfying $x_j \in B(\mathcal{A}(z_{k(j)}),\beta)$. By (5.5), Remark 5.5, (3.18) and (3.15) we obtain

$$\begin{aligned}
&\sum_{z_k\in\mathcal{V}^\beta_{\mathcal{A}}(x)} \varphi_{\lambda,x}(\mathcal{A}(z_k)) \le \sum_{z_k\in\mathbb{Z}^d} \varphi_{\lambda,x}(\mathcal{A}(z_k)) - \sum_{x_j\in\mathcal{R}^\beta_{\mathcal{A}}(x)} \varphi_{\lambda,x}(x_j)\\
&+\sum_{x_j\in\mathcal{R}^\beta_{\mathcal{A}}(x)} \Big(\varphi_{\lambda,x}(x_j)-\varphi_{\lambda,x}(\mathcal{A}(z_{k(j)}))\Big)\\
&\le\left(\frac{3^d d\omega_d\|\varphi'\|_{L^\infty(\mathbb{R})}\|A\|_*}{\lambda}\omega_d+\varepsilon_v+\frac{\varepsilon_J}{C_{W,0}}\right)\frac{\lambda^d}{\det A}\\
&+\frac{\|\varphi'\|_{L^\infty(\mathbb{R})}\beta}{\lambda}\sharp\Big(\mathcal{L}_x(\mathcal{A})\cap\Big(B(x,2\lambda+\beta)\setminus B(x,\lambda-\beta)\Big)\Big)\\
&\le\left(\frac{3^d d\omega_d\|\varphi'\|_{L^\infty(\mathbb{R})}\|A\|_*}{\lambda}\omega_d+\varepsilon_v+\frac{\varepsilon_J}{C_{W,0}}\right)\frac{\lambda^d}{\det A}\\
&+\frac{3^d d\omega_d\|\varphi'\|_{L^\infty(\mathbb{R})}\beta}{\lambda}\frac{\lambda^d}{\det A},
\end{aligned}$$

where by ξ_j we denoted a point on the segment joining x_j and $\mathcal{A}(z_{k(j)})$, and we used (3.15) to estimate $\mathcal{L}_x(\mathcal{A})\cap\Big(B(x,2\lambda+\beta)\setminus B(x,\lambda-\beta)\Big)$.

Given $x_i \in \mathcal{R}^\beta_{\mathcal{A}}(x)$ we denote by $z_{k(i)}$ an element of $\mathbb{Z}^d$ satisfying $x_i \in B(\mathcal{A}(z_{k(i)}),\beta)$. By

$$\begin{aligned}
\sum_{x_i\in\mathcal{X}}\varphi_{\lambda,x}(x_i) \le &\sum_{x_i\in\mathcal{R}^\beta_{\mathcal{A}}(x)} \big(\varphi_{\lambda,x}(x_i)-\varphi_{\lambda,x}(\mathcal{A}(z_{k(i)}))\big) + \sum_{x_i\in\mathcal{I}^\beta_{\mathcal{A}}(x)}\varphi_{\lambda,x}(x_i)\\
&+\sum_{z_k\in\mathbb{Z}^d}\varphi_{\lambda,x}(\mathcal{A}(z_k)),
\end{aligned}$$

developing up to first order $\varphi_{\lambda,x}(\cdot)$ around the elements of $\mathcal{R}^\beta_{\mathcal{A}}(x)$, we obtain (5.7) by (5.4), (3.18), (3.15). □

Remark 5.7. Let $\mathcal{X}$ be given and let $\mathcal{A}\in\widetilde{\Omega}_x(K,\beta,\varepsilon_J,\varepsilon_v,\lambda)$. For a fixed $r\in[1,2]$, as a consequence of Definition 4.1-(O4) and (5.4), we have

$$\begin{aligned}
\sharp(\mathcal{I}^\beta_{\mathcal{A}}(x)\cap B(x,2\lambda)) \le &\sum_{x_i\in\mathcal{I}^\beta_{\mathcal{A}}(x)\cap B(x,r\lambda)} \frac{\varphi_{\lambda,x}(x_i)}{\varphi(r)} + \sharp(\mathcal{X}\cap(B(x,2\lambda)\setminus B(x,r\lambda)))\\
&\le\frac{\varepsilon_J}{C_{W,0}\varphi(r)}\frac{\lambda^d}{\det A}+\frac{\omega_d(2^d-r^d)}{s_0^d}\lambda^d.
\end{aligned}$$

5.2. **Further estimates on $\widetilde{\Omega}(K,\beta,\varepsilon_J,\varepsilon_v,\lambda)$.** The main results of the present section is Lemma 5.8, where we show that a $\|\cdot\|_\lambda$- ball of radius δ centered in an element of $\widetilde{\Omega}_x(K,\beta,\varepsilon_J,\varepsilon_v,\lambda)$ is contained in $\widetilde{\Omega}_x(2K,\beta,C_2(K)(\varepsilon_J+\delta),2\varepsilon_v,\lambda)$, for every $x\in\widetilde{\Omega}_d(K,\beta,\varepsilon_J,\varepsilon_v,\lambda)$.

Lemma 5.8. *Let $(x,\mathcal{A}_0)\in\widetilde{\Omega}(K,\beta,\varepsilon_J,\varepsilon_v,\lambda)$ be such that $\mathcal{A}_0$ is a canonical representation for $\mathcal{L}_x(\mathcal{A}_0)$. There exists $\overline{\lambda}:=\overline{\lambda}(d,K)$, such that if $\lambda>\overline{\lambda}$ and $\delta<2$ then*

$$\mathfrak{B}_\lambda(\mathcal{A}_0,\delta)\subset\widetilde{\Omega}_x(2K,\beta,\frac{3C_{W,1}}{C_{W,0}}(\varepsilon_J+\frac{\delta^2C_2(K)}{\beta^2}),2\varepsilon_v,\lambda).$$

Proof. We fix $\lambda > 2$ and $\delta \in (0,2)$. By the continuity of the determinant and the norm of the inverse restrcited to $GL^+(d,\mathbb{R})$, for every $\mathcal{A} \in \mathfrak{B}_\lambda(\mathcal{A}_0,\delta) \cap \mathit{Aff}^+_\triangleright(\mathbb{R}^d_x)$ we obtain

$$\max\Big\{|A - A_0|, \Big|\frac{\det A_0}{\det A} - 1\Big|, \Big|\frac{1}{\det A_0} - \frac{1}{\det A}\Big|\Big\} < \mathcal{O}'(K, \frac{1}{\lambda}, \delta), \tag{5.8}$$

where, for any fixed $K > 0$, we have $\mathcal{O}'(K,s,t) \to 0$ as $s \to 0$ and/or $t \to 0$. In particular, for large enough λ (depending on d, K), we can conclude that

$$m_1(\mathcal{L}_x(\mathcal{A})) \leq K + \mathcal{O}'(K, \frac{1}{\lambda}, \delta).$$

Denoting by $z_{k(i)}$ the projection of x_i on $\mathcal{L}_x(\mathcal{A}_0)$, we obtain

$$\begin{aligned}
&\sum_{x_i \in \mathcal{X}} W(x_i, \mathcal{L}_x(\mathcal{A}))\varphi_{\lambda,x}(x_i) \leq C_{W,1} \sum_{x_i\in\mathcal{X}} \operatorname{dist}^2(x_i, \mathcal{L}_x(\mathcal{A}))\varphi_{\lambda,x}(x_i)\\
\leq& 2C_{W,1} \sum_{x_i \in \mathcal{X}} \Big[|x_i - \mathcal{A}_0(z_{k(i)})|^2 + |\mathcal{A}_0(z_{k(i)}) - \mathcal{A}(z_{k(i)})|^2\Big]\varphi_{\lambda,x}(x_i)\\
\leq& 2C_{W,1} \sum_{x_i \in \mathcal{X}} \Big[|x_i - \mathcal{A}_0(z_{k(i)})|^2 + 2(\|A_0 - A\|_*^2 |z_{k(i)}|^2 + |A\tau - A_0\tau_0|^2)\Big]\varphi_{\lambda,x}(x_i)\\
\leq& 2\frac{C_{W,1}}{C_{W,0}} \sum_{x\in\mathcal{X}} W(x_i, \mathcal{L}_x(\mathcal{A}_0))\varphi_{\lambda,x}(x_i) + 5C_{W,1}\delta^2 \|A_0^{-1}\|_*^2 \sum_{x_i\in\mathcal{X}} \varphi_{\lambda,x}(x_i)\\
\leq& 2\frac{C_{W,1}}{C_{W,0}}\Big(\varepsilon_J\beta^2 + \frac{5\delta^2 C_0 K^{(d-1)/d}}{2} C_{W,0}\Big(C_\varphi + \frac{(K+\beta)C_1}{\lambda} + \frac{\varepsilon_J}{C_{W,0}}\Big)\Big)\frac{\det A}{\det A_0}\frac{\lambda^d}{\det A},
\end{aligned}$$

where we used assumption (P1) on W, and in the last inequality we estimated $\sum_{x_i\in\mathcal{X}} \varphi_{\lambda,x}(x_i)$ by means of (5.7). Eventually, from the latter estimate, we get the thesis choosing λ big enough to fulfill $\det A/\det A_0 < 3/2$ for every $\mathcal{A} \in \mathfrak{B}_\lambda(\mathcal{A}_0,\delta)$ (again this is possible by (5.8)), and setting

$$C_2(K) := \frac{5C_0K^{(d-1)/d}C_{W,0}}{2}\Big(C_\varphi + \frac{(K+\beta)C_1}{\lambda} + \frac{\varepsilon_J}{C_{W,0}}\Big). \tag{5.9}$$

□

5.3. **Strict-convexity of $h_\lambda(x,\cdot,\mathcal{X})$ on $\widetilde{\Omega}(K,\beta,\varepsilon_J,\varepsilon_v,\lambda)$.** In this section we show that, for an opportune choice of the parameters $(K,\beta,\varepsilon_J,\varepsilon_v,\lambda)$, we can conclude that $\widetilde{\Omega}(K,\beta,\varepsilon_J,\varepsilon_v,\lambda) \subseteq \{D^2_{\mathcal{A}\mathcal{A}} h_\lambda(\cdot,\cdot,\mathcal{X}) > 0\}$ (see Corollary 5.11).

We begin establishing a lower bound for the Hessian of $J_\lambda(x,\mathcal{A},\mathcal{X})$ when $\mathcal{X} \cap B(x,2\lambda) = \mathcal{L}_x(\mathcal{A}) \cap B(x,2\lambda)$, and $\mathcal{A} \in \mathcal{E}$.

Proposition 5.9. *Let $x \in \Omega$. Let $\mathcal{A} = (A,\tau) \in \mathit{Aff}^+_\triangleright(\mathbb{R}^d_x)$ be such that $(A, x - A\tau) \in \mathcal{E} \subset \mathit{Aff}^+(\mathbb{R}^d)$, so that $W(\cdot,\cdot)$ is C^2-smooth in a neighborhood of $(x,\mathcal{A})$. Suppose that A is associated with a reduced, positively oriented basis of $\mathcal{L}(A)$ and $\mathcal{X} \cap B(x,2\lambda) = \mathcal{L}_x(\mathcal{A}) \cap B(x,2\lambda)$. There exists $\lambda_c := \lambda_c(K,d,W,s_0) > 0$ such that if $\lambda > \lambda_c$, then, for every $\mathcal{M} = (M,\mu) \in \mathbb{R}^{d\times d} \times \mathbb{R}^d$, we have*

$$\begin{aligned}
&\mathcal{M}^T\Big(D^2_{\mathcal{A}\mathcal{A}} \sum_{x_i\in\mathcal{X}} W(x_i,(A, x - A\tau))\varphi_{\lambda,x}(x_i)\Big)\mathcal{M} \qquad (5.10)\\
\geq& C_{W,0} \sum_{z_k\in\mathbb{Z}^d} |M(z_k - \tau) - A\mu|^2 \varphi_{\lambda,x}(\mathcal{A}(z_k)) \geq C_{\mathrm{conv}}(\|MA^{-1}\|_*^2\lambda^2 + |A\mu|^2)\frac{\lambda^d}{\det A},
\end{aligned}$$

where $C_{\rm conv} := C_{\rm conv}(W, \varphi, s_0) > 0.$

Proof. By the assumtpions (P1), (P2) on W we obtain

$$\begin{aligned}&\mathcal{M}^T\Big(D^2_{\mathcal{A}\mathcal{A}}\sum_{x_i\in\mathcal{X}} W(x_i,(A,x-A\tau))\varphi_{\lambda,x}(x_i)\Big)\mathcal{M}\\ \ge& C_{W,0}\mathcal{M}^T\Big(\sum_{x_i\in\mathcal{X}}\Big(D^2_{\mathcal{A}\mathcal{A}}|(x_i-x)-A(z_{k(i)}-\tau)|^2\Big)\varphi_{\lambda,x}(x_i)\Big)\mathcal{M}\\ =&C_{W,0}\sum_{z_k\in\mathbb{Z}^d}|M(z_k-\tau)-A\mu|^2\varphi_{\lambda,x}(\mathcal{A}(z_k)).\end{aligned}$$

Next we observe that

$$\begin{aligned}&\sum_{z_k\in\mathbb{Z}^d}|M(z_k-\tau)-A\mu|^2\varphi_{\lambda,x}(\mathcal{A}(z_k))=\int_{\mathbb{R}^d}\Big|(MA^{-1}(\mathcal{A}(v)-x)-A\mu\Big|^2\varphi_{\lambda,x}(\mathcal{A}(v))\,dv\\ &+\sum_{z_k\in\mathbb{Z}^d}\int_{Q(z_k)}\Big[|M(z_k-\tau)-A\mu|^2-|M(v-\tau)-A\mu|^2\Big]\varphi_{\lambda,x}(\mathcal{A}(z_k))\,dv\\ &+\sum_{z_k\in\mathbb{Z}^d}\int_{Q(z_k)}|M(v-\tau)-A\mu|^2\left[\varphi_{\lambda,x}(\mathcal{A}(z_k))-\varphi_{\lambda,x}(\mathcal{A}(v))\right]\,dv.\end{aligned}$$

By a change of variable in the first integral on the right hand side of the previous estimate, and expanding $\varphi_{\lambda,x}$ up to the first order, we obtain

$$\begin{aligned}&\sum_{z_k\in\mathbb{Z}^d}|M(z_k-\tau)-A\mu|^2\varphi_{\lambda,x}(\mathcal{A}(z_k))\\ =&\frac{\lambda^d}{\det A}\int_{\mathbb{R}^d}|\lambda(MA^{-1})y-A\mu|^2\varphi(|y|)\,dv \qquad (5.11)\\ -&\sum_{z_k\in\mathbb{Z}^d}\int_{Q(z_k)}\big(|M(z_k-\tau)-A\mu|^2-|M(v-\tau)-A\mu|^2\big)\varphi_{\lambda,x}(\mathcal{A}(z_k))\,dv\\ +&\sum_{z_k\in\mathbb{Z}^d}\int_{Q(z_k)}|M(v-\tau)-A\mu|^2\left[\frac{\varphi'}{\lambda}\left(\frac{|A(\xi(z_k,v)-\tau)|}{\lambda}\right)\langle\frac{A(\xi(z_k,v)-\tau)}{|A(\xi(z_k,v)-\tau)|},A(v-z_k)\rangle\right]\,dv,\end{aligned}$$

where $\xi_{z_k,v}$ denotes a suitable point on the segments joining z_k and v.
Passing to polar coordinates we get

$$\begin{aligned}\int_{\mathbb{R}^d}|\lambda(MA^{-1})y-A\mu|^2\varphi(|y|)\,dy&=\int_{\mathbb{R}^d}(\lambda^2|(MA^{-1})y|^2+|A\mu|^2)\varphi(|y|)\,dy\\ &\ge 2\widetilde{C}_\varphi(\lambda^2|MA^{-1}|^2+|A\mu|^2)\ge\frac{2\widetilde{C}_\varphi}{d}\left(\|MA^{-1}\|_*^2\lambda^2+|A\mu|^2\right).\end{aligned}$$

Now we notice that for every $z_k\in\mathbb{Z}^d$ such that $Q(z_k)\cap\mathcal{A}^{-1}(B(0,2\lambda))\neq\emptyset$, we have

$$\begin{aligned}&\Big||M(z_k-\tau)-A\mu|^2-|M(v-\tau)-A\mu|^2\Big|\\ =&|\langle M(z_k-v),M(z_k-\tau)+M(v-\tau)-2A\mu\rangle|\\ \le&\|A\|_*\|MA^{-1}\|_*\Big(\|MA^{-1}\|_*(2\lambda)+\|MA^{-1}\|_*(2\lambda+\sqrt{d})+2|A\mu|\Big) \qquad (5.12)\\ \le&\|A\|_*(5\|MA^{-1}\|_*^2\lambda+2\|MA^{-1}\|_*|A\mu|)=\frac{\|A\|_*}{\lambda}(5\|MA^{-1}\|_*^2\lambda^2+2(\|MA^{-1}\|_*\lambda)|A\mu|)\\ \le&\frac{\|A\|_*}{\lambda}(6\|MA^{-1}\|_*^2\lambda^2+|A\mu|)\le\frac{6\|A\|_*}{\lambda}(\|MA^{-1}\|_*^2\lambda^2+|A\mu|^2).\end{aligned}$$

Hence we can use (5.12) to estimate the last two terms in (5.11), and obtain

$$\begin{aligned}&\sum_{z_k\in\mathbb{Z}^d}|M(z_k-\tau)-A\mu|^2\varphi_{\lambda,x}(\mathcal{A}(z_k))\\ &\geq \lambda^d\frac{\|MA^{-1}\|_*^2\lambda^2+|A\mu|^2}{\det A}\left(\frac{2\widetilde{C}_\varphi}{d}-\frac{6\|A\|_*}{\lambda}(C_\varphi+\frac{C_1\|A\|_*}{\lambda})-\frac{2^dC_1\|A\|_*}{3^d\lambda}\right)\end{aligned}$$

hence the thesis follows from the assumption that A is associated with a positively oriented basis of $\mathcal{L}_x(\mathcal{A})$. □

Next we show that, for a given K and large enough λ, there exists a suitable choice of the parameters $\beta, \varepsilon_J, \varepsilon_v$ such that if $(x,\mathcal{A})\in\widetilde{\Omega}(K,\beta,\varepsilon_J,\varepsilon_v,\lambda)$ and A is associated to a reduced positive basis of $\mathcal{L}(A)$, then $\mathcal{A}$ belongs to the subset of $\mathit{Aff}^+_{\triangleright}(\mathbb{R}^d_x)$ where $h_\lambda(x,\cdot,\mathcal{X})$ is strictly convex.

Proposition 5.10. *Let $K\in(\frac{1}{C_0^{1/d}},\frac{1}{(C_0\overline{m_0})^{1/(d-1)}})$ be given. Suppose $\beta\in(0,\beta_0)$, and ε_J, $\varepsilon_v>0$ satisfy*

$$8\left(\varepsilon_v+\frac{\varepsilon_J}{C_{W,0}}\left(1+\mathcal{W}\right)\right)<\frac{C_{\rm conv}}{3},\tag{5.13}$$

where $\mathcal{W}$ is as in (2.16). There exists $\widehat{\lambda}_C:=\widehat{\lambda}_C(K)$ such that for every $\lambda>\widehat{\lambda}_C$, if $(x,\mathcal{A})\in\widetilde{\Omega}(K,\beta,\varepsilon_J,\varepsilon_v,\lambda)$ and A is associated with a reduced, positively oriented basis of $\mathcal{L}(A)$ then, for every $\mathcal{M}:=(M,\mu)\in\mathbb{R}^{d\times d}\times\mathbb{R}^d$ we have

$$\mathcal{M}^T:D^2_{\mathcal{A}\mathcal{A}}J_\lambda(x,\mathcal{A}_0,\mathcal{X}):\mathcal{M}>\frac{C_{{\rm conv},K}}{2}\|\mathcal{M}\|^2_\lambda,\tag{5.14}$$

where $C_{{\rm conv},K}:=C_{\rm conv}K^{-d}\big(\min\{K^{-1},s_0^d/(2^{d+1}K^{d-1})\}\big)^2$.

Proof. By (5.13), since $\beta_0<\overline{m_0}<1/(C_0K^{(d-1)})$, we can apply by Remark 5.3, and deduce that for every $x_i\in\mathcal{R}^\beta_{\mathcal{A}}(x)$ there exists an unique element of $\mathcal{L}_x(\mathcal{A})$, denoted by $z_{k(i)}$, such that $|\mathcal{A}(z_{k(i)})+x-x_i|<\beta$. Hence

$$\begin{aligned}&\mathcal{M}^T\left[\sum_{x_i\in\mathcal{X}}D^2_{\mathcal{A}\mathcal{A}}W(x_i,(A,x-A\tau))\varphi_{\lambda,x}(x_i)\right]\mathcal{M}\\ \geq&\frac{C_{W,0}}{2}\mathcal{M}^T\Big[\sum_{x_i\in\mathcal{X}\setminus\mathcal{I}^\beta_{\mathcal{A}}(x)}D^2_{\mathcal{A},\mathcal{A}}|x_i-A(z_{k(i)}-\tau)-x|^2\varphi_{\lambda,x}(x_i)\Big]\mathcal{M}\\ -&\mathcal{W}\sum_{x_i\in\mathcal{I}^\beta_{\mathcal{A}}(x)}|\mathcal{M}(\mathcal{A}(x_i))|^2\varphi_{\lambda,x}(x_i)\geq\frac{C_{W,0}}{2}\sum_{z_k\in\mathcal{A}(B(x,2\lambda))\setminus\mathcal{V}^\beta_{\mathcal{A}}(x)}|M(z_k-\tau)-A\mu|^2\varphi_{\lambda,x}(\mathcal{A}(z_k))\\ -&\frac{C_{W,0}}{2}\sum_{z_k\in\mathcal{A}(B(x,2\lambda))\setminus\mathcal{V}^\beta_{\mathcal{A}}(x)}|M(z_k-\tau)-A\mu|^2\left|\varphi_{\lambda,x}(\mathcal{A}(z_k)+x)-\varphi_{\lambda,x}(x_{i(k)})\right|\\ +&\frac{C_{W,0}}{2}\sum_{x_j\in\mathcal{X}\setminus\mathcal{I}^\beta_{\mathcal{A}}(x)}\big((x_i-x)-A(z_k-\tau)\big)^TM\mu\varphi_{\lambda,x}(x_i)-\mathcal{W}\sum_{x_i\in\mathcal{I}^\beta_{\mathcal{A}}(x)}|\mathcal{M}((\mathcal{A}(x_i))|^2\varphi_{\lambda,x}(x_i).\end{aligned}$$

By definition of $\mathcal{I}_{\mathcal{A}}^{\beta}$ we get

$$\mathcal{M}^T\Big[D^2_{\mathcal{A}\mathcal{A}}\sum_{x_i\in\mathcal{X}} W(x_i,(A,x-A\tau),)\varphi_{\lambda,x}(x_i)\Big]\mathcal{M}$$

$$\geq \frac{C_{W,0}}{2}\sum_{z_k\in\mathcal{A}(B(x,2\lambda))\setminus\mathcal{V}_{\mathcal{A}}^{\beta}(x)} |M(z_k-\tau)-A\mu|^2\varphi_{\lambda,x}(\mathcal{A}(z_k))$$

$$-C_{W,0}\|\varphi'\|_{L^\infty(\mathbb{R})}\frac{\beta}{2\lambda}\sum_{z_k\in\mathcal{A}(B(x,2\lambda))\setminus\mathcal{V}_{\mathcal{A}}^{\beta}(x)}|M(z_k-\tau)-A\mu|^2$$

$$-C_{W,0}\sqrt{d}\beta\|MA^{-1}\|_*|A\mu|\sum_{x_j\in\mathcal{X}\setminus\mathcal{I}_{\mathcal{A}}^{\beta}(x)}\varphi_{\lambda,x}(x_i)-\mathcal{W}\sum_{x_i\in\mathcal{I}_{\mathcal{A}}^{\beta}(x)}|\mathcal{M}(\mathcal{A}(x_i))|^2\varphi_{\lambda,x}(x_j)$$

$$=\frac{C_{W,0}}{2}\sum_{z_k\in\mathbb{Z}^d}|M(z_k-\tau)-A\mu|^2\varphi_{\lambda,0}(\mathcal{A}(z_k))-\frac{C_{W,0}}{2}\sum_{z_k\in\mathcal{V}_{\mathcal{A}}^{\beta}(x)}|M(z_k-\tau)-A\mu|^2\varphi_{\lambda,0}(\mathcal{A}(z_k))$$

$$-\frac{C_{W,0}\|\varphi'\|_{L^\infty(\mathbb{R})}\sqrt{d}\beta(\|MA^{-1}\|_*^2\lambda^2+|A\mu|^2)}{\lambda}\sharp\{z_k\in\mathcal{A}(B(x,2\lambda))\setminus\mathcal{V}_{\mathcal{A}}^{\beta}(x)\}$$

$$-\frac{C_{W,0}\beta\sqrt{d}(\|MA^{-1}\|_*^2\lambda^2+|A\mu|^2)}{2\lambda}\sum_{x_j\in\mathcal{R}_{\mathcal{A}}^{\beta}(x)}\varphi_{\lambda,x}(x_i)-\mathcal{W}\sum_{x_i\in\mathcal{I}_{\mathcal{A}}^{\beta}(x)}|\mathcal{M}(\mathcal{A}(x_i))|^2\varphi_{\lambda,x}(x_i).$$

By (5.10), (5.4), (5.5), (5.6), (5.7) and by

$$|\mathcal{M}(z_k-\tau)-A\mu|^2\leq 4d(\|MA^{-1}\|_*^2\lambda^2+|A\mu|^2),$$

we have

$$\frac{1}{\lambda^d}\mathcal{M}^T\Big(\sum_{x_i\in\mathcal{X}}D^2_{\mathcal{A}\mathcal{A}}W(x_i-x,\mathcal{A})\Big)\mathcal{M}$$

$$\geq\left[\left(C_{\mathrm{conv}}-8\Big(\varepsilon_v+\frac{\varepsilon_J}{C_{W,0}}(1+\mathcal{W})\Big)\right)-\frac{c\,\|A\|_*}{\lambda}\right]\frac{\|MA^{-1}\|_*^2\lambda^2+|A\mu|^2}{\det A},$$

where $c:=c(d,C_\varphi,\|\varphi'\|_{L^\infty(\mathbb{R})})>0$. Eventually the thesis follows by $\|A\|_*<\sqrt{d}K$ and (4.2) $\square$

Next we show that with same choice of the parameters, and a possibly larger λ, every $\mathcal{A}\in\widetilde{\Omega}_x(K,\beta,\varepsilon_J,\varepsilon_v,\lambda)$ belongs to a subset of $\mathit{Aff}^+(\mathbb{R}^d_x)$ where $h_\lambda(x,\cdot,\mathcal{X})$ is striclty convex.

Corollary 5.11. *Let K be given and suppose $(\beta,\varepsilon_J,\varepsilon_v)$ satisfy* (5.13)*. There exists $\lambda_C>0$ such that for every $\lambda>\lambda_C$ we have*

$$\widetilde{\Omega}_x(K,\beta,\varepsilon_J,\varepsilon_v,\lambda)\subset\{\mathcal{A}\in\mathit{Aff}^+_{\rhd}(\mathbb{R}^d_x):\,D^2_{\mathcal{A}\mathcal{A}}h_\lambda(x,\mathcal{A},\mathcal{X})>0\}.$$

More prescisely if $\mathcal{A}\in\widetilde{\Omega}_x(K,\beta,\varepsilon_J,\varepsilon_v,\lambda)$, A is associated with a reduced positively oriented basis of $\mathcal{L}(A)$ and $B\in GL^+(d,\mathbb{Z})$, we have

$$\mathcal{M}^T D_{\mathcal{A}\mathcal{A}}h_\lambda(x,(AB,\tau),\mathcal{X})\mathcal{M}\geq C^B_{\mathrm{conv,K}}\|\mathcal{M}\|^2_\lambda,\qquad\forall\mathcal{M}\in\mathbb{R}^{d\times d}\times\mathbb{R}^d,\tag{5.15}$$

where $0<C^B_{\mathrm{conv,K}}:=\frac{\min\{\|B\|_*^{-2},\|B^{-1}\|_*^{-2}\}}{4}C_{\mathrm{conv,K}}$, and $C_{\mathrm{conv,K}}>0$ is as in (5.14)*.*

Proof. We have

$$D^2_{\mathcal{A}\mathcal{A}}h_\lambda(x,\mathcal{A},\mathcal{X})=D^2_{\mathcal{A}\mathcal{A}}J_\lambda(x,\mathcal{A},\mathcal{X})+\vartheta_1 D^2_{AA}\frac{1}{\det A}+D^2_{AA}F(A).$$

Let $B \in GL^+(d,\mathbb{Z})$. For every $\mathcal{M} \in \mathit{Aff}^+(\mathbb{R}^d)$, by (5.14), we have

$$\mathcal{M}^T D^2_{\mathcal{A}\mathcal{A}} h_\lambda(x,(AB,\tau),\mathcal{X})\mathcal{M} = \begin{pmatrix} MB^{-1} \\ B\tau \end{pmatrix}^T D^2_{\mathcal{A}\mathcal{A}} h_\lambda(x,(A,B^{-1}\tau),\mathcal{X}) \begin{pmatrix} MB^{-1} \\ B\tau \end{pmatrix}$$
$$\geq \Big(\frac{C_{\mathrm{conv,K}}}{2} - \Big(\vartheta_1 |D^2_{AA}\frac{1}{\det A}| + |D^2_{AA}F(A)|\Big)\lambda^{-2}\Big)(\|MB^{-1}\|^2_\lambda + |B\tau|^2),$$

which gives (5.15) as soon as $\lambda > \lambda_C$, where λ_C is such that

$$\vartheta_1 \Big\| D^2_{AA}\frac{1}{\det(\cdot)}\Big\|_{L^\infty(\{\|A\|_*\leq K\}\cap\{\det A > C_0\})} + \Big\|D^2_{AA}F(\cdot)\Big\|_{L^\infty(\{\|A\|_*\leq K\})} = \frac{\lambda_C^2 C_{\mathrm{conv,K}}}{4}.$$

□

5.4. **Estimates on the distance between lattices in $\widetilde{\Omega}(K,\beta,\varepsilon_J,\varepsilon_v,\lambda)$.** In the present section we show that for a given $K > 0$ we can choose the parameters $(\beta,\varepsilon_J,\varepsilon_v,\lambda)$ in such a way that, if $\mathcal{A},\widetilde{\mathcal{A}} \in \widetilde{\Omega}_x(K,\beta,\varepsilon_J,\varepsilon_v,\lambda)$ and A, $\widetilde{A}$ are associated with a positive reduced basis respectively of $\mathcal{L}(A)$ and $\mathcal{L}(\widetilde{A})$, then $\mathcal{A}^{-1}\circ\widetilde{\mathcal{A}} \in \mathfrak{B}_\lambda(\mathcal{B},C\beta)$, for some $\mathcal{B} \in \mathit{Aff}^+(\mathbb{Z}^d)$ and a positive constant $C > 0$ (see Lemma 5.12). The proof of this statement is based on a more general estimate on the distance of a matrix from $GL^+(d,\mathbb{Z})$ which is proved in Section 5.4.1.

Lemma 5.12. *Let $\mathcal{A} := (A,\tau), \widetilde{\mathcal{A}} := (\widetilde{A},\widetilde{\tau}) \in \widetilde{\Omega}_x(K,\beta,\varepsilon_J,\varepsilon_v,\lambda)$, and define $\mathcal{K} := \max\{\|A\|_*, \|\widetilde{A}\|_*\}$. Suppose*

$$\Big(\frac{C_1(K+\beta)}{\lambda} + \varepsilon_v + \frac{2\varepsilon_J}{C_{W,0}}\Big) < \frac{1}{3C_0\mathcal{K}^d}, \tag{5.16}$$

$$\beta < \min\Big\{\frac{1}{18\sqrt{d}C_0\mathcal{K}^{(d-1)}}, \frac{1}{2C_0^{1/d}}\Big\}. \tag{5.17}$$

There exists $\mathcal{B} := (B,b) \in \mathbb{Z}^{d\times d}\times\mathbb{Z}^d$ such that

$$\|A^{-1}\widetilde{A} - B\|_* \leq C^{\mathcal{K}}_{\mathrm{link}}\frac{\beta}{\lambda}, \tag{5.18}$$

$$|\tau - (A^{-1}\widetilde{A}\widetilde{\tau} + b)| \leq C^{\mathcal{K}}_{\mathrm{link}}\beta, \tag{5.19}$$

where $C^{\mathcal{K}}_{\mathrm{link}} := C_d 2\sqrt{d}C_0\mathcal{K}^{(d-2)}$ and C_d is as in Theorem 5.15.

Moreover if $\lambda > \lambda_{\mathbb{Z}}$, where $\lambda_{\mathbb{Z}} := \lambda_{\mathbb{Z}}(d,\mathcal{K},s_0)$, we can conclude that $B \in GL^+(d,\mathbb{Z})$ and that it is unique.

Proof. We have

$$\min_{|v|=1}|A^{-1}v| = \frac{1}{\|A\|_*} \geq \frac{1}{\mathcal{K}}$$

and therefore

$$\tau + [-\frac{\lambda}{2\mathcal{K}},\frac{\lambda}{2\mathcal{K}}]^d =: Q^\tau_{\frac{\lambda}{\mathcal{K}}} \subset B((\tau_i,\frac{\lambda}{\mathcal{K}}) \subset \mathcal{A}^{-1}(B(x,\lambda)). \tag{5.20}$$

The same relation holds for $\widetilde{\mathcal{A}}$.

Given $z_k \in (Q^\tau_{\frac{\lambda}{\mathcal{K}}} \setminus \mathcal{V}^\beta_{\mathcal{A}}(x))$, by $x_{i(k)}$ we denote the unique element of $\mathcal{X}\cap B(x,\lambda)$ such that $|\mathcal{A}(z_k) - x_{i(k)}| \leq \beta$ (uniqueness follows by (5.17) and Remark 5.3). Next we notice that setting

$$\mathcal{S} := \{z_k \in Q^\tau_{\frac{\lambda}{\mathcal{K}}} \setminus \mathcal{V}^\beta_{\mathcal{A}}(x) : \, x_{i(k)} \notin \mathcal{I}^\beta_{\widetilde{\mathcal{A}}}\}, \tag{5.21}$$

by (5.4), (5.5), (5.6) and (4.1) we get

$$\begin{aligned}
\sharp\mathcal{S} &\geq \sharp\Big(Q^{\tau}_{\frac{\lambda}{\mathscr{k}}} \cap \mathbb{Z}^d \setminus \mathcal{V}^{\beta}_{\mathscr{A}}(x)\Big) - \sharp\mathcal{I}^{\beta}_{\widetilde{\mathscr{A}}}(x) \\
&\geq \left(\frac{\lambda}{\mathscr{k}}\right)^d - \left(\frac{3^d\omega_d\|\varphi'\|_{L^\infty(\mathbb{R})}(K+\beta)}{\lambda}\omega_d + \varepsilon_v + \frac{2\varepsilon_J}{C_{W,0}}\right)\frac{\lambda^d}{\det A} \\
&\geq \left(1 - \Big(\frac{3^d\omega_d\|\varphi'\|_{L^\infty(\mathbb{R})}(K+\beta)}{\lambda} + \varepsilon_v + \frac{2\varepsilon_J}{C_{W,0}}\Big)C_0\right)\left(\frac{\lambda}{\mathscr{k}}\right)^d \\
&\geq \frac{2}{3}\left(\frac{\lambda}{\mathscr{k}}\right)^d .
\end{aligned}$$

Let $z_k \in \mathcal{S}$ and let $z_{l(k)} \in \mathbb{Z}^d \cap \widetilde{\mathscr{A}}^{-1}(B(x,\lambda))$ be such that $|\widetilde{\mathscr{A}}(z_{l(k)}) - x_{i(k)}| < \beta$. We have

$$\begin{aligned}
|\widetilde{\mathscr{A}}^{-1}(\mathscr{A}(z_k)) - z_{l(k)}| \leq& |\widetilde{\mathscr{A}}^{-1}(\mathscr{A}(z_k)) - \widetilde{\mathscr{A}}^{-1}(x_{i(k)})| + |\widetilde{\mathscr{A}}^{-1}(x_{i(k)}) - z_{l(k)}| \\
=& |\widetilde{A}^{-1}\left(\mathscr{A}(z_k) - x_{i(k)}\right)| + |\widetilde{\mathscr{A}}^{-1}(x_{i(k)}) - \widetilde{\mathscr{A}}^{-1}\widetilde{\mathscr{A}}(z_{l(k)}))| \\
\leq& \|\widetilde{A}^{-1}\|_*\beta + |\widetilde{A}^{-1}\Big(x_{i(k)} - \widetilde{\mathscr{A}}(z_{l(k)})\Big)| \\
\leq& 2\|\widetilde{A}^{-1}\|_*\beta < 2\sqrt{d}\mathscr{k}^{(d-1)}C_0\beta.
\end{aligned}$$

Since by (5.17) we have $\overline{\beta} := 2\sqrt{d}C_0\mathscr{k}^{(d-1)}\beta < 1/9$, we are in a position to apply Theorem 5.15 with repsect to $R = \lambda/\mathscr{k}$ and $\overline{\beta}$, and so we obtain the existence of $\mathscr{B} = (B,b) \in \mathbb{Z}^{d\times d} \times \mathbb{Z}^d$ such that

$$\|\widetilde{A}^{-1}A - B_{21}\|_* \leq C^{\mathscr{k}}_{\text{link}}\frac{\beta}{\lambda}, \tag{5.22}$$

$$|\widetilde{\tau} - (\widetilde{A}^{-1}A\tau + b)| \leq C^{\mathscr{k}}_{\text{link}}\beta, \tag{5.23}$$

where $C^{\mathscr{k}}_{\text{link}} := C_d 2\sqrt{d}C_0\mathscr{k}^{(d-2)}$. Applying the same argument to $\mathscr{A}^{-1}\circ\widetilde{\mathscr{A}}$ we obtain $\mathscr{B}' = (B', b') \in \mathbb{Z}^{d\times d} \times \mathbb{Z}^d$ such that

$$\|A^{-1}\widetilde{A} - B'\|_* \leq C^{\mathscr{k}}_{\text{link}}\frac{\beta}{\lambda}, \tag{5.24}$$

$$|\tau - (A^{-1}\widetilde{A}\widetilde{\tau} + b)| \leq C^{\mathscr{k}}_{\text{link}}\beta. \tag{5.25}$$

Next we show that, for big enough λ, we have we show that $B'B = BB' = Id$, that is $B, B' \in GL(d,\mathbb{Z})$.

By (5.22)-(5.25) and hypothesis (O1) in Definiton 4.1 we get

$$\begin{aligned}
\|B'B - Id_d\|_* \leq& \|B'\left(B - \widetilde{A}^{-1}A\right)\|_* + \|B'\widetilde{A}^{-1}A - A^{-1}\widetilde{A}\widetilde{A}^{-1}A\|_* \\
\leq& \|B_{12}\|_*\|B_{21} - A_2A_1^{-1}\|_* + \|B_{12} - A_1A_2^{-1}\|_*\|A_2A_1^{-1}\|_* \\
\leq& \left(\|B'\|_* + \|\widetilde{A}^{-1}A\|_*\right)C^{\mathscr{k}}_{\text{link}}\frac{\beta}{\lambda} \\
\leq& \left(\|A^{-1}\widetilde{A}\|_* + \|\widetilde{A}^{-1}A\|_* + 2C^{\mathscr{k}}_{\text{link}}\frac{\beta}{\lambda}\right)C^{\mathscr{k}}_{\text{link}}\frac{\beta}{\lambda} \\
\leq& 2\frac{(2\mathscr{k})^d}{s_0^d(1-\varepsilon_v)}C^{\mathscr{k}}_{\text{link}}\frac{\beta}{\lambda} + 2\left(C^{\mathscr{k}}_{\text{link}}\frac{\beta}{\lambda}\right)^2 .
\end{aligned} \tag{5.26}$$

Hence, as we assumed $\beta < s_0/2$ and $\varepsilon_v < 1/2$, we can find $\lambda' := \lambda'(d, \kappa, s_0)$ such that, for $\lambda > \lambda'$, we have

$$2\frac{(2\kappa)^d}{s_0^d(1-\varepsilon_v)} C^{\kappa}_{\text{link}} \frac{\beta}{\lambda} + 2\left(C^{\kappa}_{\text{link}} \frac{\beta}{\lambda}\right)^2 \le 2\frac{(2\kappa)^{d+1}}{s_0^d} C^{\kappa}_{\text{link}} \frac{s_0}{\lambda'} + 2\left(C^{\kappa}_{\text{link}} \frac{s_0}{\lambda'}\right)^2 < \frac{1}{2}.$$

This latter relation together with the discreteness of $\mathbb{Z}^{d\times d}$ implies that $B'B = I$. Repeating the same argument for BB' we eventually get $B', B \in GL(d, \mathbb{Z})$. Since by (4.1) we have that $\det A^{-1}\widetilde{A} > \kappa^{-d} s_0^d / 2^{d+1}$, we can find $\lambda_{\mathbb{Z}} := \lambda_{\mathbb{Z}}(d, \kappa, s_0)$ such that for $\lambda > \lambda_{\mathbb{Z}}$ we have $\det B' > 0$, that is $B', B \in GL^+(d, \mathbb{Z})$. $\square$

Remark 5.13. Let us notice that if A, $\widetilde{A}$ are respectively associated with reduced positively oriented basis of $\mathcal{L}(A)$ and $\mathcal{L}(\widetilde{A})$, from (5.18) and (5.19) we deduce that

$$\mathcal{A}^{-1} \circ \widetilde{\mathcal{A}} \in \mathfrak{B}_\lambda(\mathcal{B}, 2C^K_{\text{link}}\beta).$$

5.4.1. *Estimates on the distance from $GL^+(d, \mathbb{Z})$ for matrices.* We begin with an easy Lemma that we will need in order to prove the main result of the present section, namely Theorem 5.15.

Lemma 5.14. *Let $m, N \in \mathbb{N}$ be such that $l < (2N+1)/3$ and let e_j be an element of the canonical basis of $\mathbb{R}^d$. If $\mathcal{S} \subset [-N, N]^d \cap \mathbb{Z}^d$ verifies*

$$z_k \in K \Longrightarrow \{z_k + le_j,\, z_k - le_j\} \cap \mathcal{S} = \emptyset, \tag{5.27}$$

then

$$\sharp\mathcal{S} \le \left(\frac{1}{2} + \frac{l}{2N+1}\right)(2N+1)^d \tag{5.28}$$

Proof. Let us suppose for simplicity that $j = 1$.

Firstly we notice that due to (5.27) we maximize $\sharp\mathcal{S}$ if for every $\widehat{z}_k \in \{0\} \times [-N, N]^{d-1}$ we maximize $\sharp\mathcal{S}_1(\widehat{z}_k)$, where

$$\mathcal{S}_1(\widehat{z}_k) := \mathcal{S} \cap [-N, N] \times \{\widehat{z}_k\}.$$

We are thus reduced to study the problem in one dimension.

Since $l < (2N+1)/3$ we have $(2N+1) = k(2l) + n$, where $k, n \in \mathbb{N}$ and $0 \le n < 2l$. Let $\widehat{z}_k \in \{0\} \times [-N, N]^{d-1}$. If $z_h \in \mathcal{S}_1(\widehat{z}_k)$ with $\langle z_h, e_1\rangle \le (N+1) - l$ then $z_h + le_1 \in [-N, N] \times \{\widehat{z}_k\} \setminus \mathcal{S}_1(\widehat{z}_k)$. Now If $0 \le n < l$ then $\sharp\mathcal{S}_1(\widehat{z}_k) \le kl + n$, if $l \le n < 2l$ then $\sharp\mathcal{S}_1(\widehat{z}_k) \le (k+1)l$. Hence we can conlcude that

$$\sharp\mathcal{S}_1(\widehat{z}_k) \le \frac{(2N+1)+l}{2},$$

and eventually that

$$\sharp\mathcal{S} = \sum_{\widehat{z}_k \in \{0\}\times[-N,N]^{d-1}} \sharp\mathcal{S}_1(\widehat{z}_k) \le (\frac{2N+1}{2} + \frac{l}{2})(2N+1)^{d-1}$$

$\square$

Theorem 5.15. *Let $(M, \mu) \in GL^+(d, \mathbb{R}) \times \mathbb{R}^d$. Suppose that for some $\beta < 1/9$ and $R > 27$ there exists*

$$\mathcal{S} \subseteq \mathbb{Z}^d \cap Q_R, \qquad \sharp\mathcal{S} \ge \frac{2}{3}(2R+1)^d, \tag{5.29}$$

such that

$$\text{dist}(Mz + \mu, \mathbb{Z}^d) \le \beta, \qquad \forall z \in \mathbb{Z}^d \cap \mathcal{S}. \tag{5.30}$$

Then there exist $B \in \mathbb{Z}^{d\times d}$, $b \in \mathbb{Z}^d$ such that

$$|M - B| \leq C_d \frac{\beta}{R}, \tag{5.31}$$

$$|\mu - b| \leq C_d \beta, \tag{5.32}$$

where $C_d > 0$ is a constant depending only on the dimension d.

Proof. Since $R/[R] \leq 3/2$ it is sufficient to prove the thesis for $R \in \mathbb{N}$.
We split the proof in several steps.

Step 1. Let e_j be an element of the canonical basis of $\mathbb{R}^d$ and let $l \in \mathbb{N}$ such that $1 \leq l \leq R/3$.

We claim that there exists $z_k \in \mathcal{S}$ such that either $(z_k + le_j) \in \mathcal{S}$ or $(z_k - le_j) \in \mathcal{S}$.

We will proceed by contradiction, supposing that for every $z_k \in \mathcal{S}$ nor $z_k + le_j \in \mathcal{S}$, nor $z_k - le_j \in \mathcal{S}$. Then, by Lemma 5.14, we would have

$$\begin{aligned} \mathcal{S} \cap [-R, R]^d &\leq \left(\frac{2R+1}{2} + \frac{l}{2}\right)(2R+1)^{d-1} \\ &\leq \left(\frac{2R+1}{2} + \frac{2R+1}{6}\right)(2R+1)^{d-1} = \frac{2}{3}(2R+1)^d, \end{aligned}$$

which is in contrast with (5.29).

Step 2. In this step we prove that for every element of the canonical basis e_j $(j = 1, \ldots, d)$ and every $l \in \mathbb{N}$ with $1 \leq l \leq R/3$, we have

$$\operatorname{dist}(M(le_j), Z^d) < 2\beta. \tag{5.33}$$

Let $z_k \in \mathcal{S}$ satisfy the statement of *Step 1* and suppose that $z_k + le_j \in \mathcal{S}$. By $z_{h(k)}$ (resp. $z_{h(k,j,l)}$) we denote the element of $\mathbb{Z}^d$ such that $\operatorname{dist}(Mz_k + \mu, \mathbb{Z}^d) = |z_k - z_{h(k)}|$ (resp. such that $\operatorname{dist}(M(z_k + le_j) + \mu, \mathbb{Z}^d) = |(z_k + le_j) - z_{h(k,j,l)}|$). Hence

$$\begin{aligned} \operatorname{dist}(M(le_j), \mathbb{Z}^d) \leq& |M(le_j) - (z_{h(k,j,l)} - z_{l(k)})| \\ =& |(M(z_k + le_j) + \mu - z_{h(k,jl)}) - (Mz_k + \mu - z_{h(k)})| \leq 2\beta. \end{aligned}$$

Step 3. By (5.33) we get that for every m_{ij} and $l \in \{1, 2, \ldots, (2R+1)/3\}$, denoting by $\widehat{z}^i_{h(l,j)} \in \mathbb{Z}$ the i-th component of the (unique) projection $\widehat{z}_{h(l,j)}$ of $M(le_j)$ on $\mathbb{Z}^d$, we get

$$\operatorname{dist}(lm_{ij}, \mathbb{Z}) \leq |lm_{ij} - \widehat{z}^i_{h(l,j)}| \leq |M(le_j) - \widehat{z}_{h(l,j)}| = \operatorname{dist}(M(le_j 2), \mathbb{Z}^d) < 2\beta.$$

We can thus conclude that

$$\operatorname{dist}(m_{ij}, \mathbb{Z}) \leq \frac{3\beta}{R}. \tag{5.34}$$

Setting $B = (b_{ij}) \in \mathbb{Z}^{d\times d}$, where $b_{ij} \in \mathbb{Z}$ is a projection of m_{ij} on $\mathbb{Z}$, we get

$$\|M - B\|_* \leq \sqrt{d}\sqrt{\sum_{i,j=1}^{d}(m_{ij} - b_{ij})^2} \leq (3d^{3/2})\frac{\beta}{R},$$

which implies (5.31).

Next we prove (5.32). Let $z_k \in \mathcal{S}$ and denote by $z_{h(k)}$ the element of $\mathbb{Z}^d$ such that (5.30) holds. We have

$$\begin{aligned}\operatorname{dist}(\mu, \mathbb{Z}^d) \leq & |\mu - (z_{h(k)} - Bz_k)| \\ \leq & |(Mz_k + \mu) - z_{h(k)}| + |(M - B)z_k| \\ \leq & \beta + \|M - B\|_* |z_k| \leq \beta(1 + 3d^{3/2}),\end{aligned}$$

which implies (5.32). □

6. Proof of Theorem 4.4

Let us recall that, assuming $\beta < \beta_0$, Theorem 4.4 (A) follows from Remark 5.3, (5.5) and (5.7). Hence it remains to prove Theorem 4.4 (B)-(C). To this aim firstly we introduce, in Definition 6.1, a criterion to choose the parameters $(K, \beta, \varepsilon_J, \varepsilon_v, \lambda)$. Then, in Theorem 6.3, we prove Theorem 4.4 (B)-(C).

Definition 6.1. *Given* $K \in (\frac{1}{C_0^{1/d}}, \overline{m_1})$ *we say that* $(K, \beta, \varepsilon_J, \varepsilon_v, \lambda)$ *are proper if:*

(i) $\beta \in (0, \beta_0)$*, verifies* (5.17)*;*
(ii) ε_J, ε_v *satisfy* (5.13)*;*
(iii) λ *is big enough with respect to* $K, \beta, \varepsilon_J, \varepsilon_v$ *to satisfy*

$$\lambda > \max\{\overline{\lambda}, \lambda_C, \lambda_{\mathbb{Z}^d}\}, \tag{6.1}$$

where $\overline{\lambda}, \lambda_C, \lambda_{\mathbb{Z}^d}$ *are respectively defined in Lemma 5.8, Corollary 5.11, Lemma 5.12;*
(iv) $(K, \beta, \varepsilon_J, \varepsilon_v, \lambda)$ *satisfy* (5.16)

By Proposition 5.10 and Lemma 5.12 we have the following

Lemma 6.2. *If* $(K, \beta, \varepsilon_J, \varepsilon_v, \lambda)$ *are proper, then:*

$$\widetilde{\Omega}_x(K, \beta, \varepsilon_J, \varepsilon_v, \lambda) \subset \{\mathcal{A} \in \mathit{Aff}^+_{\triangleright}(\mathbb{R}^d_x) : D^2_{\mathcal{A}\mathcal{A}} h_\lambda(x, \mathcal{A}, \mathcal{X}) > 0\}. \tag{6.2}$$

Moreover, if $\mathcal{A}_0, \widehat{\mathcal{A}}_0 \in \widetilde{\Omega}_x(K, \beta, \varepsilon_J, \varepsilon_v, \lambda)$*, and* $\mathcal{A}_0, \widehat{\mathcal{A}}_0$ *are canonical representations respectively of* $\mathcal{L}_x(\mathcal{A}_0)$*,* $\mathcal{L}_x(\widehat{\mathcal{A}}_0)$*, then there exists an unique* $\mathcal{B} \in \mathit{Aff}^+(\mathbb{Z}^d)$ *such that*

$$\mathcal{A}_0^{-1} \circ \widehat{\mathcal{A}}_0 \in \mathfrak{B}_\lambda(\mathcal{B}, 2C^K_{\text{link}}\beta), \quad (\widehat{\mathcal{A}}_0)^{-1} \circ \mathcal{A}_0 \in \mathfrak{B}_\lambda(\mathcal{B}^{-1}, 2C^K_{\text{link}}\beta). \tag{6.3}$$

We are now in a position to prove Theorem 4.4 (B)-(C).

Theorem 6.3. *Let* $P_0 := (x_0, \widetilde{\mathcal{A}}_0) \in \widetilde{\Omega}(K, \beta, \varepsilon_J, \varepsilon_v, \lambda)$*,* $\widetilde{\mathcal{A}}_0$ *being a canonical representation for* $\mathcal{L}_{x_0}(\widetilde{\mathcal{A}}_0)$*. We assume that there exists* $\overline{\varepsilon}_J > 0$ *such that*

$$\frac{9}{8}\varepsilon_J < \overline{\varepsilon}_J, \quad \sqrt{\varepsilon_J} < \frac{\overline{\varepsilon}_J}{3KC_2(K)\sqrt{2C^K_{\text{link}}d}}, \tag{6.4}$$

where $C_2(K)$*,* C^K_{link} *are defined in Lemma 5.8 and Lemma 5.12 respectively. Moreover we suppose that* $(2K, \beta, 9\frac{C_{W,1}}{C_{W,0}}\overline{\varepsilon}_J, 2\varepsilon_v, \lambda)$ *are proper. Under such assumptions setting*

$$\delta_0^2 := \frac{\overline{\varepsilon}_J \beta^2}{2C_2(K)}, \tag{6.5}$$

we can find $\Lambda := \Lambda(K, \beta, \varepsilon_J, \varepsilon_v) > 0$*, such that, if* $\lambda > \Lambda$*, the problem*

$$\min\{h_\lambda(x_0, \mathcal{A}, \mathcal{X}) : \mathcal{A} \in \overline{\mathfrak{B}_\lambda(\mathcal{A}_0, \delta_0)}\}, \tag{6.6}$$

admits an unique solution $\mathcal{A}_{0,x_0} \in \mathfrak{B}_\lambda(\mathcal{A}_0, \delta_0) \cap \widetilde{\Omega}_{x_0}(\frac{3}{2}K, \beta, \frac{10}{9}\varepsilon_J, \frac{3}{2}\varepsilon_v, \lambda)$.
Moreover the elements of $[\![\mathcal{A}_{0,x_0}]\!]_{Aff^+(\mathbb{Z}^d)}$ *are the unique stationary points of* $h_\lambda(x_0, \cdot, \mathcal{X})$ *in* $\widetilde{\Omega}_{x_0}(2K, \beta, \frac{9}{8}\varepsilon_J, 2\varepsilon_v, \lambda)$.

Proof. The existence of a solution to (6.6) trivially follows from the compactness of $\overline{\mathfrak{B}_\lambda(\widetilde{\mathcal{A}}_0, \delta_0)}$ and the continuity of $h_\lambda(x_0, \cdot, \mathcal{X})$ with respect to $\mathcal{A} \in Aff^+_\triangleright(\mathbb{R}^d_x)$.

Let $\mathcal{A}_{P_0} := (A_{P_0}, \tau_{P_0})$ be a solution of (6.6). By Lemma 5.8, the choice of δ_0 and the assumption that $(2K, \beta, \frac{9C_{W,1}}{C_{W,0}}\overline{\varepsilon}_J, 2\varepsilon_v, \lambda)$ are proper, we have $\mathcal{A}_{P_0} \in \overline{\mathfrak{B}_\lambda(\widetilde{\mathcal{A}}_0, \delta_0)} \subset \widetilde{\Omega}(2K, \beta, \frac{9C_{W,1}}{C_{W,0}}\overline{\varepsilon}_J, 2\varepsilon_v, \lambda)$ and

$$A_{P_0} \in \mathcal{H} := \{\|A\|_* < 2K\} \cap \{\|A^{-1}\|_* \leq \frac{2^{d+2}K^{d-1}}{s_0^d}\}.$$

By the uniform continuity of the functions $1/\det A$ and $F(A)$ on $\mathcal{H}$ we can deduce the existence of $\lambda' = \lambda'(K, \beta, \varepsilon_J, \varepsilon_v)$ such that for $\lambda > \lambda'$ we have

$$\begin{aligned}
&\frac{1}{\lambda^d}\sum_{x_i \in \mathcal{X}} W\big(x_i, \mathcal{L}_{x_0}(\mathcal{A}_{P_0})\big)\varphi_{\lambda,x_0}(x_i) \\
\leq &\frac{1}{\lambda^d}\sum_{x_i \in \mathcal{X}} W\big(x_i, \mathcal{L}_{x_0}(\widetilde{\mathcal{A}}_0)\big)\varphi_{\lambda,x_0}(x_i) + \vartheta_1\Big(\frac{1}{\det \widetilde{A}_0} - \frac{1}{\det A_{P_0}}\Big) + \Big[F\Big(\widetilde{A}_0\Big) - F\Big(A_{P_0}\Big)\Big] \\
< &\frac{10}{9}\frac{\varepsilon_J\beta^2}{\det\big(A_{P_0}\big)} < \frac{\overline{\varepsilon}_J(3\beta\sqrt{\varepsilon_J/8\overline{\varepsilon}_J})^2}{\det\big(A_{P_0}\big)}.
\end{aligned}$$

and $\mathcal{A}_{P_0}, \widetilde{\mathcal{A}}_0 \in \widetilde{\Omega}(\frac{3K}{2}, \frac{\sqrt{10}}{3}\sqrt{\frac{\varepsilon_J}{\overline{\varepsilon}_J}}\beta, \overline{\varepsilon}_J, \frac{3}{2}\varepsilon_v, \lambda) \subseteq \widetilde{\Omega}(\overline{K}, \frac{3}{2\sqrt{2}}\sqrt{\frac{\varepsilon_J}{\overline{\varepsilon}_J}}\beta, \overline{\varepsilon}_J, 2\varepsilon_v, \lambda)$. Since by (6.4) we have $\frac{3}{2\sqrt{2}}\sqrt{\frac{\varepsilon_J}{\overline{\varepsilon}_J}}\beta < \beta$ and $(\overline{K}, \beta, \overline{\varepsilon}_J, 2\varepsilon_v, \lambda)$ are proper, we can apply Lemma 5.12 and deduce by (6.4), (6.5) that

$$\begin{aligned}
\|\widetilde{\mathcal{A}}_0 - \mathcal{A}_{P_0}\|_\lambda < &C^K_{\text{link}}\frac{3\sqrt{\varepsilon_J/\overline{\varepsilon}_J}}{2\sqrt{2}}\beta\sqrt{d}\|\widetilde{A}_0\|_* \\
\leq &C^K_{\text{link}}\frac{3\sqrt{\varepsilon_J/\overline{\varepsilon}_J}}{\sqrt{2}}\beta\sqrt{d}K < \delta_0.
\end{aligned} \tag{6.7}$$

The uniqueness of a solution to (6.6) is then a consequence of (6.2) which implies the strict convexity of $h_\lambda(x, \cdot, \mathcal{X})$ on $\overline{\mathfrak{B}_\lambda(\mathcal{A}_0, \delta_0)}$.

In order to prove that $[\![\mathcal{A}_{P_0}]\!]_{Aff^+(\mathbb{Z}^d)}$ are the unique stationary points for $h_\lambda(x_0, \cdot, \lambda)$ in $\widetilde{\Omega}(2K, \beta, \frac{9}{8}\varepsilon_J, 2\varepsilon_v, \lambda)$ we proceed by contradiction. Suppose that there exists $\widehat{\mathcal{A}}_0 \in \widetilde{\Omega}(2K, \beta, \frac{9}{8}\varepsilon_J, 2\varepsilon_v, \lambda) \notin [\![\mathcal{A}_{P_0}]\!]_{Aff^+(\mathbb{Z}^d)}$ which is a stationary point of $h_\lambda(x_0, \cdot, \mathcal{X})$. By Remark 2.6 we can suppose that $\widehat{\mathcal{A}}_0$ is a canonical representation for $\mathcal{L}_{x_0}(\widehat{\mathcal{A}}_0)$. Repeating the same argument we used to deduce (6.7), we obtain the existence of $\widehat{\mathcal{A}}_{0,\mathcal{B}} \in [\![\widehat{\mathcal{A}}_0]\!]_{Aff^+(\mathbb{Z}^d)}$ such that $\widehat{\mathcal{A}}_{0,\mathcal{B}} \in \mathfrak{B}_\lambda(\mathcal{A}_{P_0}, \delta_0)$. By the choice of δ_0 and Lemma 5.8 we obtain

$$\mathfrak{B}_\lambda(\mathcal{A}_{P_0}, \delta_0) \subset \widetilde{\Omega}_{x_0}(2K, \beta, 9\frac{C_{W,1}}{C_{W,0}}\overline{\varepsilon}_J, 2\varepsilon_v, \lambda),$$

hence, by the assumption on the properness of $(2K, \beta, 9\frac{C_{W,1}}{C_{W,0}}\overline{\varepsilon}_J, 2\varepsilon_v, \lambda)$, we obtain the strict convexity of $h_\lambda(x_0, \cdot, \mathcal{X})$ on $\mathfrak{B}_\lambda(\mathcal{A}_{P_0}, \delta_0)$, and hence the contradiction. ☐

7. Proof of Theorem 4.5

In the present Section we will always assume that the set $\widetilde{\Omega}(K,\beta,\varepsilon_J,\varepsilon_v,\lambda)$ satisfies the hypothesis of Theorem 6.3. Moreover for ease of notation we set $\widetilde{\omega}_d := \widetilde{\Omega}_d(\frac{K}{2},\beta,\frac{9}{8}\varepsilon_J,\frac{\varepsilon_v}{2},\lambda)$ and $\widetilde{\Omega} := \widetilde{\Omega}(K,\beta,\varepsilon_J,\varepsilon_v,\lambda)$. We begin proving a local version of Theorem 4.5, and then complete its proof by an easy argument.

Proposition 7.1. *Let* $\mathrm{Argmin}_{\widetilde{\Omega}} : \widetilde{\omega}_d \to \widetilde{\Omega}$ *be the multi-valued map defined in* (4.5). *Let* $x_0 \in \widetilde{\omega}_d$ *and* $\mathcal{A}_{\mathcal{B}} \in [\![\mathcal{A}_{0,x_0}]\!]_{A\!f\!f^+(d,\mathbb{Z})}$, *where* $\mathcal{A}_{0,x_0}$ *is a canonical representation for* $\mathcal{L}_{x_0}(\mathcal{A}_{0,x_0})$. *There exist open neighborhoods* $U \subset\subset \widetilde{\omega}_d$ *of* x_0, $V \subset \widetilde{\Omega}_x$ *of* $\mathcal{A}_{\mathcal{B},x_0}$ *and a smooth (single-valued) map* $\mathcal{A}_{\mathcal{B}}(\cdot) \in C^1(U,V)$ *such that* (4.6) *is satisfied. Moreover there exists* $C_\nabla := C_\nabla(\widetilde{\Omega}) > 0$, *such that* (4.7) *holds.*

Proof. We consider the map

$$D_{\mathcal{A}}h_\lambda(\cdot,\cdot,\mathcal{X}) : \bigcup_{x\in\widetilde{\omega}_d} \{x\}\times\widetilde{\Omega}_x \to A\!f\!f(\mathbb{R}^d),$$
$$(x,\mathcal{A}) \mapsto D_{\mathcal{A}}h_\lambda(x,\mathcal{A},\mathcal{X}).$$

By Theorem 6.3 we have

$$\mathrm{Argmin}_{\widetilde{\Omega}}(\widetilde{\omega}_d) = \{D_{\mathcal{A}}h_\lambda(\cdot,\cdot,\mathcal{X}) = 0\} \cap \{D^2_{\mathcal{A}\mathcal{A}}h_\lambda(\cdot,\cdot,\mathcal{X}) > 0\} \cap \bigcup_{x\in\widetilde{\omega}_d}\{x\}\times\widetilde{\Omega}_x.$$

The existence of the neighborhoods U of x_0 and V of $\mathcal{A}_{\mathcal{B},x_0}$ and of a map $\mathcal{A}_{\mathcal{B}} \in C^1(U,V)$ verifying (4.6) is then a direct consequence of the Implicit Function Theorem. For ease of notation in the rest of the proof we set $\mathcal{A}_{\mathcal{B}}(x) = (A(x),\tau(x))$. Again by the Implicit Function Theorem, we have

$$\begin{pmatrix} \nabla_x A(x) \\ \nabla_x \tau(x) \end{pmatrix} = -\left[D^2_{\mathcal{A}\mathcal{A}}h_\lambda(x,\mathcal{A}(x),\mathcal{X})\right]^{-1}\left[\nabla_x D_{\mathcal{A}}h_\lambda(x,\mathcal{A}(x),\mathcal{X})\right]. \tag{7.1}$$

Next we notice that

$$\begin{aligned} &\nabla_x D_{\mathcal{A}}h_\lambda(x,\mathcal{A},\mathcal{X}) \\ &= -\frac{1}{\lambda^d}\sum_{x_i\in\mathcal{X}} D_{\mathcal{A}}W(x_i,(A,x-A\tau))\otimes\nabla_x\varphi_{\lambda,x}(x_i) - D^2_{\mathcal{A}\mathcal{A}}h_\lambda(x,\mathcal{A},\mathcal{X})\begin{pmatrix} 0 \\ A^{-1}\end{pmatrix} \\ &\quad+\frac{1}{\lambda^d}\Big(D_\tau\sum_{x_i\in\mathcal{X}} W(x_i,(A,x-A\tau))\varphi_{\lambda,x}(x_i)\Big)^T (A^{-1})^2. \end{aligned}$$

Since by $A(x) \in Argmin_{\widetilde{\Omega}}(\widetilde{\omega}_d)$ we have

$$D_\tau\sum_{x_i\in\mathcal{X}} W(x_i,(A(x),x-A(x)\tau(x)))\varphi_{\lambda,x}(x_i) = 0,$$

we conclude that

$$\begin{aligned} &D^2_{\mathcal{A}\mathcal{A}}h_\lambda(x,\mathcal{A}(x),\mathcal{X})\begin{pmatrix} \nabla_x A(x) \\ \nabla_x\tau(x) - A^{-1}(x)\end{pmatrix} \\ &= -\frac{1}{\lambda^d}\sum_{x_i\in\mathcal{X}} D_{\mathcal{A}}W\big(x_i,\big(A(x),x-A(x)\tau(x)\big)\big)\otimes\nabla_x\varphi_{\lambda,x}(x_i). \end{aligned}$$

We set

$$\begin{pmatrix} \partial_{x^{(k)}}A(x) \\ \partial_{x^{(k)}}\tau(x) - (a^{-1})_{\cdot,k}\end{pmatrix} := \begin{pmatrix} \big(\partial_{x^{(k)}}(a(x))_{pq}\big)_{\alpha(p,q)} \\ \big(\partial_{x^{(k)}}\tau^{(l)}(x) - (a^{-1}(x))_{l,k}\big)_{d^2+l}\end{pmatrix} \in \mathbb{R}^{d^2+d},$$

and

$$\frac{1}{\lambda^d}\Big[\sum_{x_i\in X}\Big(D_{\mathcal{A}}W\big(x_i,\big(A(x),x-A(x)\tau(x)\big)\big)\Big)^T\partial_{x^{(k)}}\varphi_{\lambda,x}(x_i)\Big]\begin{pmatrix}\partial_{x^{(k)}}A(x)\\ \partial_{x^{(k)}}\tau(x)-(a^{-1}(x))_{\cdot,k}\end{pmatrix} \tag{7.2}$$

$$=:\Big\langle\Big(L(p,q,k)\Big)_{\alpha(p,q)},\,\partial_{x^{(k)}}A(x)\Big\rangle+\Big\langle\Big(R(m,k)\Big)_m,\,(\partial_{x^{(k)}}\tau(x)-(a^{-1}(x))_{\cdot,k})\Big\rangle.$$

Next, we notice that if $x_i\in\mathcal{R}^{\mathcal{A}}_{\beta}(x)\cap B(x,2\lambda)$ then, by assumption (P2) on $W(\cdot,\cdot)$, we have

$$\begin{aligned}\Big|\partial_{a_{pq}}W(x_i,(A,x-A\tau))\Big|\leq&2C_{W,1}\Big|x_i^{(p)}-x^{(p)}-\sum_{l=1}^{d}a_{pl}(z^{(l)}_{k(i)}-\tau^{(l)}))\Big|\;|z^{(q)}_{k(i)}-\tau^{(q)}|\\ \leq&2\beta C_{W,1}\sqrt{d}\|A^{-1}\|_*\Big|\Big(A(z_{k(i)}-\tau)\Big)^{(q)}\Big|\leq4\beta\sqrt{d}\|A^{-1}\|_*\lambda.\end{aligned}$$

Hence

$$\begin{aligned}\Big|\Big(L(p,q,k)\Big)_{\alpha(p,q)}\Big|\leq&\frac{\|\varphi'\|_{L^\infty(\mathbb{R})}}{\lambda^{d+1}}\Big(4\beta\sqrt{d}\|A^{-1}\|_*\lambda\;\sharp(\mathcal{R}^{\beta}_{\mathcal{A}(x)}(x)\cap B(x,2\lambda))\\ &+\|D_AW\big(\cdot,(A(x),-A(x)\tau(x))\big)\|_{L^\infty(B(0,2\lambda))}\;\sharp(\mathcal{I}^{\beta}_{\mathcal{A}(x)}(x)\cap B(x,2\lambda))\Big),\end{aligned}$$

finally, applying Remark 5.7 with $r:=\varphi^{-1}(\varepsilon_J)$ and by Definition 4.1-(O4), setting $C(W,U):=\|D_AW\big(\cdot,(A(\cdot),-A(\cdot)\tau(\cdot))\big)\|_{L^\infty(B(0,2\lambda)\times U)}$, we obtain

$$\begin{aligned}&\Big|\Big(L(p,q,k)\Big)_{\alpha(p,q)}\Big|\\ \leq&\|\varphi'\|_{L^\infty(\mathbb{R})}\left(\frac{\beta s_0^d\sqrt{d}\|A^{-1}(x)\|_*}{2^{d-1}}+\frac{C(W,U)}{\lambda}\left(\frac{\varepsilon_J^{1/2}4^{(d+1)}}{s_0^dC_{W,0}}+\frac{\omega_d(2^d-\varphi^{-1}(\varepsilon_J^{1/2}))}{s_0^d}\right)\right)\\ &=:C_{1,\nabla}(s_0,W,\varphi,\beta,\varepsilon_J,\|\mathcal{A}_{\mathcal{B}}(\cdot)\|_{L^\infty(U)}),\end{aligned}$$

and $C_{1,\nabla}\to0$, as $\varepsilon_J,\beta\to0$. Similarly, we get

$$|(R(m,k))_m|\leq\frac{C_{2,\nabla}(s_0,W,\varphi,\beta,\varepsilon_J,\|\mathcal{A}_{\mathcal{B}}(\cdot)\|_{L^\infty(U)})}{\lambda},$$

where again $C_{2,\nabla}\to0$, as $\varepsilon_J,\beta\to0$.

Hence by (5.15), we can find a positive constant $C^{\mathcal{A}_{\mathcal{B}}}_{conv}$ such that, setting $C_\nabla=\max\{C_{1,\nabla},C_{2,\nabla}\}/C^{\mathcal{A}_{\mathcal{B}}}_{conv}$, we have

$$\begin{aligned}&(\lambda^2|\partial_{x^{(k)}}A(x)|^2+|\partial_{x^{(k)}}\tau^{(l)}(x)-(a^{-1}(x))_{\cdot,k}|^2)\\ &\leq\frac{C_\nabla}{\lambda}(\lambda|\partial_{x^{(k)}}A(x)|+|\partial_{x^{(k)}}\tau^{(l)}(x)-(a^{-1}(x))_{\cdot,k}|)\\ &\leq\frac{\sqrt{2}C_\nabla}{\lambda}\sqrt{(\lambda^2|\partial_{x^{(k)}}A(x)|^2+|\partial_{x^{(k)}}\tau^{(l)}(x)-(a^{-1}(x))_{\cdot,k}|^2)},\end{aligned}$$

and finally

$$\begin{aligned}&\lambda|\partial_{x^{(k)}}A(x)|^2+|\partial_{x^{(k)}}\tau^{(l)}(x)-(a^{-1}(x))_{\cdot,k}|\\ &\leq\sqrt{2}\sqrt{(\lambda^2|\partial_{x^{(k)}}A(x)|^2+|\partial_{x^{(k)}}\tau^{(l)}(x)-(a^{-1}(x))_{\cdot,k}|^2)}\leq\frac{2C_\nabla}{\lambda},\end{aligned}$$

which is our thesis. □

Let us now consider an open simply connected subset U of $\widetilde{\omega}_d$. We can apply a global version of the Implicit Function Theorem (see for example [1]) and deduce that the map $\mathcal{A}_{\mathcal{B}}(\cdot)$ can be extended to the whole of U.

Finally as a consequence of Lemma 5.12, the discreteness of $Aff(\mathbb{Z}^d)$ and the smoothness of the map Φ_{P_0}, we obtain that (4.8) holds and the proof of Theorem 4.5 is completed.

8. Proof of Corollary 4.6

Let $x_0 \in \{h_\lambda(\cdot, \mathcal{X}) + \vartheta_0 \rho_\lambda(\cdot, \mathcal{X}) < \eta\}$. By the definition of $h_\lambda(x_0, \mathcal{X})$ we can find $\mathcal{A} = (A, \tau) \in Aff^+(\mathbb{R}^d_{x_0})$ such that

$$h_\lambda(x_0, \mathcal{A}, \mathcal{X}) + \vartheta_0 \rho_\lambda(x_0, \mathcal{X}) < 2\eta.$$

By the assumption (P1) made on W, and the non-negativity of the function $F(\cdot)$, we have

$$\begin{aligned}\frac{C_{W,0}}{\lambda^d} &\sum_{x_i \in \mathcal{X}} \operatorname{dist}^2(x_i, \mathcal{L}_x(\mathcal{A})) \varphi_{\lambda,x}(x_i) + \mathcal{V}(x, A, \lambda) \\ &\leq h_\lambda(x_0, \mathcal{A}, \mathcal{X}) + \vartheta_0 \rho_\lambda(x_0, \mathcal{X}) < 2\eta.\end{aligned}$$

Hence if we choose $\eta > 0$ to satisfy (3.11), we can apply Proposition 3.3, and, restricting ourselves to $\lambda > \lambda_{m_1}$, we deduce that $m_1(\mathcal{L}_x(\mathcal{A})) < \widehat{C}$. Moreover, by Proposition 3.2 we obtain

$$F(A) - \frac{d\vartheta_1 \widehat{C} + \sqrt{\vartheta_1 / C_{W,0} C_\varphi}}{\lambda} \leq h_\lambda(x_0, \mathcal{A}, \mathcal{X}) + \vartheta_0 \rho_\lambda(x_0, \mathcal{X}) < 2\eta.$$

Hence, after choosing a possibly smaller η, for $\lambda \geq \overline{\lambda} := \overline{\lambda}(C_{W,0}, \vartheta_1, \varphi, \widehat{C})$ we obtain

$$\det A_0 < C_{\mathrm{el}},$$

Consequently

$$\begin{aligned}&\vartheta_1 \Big(\frac{1}{\det A} - \frac{1}{C_\varphi \lambda^d} \sum_{x_i \in \mathcal{X}} \varphi_{\lambda,x_0}(x_i) \Big) \\ &\leq h_\lambda(x_0, \mathcal{A}, \mathcal{X}) + \frac{\vartheta_0}{\lambda^d} \sum_{x_i \in \mathcal{X}} \varphi_{\lambda,x_0}(x_i) < \frac{2\eta C_{\mathrm{el}}}{\det A},\end{aligned}$$

and eventually, setting $\eta' := (2\eta C_{\mathrm{el}} C_\varphi)/\vartheta_1$, we obtain

$$(C_\varphi - \eta') \frac{\lambda^d}{\det A} \leq \sum_{x_i \in \mathcal{X}} \varphi_{\lambda,x_0}(x_i). \tag{8.1}$$

By (2.22) we can find $\sigma > 0$ (dependent on $(C_{W,0} s_0^2/4 - \vartheta_1/C_\varphi) > 0$) such that

$$\begin{aligned}
2\eta > & h_\lambda(x_0, \mathcal{A}, X) + \vartheta_0 \rho_\lambda(x_0, X) = \frac{1}{\lambda^d} \sum_{x_i \in \mathcal{R}_{\mathcal{A}}^{\frac{s_0}{4}}(x_0)} W(x_i - x, \mathcal{A}) \varphi_{\lambda,x_0}(x_i) \\
& + \frac{1}{\lambda^d} \sum_{x_i \notin \mathcal{R}_{\mathcal{A}}^{\frac{s_0}{4}}(x_0)} \left[W(x_i - x, \mathcal{A}) - \frac{\vartheta_1}{C_\varphi} \right] \varphi_{\lambda,x_0}(x_i) \\
& + \vartheta_1 \left(\frac{1}{\det A} - \frac{1}{C_\varphi \lambda^d} \sum_{x_i \in \mathcal{R}_{\mathcal{A}}^{s_0/4}(x_0)} \varphi_{\lambda,x_0}(x_i) \right) + F(A) \\
\geq & \sigma \left(\frac{1}{\lambda^d} \sum_{x_i \in X} W(x_i - x, \mathcal{A}) \varphi_{\lambda,x_0}(x_i) \right) - \frac{3^d \omega_d \|\varphi'\|_{L^\infty(\mathbb{R})} (\widehat{C} + s_0/4)}{\lambda}.
\end{aligned}$$

This means that, possibly further restricting to a larger $\lambda \geq \overline{\lambda}$, we can conclude that

$$\sum_{x_i \in X} W(x_i - x, \mathcal{A}) \varphi_{\lambda,x_0}(x_i) < \frac{3\eta C_{\text{el}}}{\sigma} \frac{\lambda^d}{\det A} =: \eta'' \frac{\lambda^d}{\det A}. \tag{8.2}$$

By (8.1), (8.2) and (3.10), for $\lambda \geq \overline{\lambda}$, we obtain that $(x_0, \widetilde{\mathcal{A}}) \in \widetilde{\Omega}(K, \beta, \varepsilon_J, \varepsilon_v, \lambda)$, where

$$K = 3\widehat{C}, \quad \varepsilon_v = 3\eta', \quad \beta^2 \varepsilon_J = 2\eta''.$$

Since letting $\eta \to 0$ we have $\eta', \eta'' \to 0$, we can conclude that, for small enough η and $\lambda \geq \overline{\lambda}$, the set $\widetilde{\Omega}(K, \beta, \varepsilon_J, \varepsilon_v, \lambda)$ verifies the hypothesis of Theorem 4.4 and $\widetilde{\Omega}(\frac{K}{2}, \beta, \frac{8}{9}\varepsilon_J, \frac{\varepsilon_v}{2}, \lambda)$ is not empty.
Next we show that $h_\lambda(x_0, X) = h_\lambda(x_0, \mathcal{A}_{0,x_0}, X)$. To this aim we chose a minimizing sequence $\{\mathcal{A}_n\}_n \subset \mathit{Aff}^+_\triangleright(\mathbb{R}^d_{x_0})$ such that $\mathcal{A}_n$ is a canonical representation for $\mathcal{L}_{x_0}(\mathcal{A}_n)$. Repeating th same argument as above, we obtain $\|A_n\|_* \leq \sqrt{d} m_1(\mathcal{L}_{x_0}(\mathcal{A}_n)) < K$. Hence the sequence $\{\mathcal{A}_n\}_n$ is pre-compact in $\mathbb{R}^{d\times d} \times \mathbb{R}^d$. Let $\widetilde{\mathcal{A}}_0 \in \mathit{Aff}^+_\triangleright(\mathbb{R}^d_{x_0})$ be a limit point of $\{\mathcal{A}_n\}_n$. By the continuity of $h_\lambda(x_0, \cdot, X)$ we obtain that $\widetilde{\mathcal{A}}_0 \in \widetilde{\Omega}(K, \beta, \varepsilon_J, \varepsilon_v, \lambda)$ and that it is a minimizer of $h_\lambda(x_0, \cdot, X)$. The thesis is then a consequence of the uniqueness of the local minimizers proved in Theorem 4.4.
In order to conclude the proof we have to estimate the measure of $\widetilde{\Omega}(K, \beta, \varepsilon_J, \varepsilon_v, \lambda)$. Keeping the notation introduced above, we notice that, by the assumptions $\eta' < \eta$ and

$$H_\lambda(X, \Omega) + \vartheta_0 \int_\Omega \rho_\lambda(x, X)\, dx = \int_\Omega h_\lambda(x, X) + \vartheta_0 \rho_\lambda(x, X)\, dx < \eta' L^d,$$

we deduce that $Y := \{h_\lambda(\cdot, \mathcal{X}) + \vartheta_0\rho_\lambda(\cdot, \mathcal{X}) < \eta\} \subset \Omega$ is non-void. Moreover, by Proposition 3.3 and Proposition 3.2, we have

$$|\Omega \setminus \widetilde{\Omega}_d| \leq |\Omega \setminus Y| \leq \frac{1}{\eta}\int_{\Omega\setminus Y} h_\lambda(x, \mathcal{X}) + \vartheta_0\rho_\lambda(x, \mathcal{X})\, dx$$

$$\leq \frac{1}{\eta}\Big(\int_\Omega h_\lambda(x, \mathcal{X}) + \vartheta_0\rho_\lambda(x, \mathcal{X})\, dx + \frac{d\vartheta_1\widehat{C} + \sqrt{\vartheta_1/(C_{W,0}c_\varphi)}}{\lambda}|\widetilde{\Omega}_d|\Big)$$

$$< \Big(\frac{\eta'}{\eta} + \frac{d\vartheta_1\widehat{C} + \sqrt{\vartheta_1/(C_{W,0}c_\varphi)}}{\lambda\eta}\Big)L^d,$$

which is our thesis.

9. Dislocations

In the present section we briefly discuss how dislocations can be related to the topology of $\widetilde{\Omega}(K, \beta, \varepsilon_J, \varepsilon_v, \lambda)$. We begin with a (sloppy) analysis of a configuration containing a single dislocation and fulfilling some additional, simplifying, assumptions. Let $\mathcal{X}_L \subset \Omega_L := (0, L)^3$ and $\mathcal{C} := \{t(0, 0, 1) : \ t \in (0, L)\}$. We suppose that for large L we can choose $1 << \lambda << \sqrt{L}$, such that for every simply connected

$$U \subset\subset \Omega \setminus (\mathcal{C})_\lambda, \quad (\mathcal{C})_\lambda := \{\mathrm{dist}(\cdot, \mathcal{C}) < 4\lambda\},$$

we can find a smooth diffeomorphism $\Phi_U^{-1} : U \to \Phi_U^{-1}(U)$, such that $\Phi_U^{-1}(\mathcal{X}_L \cap U) \subset \mathcal{L}(G)$, and $\|\nabla\Phi_U(\cdot) - Id\|_{L^\infty(\Phi_U^{-1}(U))}$ is small. More precisely we suppose that for every $y \in U$ the matrix $\nabla\Phi_U(y)G$ belongs to a neighborhood V of G such that $\overline{V} \cap \{B^{-1}GB : \ B \in GL^+(d, Z)\} = \{G\}$. As a consequence we can suppose that, if L is large enough, we have $\Omega \setminus (\mathcal{C})_\lambda \subset \widetilde{\Omega}(K, \beta, \varepsilon_J, \varepsilon_v, \lambda)$, that Theorem 4.4, Theorem 4.5 hold on this set, and that, as in Section 3, for every $x \in \Omega \setminus (\mathcal{C})_\lambda$ we have $(\nabla\Phi_U(\Phi_U^{-1}(x))G, G^{-1}\Phi_U^{-1}(x)) \in \widetilde{\Omega}_x(K, \beta, \varepsilon_J, \varepsilon_v, \lambda)$. Next we let $\Gamma \subset\subset \Omega \setminus (C)_\lambda$ be a Burgers-circuit (i.e. a simple, closed curve with non-trivial link with $\mathcal{C}$), and consider $\widehat{U} \subset\subset \Omega \setminus (C)_\lambda$ to be an open neighborhood of Γ such that $B(x, 2\lambda) \subset\subset \widehat{U}$ for every $x \in \Gamma$. Fixed $x_0 \in \Gamma$ we define U to be the simply connected open set obtained removing from $\widehat{U}$ a "disc-like" surface Σ passing through x_0. Since we assumed that $\mathcal{C}$ is a dislocation line of Burgers vector Gb, the vector Gb represents also the jump performed by the map $\Phi_U^{-1}(\cdot)$ when approaching x_0 along Γ from the two opposite side of Σ with respect to x_0. However, by Theorem 4.4 and Theorem 4.5, we can conclude that, at least for large λ, the same relations hold true for the map $\mathcal{A}_0(\cdot) \in C^1(U, V)$ such that $\mathcal{A}_0(x) \in Argmin_{\widetilde{\Omega}}(x)$ and $\|A_0(\cdot) - \nabla\Phi_U(\Phi_U^{-1}(\cdot))G\|_{L^\infty(\Phi_U^{-1}(U))} \approx 1/\lambda$. Moreover, by the smallness of $\|\nabla\Phi_U(\cdot) - Id\|_{L^\infty(\Phi_U^{-1}(U))}$ we can conclude that, as $x \to x_0$ from both sides of Σ, the limits of $\nabla\Phi_U(x)$ coincide.

Motivated by this example, we proceed as follows in order to give a definition of *generalized dislocation line*.

Let Ω be simply connected, and let $\mathcal{X} \subset \Omega$ be such that (4.10) holds. In what follows we will adopt the same notation used in the proof of Theorem 4.5 (see Section 7). We set $\mathcal{P} := Argmin_{\widetilde{\Omega}}(\widetilde{\omega}_d) \subset \Omega \times \mathit{Aff}^+(\mathbb{R}^d)$. By the results of Theorem 4.5, we can conclude that $\mathcal{P}$ is a d-dimensional C^1-differentiable manifold embedded in $\mathbb{R}^d \times \mathit{Aff}^+(\mathbb{R}^d)$. Next, we consider $\mathit{Aff}^+(\mathbb{Z}^d)$ as a group with product rule

$$\mathcal{B}_1 \cdot \mathcal{B}_2 = (B_1B_2, B_2^{-1}b_1 + b_2), \quad \forall \mathcal{B}_i = (B_i, b_i) \in \mathit{Aff}^+(\mathbb{Z}^d),\ i = 1, 2,$$

acting (freely and transitively) on the elements of $(x, \mathcal{A}_x) \in \mathcal{P}$ via

$$(x, \mathcal{A}_x) \cdot \mathcal{B} = (x, \mathcal{A}_{x,\mathcal{B}}) := \big(x,\, (A_x B, B^{-1}\tau_x + b)\big) \in \{x\} \times \mathit{Aff}^{+}_{\triangleright}(\mathbb{R}^d_x) \cap \mathcal{P}.$$

(Let us remark that $(x, \mathcal{A}_{x,\mathcal{B}}) \in \mathcal{P}$ holds because we identify $(A, \tau) \in \mathit{Aff}^{+}_{\triangleright}(\mathbb{R}^d_x)$ with $(A, x - A\tau) \in \mathit{Aff}^{+}(\mathbb{R}^d)$, hence $\mathcal{A}_{x,\mathcal{B}} = \big(A_x B, x - A_x B(B^{-1}\tau_x + b)\big) \in \mathit{Aff}^{+}(\mathbb{R}^d)$, and therefore $\mathcal{L}_x(\mathcal{A}_x) = \mathcal{L}_x(\mathcal{A}_{x,\mathcal{B}})$). Since the action of $\mathit{Aff}^{+}(\mathbb{Z}^d)$ on $\mathcal{P}$ is properly discontinuous, the projection map $\mathrm{p} : \mathcal{P} \to \mathcal{P}/\mathit{Aff}^{+}(\mathbb{Z}^d)$ is a G-covering. However, since $\mathcal{P}/\mathit{Aff}^{+}(\mathbb{Z}^d) = \{(x, \mathcal{L}_x(\mathcal{A}_x)) : x \in \widetilde{\omega}_d\}$, by Theorem 4.4 and Theorem 4.5 we can conclude that $\mathcal{P}/\mathit{Aff}^{+}(\mathbb{Z}^d)$ is homeomorphic to $\widetilde{\omega}_d$. Hence, given a simple, regular path $\gamma \in C^{0,1}([0,1], \widetilde{\omega}_d)$ such that $\gamma(0) = x_0$, $\gamma([0,1]) \subset\subset \widetilde{\omega}_d$, and fixed $(x_0, \mathcal{A}_{x_0}) \in \mathcal{P}$, we can use the map p to lift γ to a path $\mathrm{p}_{\sharp,\mathcal{A}_{x_0}}\, \gamma \in C^1([0,1], \mathcal{P})$ such that $\mathrm{p}_{\sharp,\mathcal{A}_{x_0}}\, \gamma(0) = (x_0, \mathcal{A}_{x_0})$. Next, by means of the lifting map p, we define a function between $\Pi_1(\widetilde{\omega}_d, x_0)$, the fundamental group of $\widetilde{\omega}_d$ with base point x_0, and $\mathit{Aff}^{+}(\mathbb{Z}^d)/\sim$, where $\sim$ denotes the conjugacy in $\mathit{Aff}^{+}(\mathbb{Z}^d)$. Finally, we use such map to define when a loop in $\widetilde{\omega}_d$ is linked to a *generalized dislocation*. More precisely we proceed as follows. We consider a closed loop γ as above, and pick $\mathcal{A}_{x_0} \in \mathit{Argmin}_{\widetilde{\Omega}}(x_0)$. Then, since $\gamma(0) = \gamma(1) = x_0$, we can find an unique $\mathcal{B}_{\mathcal{A}_{x_0},\gamma} \in \mathit{Aff}^{+}(\mathbb{Z}^d)$ such that

$$\mathrm{p}_{\sharp,\mathcal{A}_{x_0}}\, \gamma(0) \cdot \mathcal{B}_{\mathcal{A}_{x_0},\gamma} = \mathrm{p}_{\sharp,\mathcal{A}_{x_0}}\, \gamma(1).$$

We can rephrase the definition of $\mathcal{B}_{\mathcal{A}_{x_0},\gamma}$ in the following, less abstract, way. As $\gamma([0,1]) \subset\subset \widetilde{\omega}_d$, we can find a connected, open neighborhood $\widehat{U} \subset\subset \widetilde{\omega}_d$ of $\gamma([0,1])$, and a "disc-like surface" Σ, such that $x_0 \in \Sigma$ and $U := \widehat{U} \backslash \Sigma$ is simply connected. By Theorem 4.5, we can find a map $\mathcal{A}(\cdot) \in C^1(U, V)$ such that $\lim_{t\to 0} \mathcal{A}(\gamma(t)) = \mathcal{A}_{x_0}$, and $\big(\gamma(t), \mathcal{A}(\gamma(t))\big) = \mathrm{p}_{\sharp,\mathcal{A}_{x_0}}\, \gamma(t) \in \mathcal{P}$. Moreover, again by Theorem 4.4, Theorem 4.5, we have $\lim_{t\to 1} \mathcal{A}(\gamma(t)) \in \mathit{Argmin}_{\widetilde{\Omega}}(x_0)$. Hence $\mathcal{B}_{\mathcal{A}_{x_0},\gamma}$ is the unique element of $\mathit{Aff}^{+}(\mathbb{Z}^d)$ such that

$$\lim_{t\to 1} \mathcal{A}(\gamma(t)) = \lim_{t\to 0} \mathcal{A}(\gamma(t)) \cdot \mathcal{B}_{\mathcal{A}_{x_0},\gamma} = \mathcal{A}_{x_0} \cdot \mathcal{B}_{\mathcal{A}_{x_0},\gamma}.$$

From the above construction, and Theorem 4.5, it follows that

- chosen any $\mathcal{B} \in \mathit{Aff}^{+}(\mathbb{Z}^d)$, we have
$$\mathcal{B}_{\mathcal{A}_{x_0}\cdot\mathcal{B},\gamma} = \mathcal{B}^{-1} \cdot \mathcal{B}_{\mathcal{A}_0,\gamma} \cdot \mathcal{B}. \tag{9.1}$$
- If $\widehat{\gamma} \in C^1([0,1], \widehat{\omega}_d)$ is homotopic to γ in $\widetilde{\omega}_d$ (and with same orientation of γ), setting $\widehat{\gamma}(0) =: x_1$, for every $(x_1, \mathcal{A}_{x_1}) \in \mathcal{P}$ we can find an element $\mathcal{B} \in \mathit{Aff}^{+}(\mathbb{Z}^d)$ such that
$$\mathcal{B}_{\mathcal{A}_{x_1},\widehat{\gamma}} = \mathcal{B}^{-1} \cdot \mathcal{B}_{\mathcal{A}_{x_0},\gamma} \cdot \mathcal{B}. \tag{9.2}$$

All in all we defined

$$\Psi : \Pi_1(\widetilde{\omega}_d, x_0) \to \frac{\mathit{Aff}^{+}(\mathbb{Z}^d)}{\sim}, \qquad (\gamma) \mapsto [\mathcal{B}_{p_\sharp(\gamma)}]_\sim,$$

where, for every closed loop $\widehat{\gamma}$ in the homotopy class of γ in $\widetilde{\omega}_d$, and $\mathcal{A}_{\widehat{\gamma}(0)} \in \mathit{Argmin}_{\widetilde{\Omega}}(\widehat{\gamma}(0))$, we can find an element $\mathcal{B}_{\mathcal{A}_{\widehat{\gamma}(0)}}$ in the conjugacy class of $\mathcal{B}_{p_\sharp(\gamma)}$ in $\mathit{Aff}^{+}(\mathbb{Z}^d)$ such that

$$\mathrm{p}_{\sharp,\mathcal{A}_{\widehat{\gamma}(0)}}\, \widehat{\gamma}(0) \cdot \mathcal{B}_{\mathcal{A}_{\widehat{\gamma}(0)}} = \mathrm{p}_{\sharp,\mathcal{A}_{\widehat{\gamma}(0)}}\, \widehat{\gamma}(1). \tag{9.3}$$

We call the map Ψ the *holonomy representation* of $\widetilde{\omega}_d$. We remark that actually the map Ψ does not depend on the base point x_0 as soon as we let vary the base point in the connected component C_{x_0} of $\widetilde{\omega}_d$ containing x_0. We are now in a position to state the following

Proposition 9.1. *Let x_0, C_{x_0} be as above. We have $\Psi(\Pi_1(C_{x_0}, x_0)) = \{(Id, 0)\}$ if and only if for every $U \subset\subset C_{x_0}$ and $\mathcal{A}_{x_0} \in Argmin_{\widetilde{\Omega}}(x_0)$ we can find $\mathcal{A}(\cdot) \in C^1(U, Aff^+(\mathbb{R}^d))$ verifying the conclusions of Theorem 4.5. Moreover if the fundamental group $\Pi_1(C_{x_0}\, x_0)$ of C_{x_0} with base point x_0 is trivial, then $\Psi(\Pi_1(C_{x_0}, x_0)) = \{(Id, 0)\}$.*

Proof. The proof of the proposition is elementary, and can be obtained via a straightforward adaptation of the proof of [3, Corollary 2.4]. □

The purpose of Proposition 9.1 is that of showing the relations holding between the image of the map Ψ and the possibility of defining global approximate lagrangian coordinates on the whole of a connected component C_{x_0} of $\widetilde{\omega}_d$. In a way Proposition 9.1 gives us a tool to check wether or not, at the "meso-scale" λ, we can approximate the set $\mathcal{X} \cap C_{x_0}$ via an elastically deformed portion of the ground state (up to errors due to higher order derivatives of the elastic deformation, and "small" percentages of "point-defects"). Moreover, we can interpret the case $\Psi(\Pi_1(\widetilde{\omega}_d, x_0)) \supsetneq \{(Id, 0)\}$ as revealing the presence of some kind of topological defect in $\mathcal{X} \cap Q$, where Q is the portion of $\Omega \setminus \widetilde{\omega}_d$ not trivially linked to those loops $\gamma \in C^1([0,1], \widetilde{\omega}_d)$ such that $\Psi(\gamma) \neq (Id, 0)$. In particular, we are lead to give the following

Definition 9.2. . *Let $\gamma \in C^1([0,1], \widetilde{\omega}_d)$. We say that γ links a generalized dislocation in Ω if and only if $\Psi(\gamma) = [(Id, b_\gamma)]_\sim$, for some $b_\gamma \in \mathbb{Z}^d \setminus \{0\}$.*

Remark 9.3. Suppose that $\mathcal{X}$ contains two (classical) dislocations lines ℓ_1, ℓ_2 of Burgers vectors Gb_1, $Gb_2 \in \mathcal{L}(G)$. Due to the way our Hamiltonian depends on the parameter λ, we will recognize the presence of both dislocations only if the distance between ℓ_1 and ℓ_2 is larger than λ. Otherwise we will observe just one generalized dislocation such that $\Psi(\gamma) = [(Id, b_1 + b_2)]_\sim$, for every γ which is not trivially linked to a λ-neighborhood of $\ell_1 \cup \ell_2$.

Next we define an appropriate notion of Burgers vector for a *generalized dislocation.* Since $[(Id, b_\gamma)]_\sim = \{(Id, B^{-1}b_\gamma) : B \in GL^+(d, \mathbb{Z})\}$, the only quantity we can define by means of $\Psi(\gamma)$, requiring that it is stable with respect to homotopies and changes of the base point within the same connected component of $\widetilde{\omega}_d$, is the *sign* of a generalized dislocation linked to γ (once a notion of positive orientation for the loops is defined). This is not surprising at all for two reasons. Firstly, being $H_\lambda(\mathcal{X}, \Omega)$ reference free, we cannot expect to be able to define the Burgers vector as an element of $\mathcal{L}(G)$, and obtain that it is invariant with respect to homotopies, unless we do not specify a particular basis for the ground state. The second reason is related to the fact that, in contrast with the classical theory of dislocations, Definition 9.2 is given without making any assumption on the distance between the "(approximate) deformation gradient" and the identity, therefore in general we cannot exclude that the Burgers vector depends on the base point. However, we can define a notion of Burgers vector of a generalized dislocation,which depends on the base point x_0 but it is stable with respect to homotopy, if we look at the jump of the approximate deformation. More precisely we consider $\mathcal{A}(\cdot)$ as a map taking values in the linear space $\mathit{Aff}^+(\mathbb{R}^d)$, we denote by $\pi_d : \mathit{Aff}^+(\mathbb{R}^d) = GL^+(d,\mathbb{R}) \times \mathbb{R}^d \to \mathbb{R}^d$ the projection on $\mathbb{R}^d$, and finally we define

$$\mathcal{b}_{\Omega,x_0}[(\gamma)] := \pi_d\big(\mathcal{A}(\gamma(0)) - \mathcal{A}(\gamma(1))\big) = A_{x_0}\big(\tau_{x_0} - \tau(\gamma(1))\big). \tag{9.4}$$

By Definition 9.2, and the relations (9.3), (9.1), (9.2), the Burgers vector $\mathcal{b}_{\Omega,x_0}[(\gamma)]$ is an element of the lattice $\mathcal{L}_{x_0}(\mathcal{A}_{x_0})$ which does not depend on the choice of the loop γ within the set of homotopic loops with base point x_0.

Remark 9.4. An assumption on $\mathcal{X}$ that, in our context, corresponds to the hypothesis that the deformation gradient far away from the dislocation core, belongs to a small neighborhood of the identity, is the following. For every $U \subset\subset \widetilde{\omega}_d$ simply connected and $x_0 \in U$, we require that we can find $(x_0, \mathcal{A}_{0,x_0}) \in \mathcal{P}$ such that $\mathcal{A}_{0,x_0}$ is a canonical representation of $\mathcal{L}_{x_0}(\mathcal{A}_{0,x_0})$ and, denoted by $\mathcal{A}(\cdot) \in C^1(U, \widetilde{\Omega})$ the corresponding approximate local lagrangian coordinates, we have

$$[A(x)]G^{-1} \in \mathcal{U}, \qquad \forall x \in U,$$

where $\mathcal{U}$ is an open neighborhood of the identity, whose closure has positive distance from the finite set of the proper symmetries (that is orientation preserving isometries) of the ground state into itself. Under this assumption a canonical choice between the elements of $[(Id, b_\gamma)]_\sim$ is given by the one verifying

$$\mathrm{p}_{\sharp,\mathcal{A}_{0,x_0}}\,\gamma(0)\cdot(Id, b_{(\gamma)}) = \mathrm{p}_{\sharp,\mathcal{A}_{0,x_0}}\,\gamma(1),$$

where $\mathcal{A}_{0,x_0}$ is as above. It can be easily checked that under such an assumption, the vector $Gb_{(\gamma)}$ coincides with the classical Burgers vector, and that it is stable with respect to homotopies and changes of the base point.

Remark 9.5. The whole matter of the present section is very closely related to the formalism introduced in [3]. Moreover there exists a strong link between the assumption discussed in the previous remark and the setting in which dislocations are treated in [3, Section 3].

We conclude our discussion on generalized dislocations deriving a (very) rough estimate on the asymptotic behavior of the value of our Hamiltonian along a sequence of configurations containing at least one of such dislocations. For the sake of simplicity let us firstly consider the case $d = 2$.We choose $\{L_n\}_n$, $\{\lambda_n\}_n \subset \mathbb{R}^+$ to be such that

$$\lim_{n\to\infty} L_n = \lim_{n\to\infty} \lambda_n = \lim_{n\to\infty} \frac{L_n}{\lambda_n^2} = +\infty,$$

and consider $\mathcal{X}_n = \{x_{n,i}\}_{i\in I_n} \subset \Omega_n = [0, L_n]^2$. We suppose that there exist ρ, $\eta' > 0$ such that (3.10), (4.10) hold, and $\mathcal{X}_n$ satisfies the conclusions of Corollary 4.6 for every $n \in \mathbb{N}$. Finally we suppose that for every $n \in \mathbb{N}$ we can find a path $\gamma_n \in C^0([0,1], (\widetilde{\omega}_n)_d)$, such that $\Psi(\gamma_n) = (Id, b_n)$, where $b_n \in \mathbb{Z}^d \setminus \{0\}$. Since Ω_n is simply connected, by Proposition 9.1, we can conclude that $\Omega_n \setminus \widetilde{\omega}_{d,n} \neq \emptyset$ so that $|\{h_{\lambda_n}(x, \mathcal{X}_n) > \eta_0\}| \geq c\lambda_n^2$, and

$$\begin{aligned}\liminf_{n\to\infty} \frac{1}{\lambda_n^2} H_{\lambda_n}(\mathcal{X}_n, \Omega_n) \geq& \liminf_{n\to\infty} \int_{\Omega_n\setminus\widetilde{\omega}_d} h_{\lambda_n}(x, \mathcal{X}_n)\,dx + \liminf_{n\to\infty} \int_{\widetilde{\omega}_d} h_{\lambda_n}(x, \mathcal{X}_n)\,dx \\ \geq& c\eta_0 - \liminf_{n\to\infty} O(1/\lambda_n) = c\eta_0,\end{aligned}$$

When $d = 3$, making some assumptions on the geometry of $\Omega \setminus \widetilde{\omega}_d$, we can repeat the same argument and obtain that

$$\liminf_{n\to\infty} \frac{1}{L_n \lambda_n^2} H_{\lambda_n}(\mathcal{X}_n, \Omega_n) \geq c\eta_0.$$

Clearly by these estimates we can deduce only a very rough clue on the scaling of $H_{\lambda_n}(\mathcal{X}_n, \Omega_n)$ when $\mathcal{X}$ contains (generalized) dislocations. However, although we expect that for some choices of λ_n, L_n a more careful analysis would furnish some interesting (and more "realistic") estimates, we have to keep in mind that we cannot expect to get a reasonable energy estimate in the dislocation core because of the definition of H_λ itself.

Remark 9.6. By (4.7) we can conclude that if γ is such that $\Psi(\gamma) = [(B_\gamma, b_\gamma)]_\sim$ for some $B_\gamma \neq Id$, then the length of the γ has to be at least of order λ^2. Hence, by a simple argument (similar to the one used above to estimate the "dislocation-core") we can conclude that configurations containing topological defects such that $\Psi(\Pi_1(C_{x_0}, x_0)) \supset \{[(B, b)]_\sim\}$ for some $B \neq Id$, have an energy higher than that of configuration containing dislocations.

Remark 9.7. We conclude this section noticing that we can also derive a (rough) upper bound estimate on the asymptotic behavior of $H_{\lambda_n}(\mathcal{X}_n, \Omega_n)$ that is related to the presence of some "*grain boundaries*" in $\mathcal{X}_n$. More precisely, suppose $\mathcal{X}_n = \big(\mathcal{L}(\mathcal{A}_0) \cap U_n\big) \cup \big(\mathcal{L}(\mathcal{A}_1) \cap \Omega_n \setminus \overline{U_n}\big)$, where U_n are open subsets of Ω_n, such that ∂U_n is (Lipschitz) smooth and the volume of U_n is of order L_n^d, we obtain

$$\liminf_{n\to\infty} \Big[H_{\lambda_n}(\mathcal{X}_n) - \eta \mathcal{H}^{d-1}(\partial U_n)\lambda_n \Big] \geq 0.$$

Appendix A.

In the present section we exhibit an example of a function $W(\cdot,\cdot) \in C^0(\mathbb{R}^d \times \mathit{Aff}^+(\mathbb{R}^d))$ satisfying (P1)-(P3).

A.1. **Example.** Let $0 < \overline{m_0} < \overline{m_1}$ verifying (2.15), and define

$$\mathcal{E} := \{\mathcal{M} \in \mathit{Aff}^+(\mathbb{R}^d) : \ \overline{m_0} < m_0(\mathcal{L}(\mathcal{M})) \leq m_1(\mathcal{L}(\mathcal{M})) < \overline{m_1}\},$$
$$\mathcal{E}' := \{\mathcal{M} \in \mathit{Aff}^+(\mathbb{R}^d) : \ \frac{\overline{m_0}}{2} < m_0(\mathcal{L}(\mathcal{M})) \leq m_1(\mathcal{L}(\mathcal{M})) < \frac{3\overline{m_1}}{2}\} \supset \mathcal{E}.$$

Let $\psi \in C^2([0,1] \times [1,2])$ be such that: there exists $\sigma \in (0,1)$ such that $\psi(s,t) = s^2$ for $(s,t) \in [0,\sigma] \times [1,2]$; for every $t \in [1,2]$ we have $\partial_s \psi(s,t) > 0$ for $s \in [0,1)$; for every $t \in [1,2]$ we have $\psi(1,t) = t$ and $\partial_s \psi(1,t) = \partial^2_{ss}\psi(1,t) = 0$.

For every $(y, \mathcal{M} = (M,\mu)) \in \mathbb{R}^d \times \mathcal{E}'$ we define

$$\Psi(y,\mathcal{M}) := \sum_{z\in\mathbb{Z}^d} \psi\Big(\frac{|y - \mathcal{M}(z)|}{f(M)}, 2\det M\Big)\, \chi_{B(\mathcal{M}(z), f(M))}(y) \\ +2(\det M)\chi_{\mathcal{D}}(y),$$

where $f(M) := \frac{2^{(d-2)}\det M}{(3\overline{m_1})^{(d-1)}}$ and $\mathcal{D} := \mathbb{R}^d \setminus \cup_{z\in\mathbb{Z}^d} B(\mathcal{M}(z), f(M))$.

By Proposition 2.2 we obtain that

$$\Big(\frac{\overline{m_0}}{2}\Big)^{(d-1)}\frac{1}{C_d}m_1(M) \le \det M \le \Big(\frac{3\overline{m_1}}{2}\Big)^{(d-1)} m_1(M), \tag{A.1}$$

$$\frac{m_0(M)}{2C_d}\Big(\frac{\overline{m_0}}{3\overline{m_1}}\Big)^{(d-1)} \le f(M) = \frac{2^{(d-2)}\det M}{(3\overline{m_1})^{(d-1)}} \le \frac{m_0(M)}{2}, \tag{A.2}$$

hold for every $M \in \mathcal{E}'$. As a consequence for every $M \in \mathcal{E}'$ and $z \in \mathbb{Z}^d$ we have $B(\mathcal{M}(z), f(M)) \subset B(\mathcal{M}(z), m_0(M))$ and hence $B((z_i), f(M)) \cap B((z_j), f(M)) = \emptyset$ for every $z_i \neq z_j$, $z_i, z_j \in \mathbb{Z}^d$. Therefore the sum defining $\Psi(\cdot, \mathcal{M})$ has at most one non-zero term.

In order to construct $W(\cdot,\cdot)$ we also need to define the functions

$$\Phi_0, \Phi_1 : \mathit{Aff}^+(\mathbb{R}^d) \to [0,1],$$

$$\Phi_0(\mathcal{M}) := \begin{cases} 0 & \text{if } m_0(\mathcal{L}(\mathcal{M})) \le \frac{\overline{m_0}}{2} \\ \frac{4m_0(\mathcal{L}(\mathcal{M})) - 2\overline{m_0}}{\overline{m_0}} & \text{if } m_0(M) \in [\frac{\overline{m_0}}{2}, \frac{3\overline{m_0}}{4}], \\ 1 & \text{if } m_0(\mathcal{L}(\mathcal{M})) \ge \frac{3\overline{m_0}}{4} \end{cases}$$

$$\Phi_1(\mathcal{M}) := \begin{cases} 1 & \text{if } m_1(\mathcal{L}(\mathcal{M})) \le \frac{5\overline{m_1}}{4} \\ \frac{6\overline{m_1} - 4m_1(\mathcal{L}(\mathcal{M}))}{\overline{m_1}} & \text{if } m_1(M) \in [\frac{5\overline{m_1}}{4}, \frac{3\overline{m_1}}{2}], \\ 0 & \text{if } m_1(\mathcal{L}(\mathcal{M})) \ge \frac{3\overline{m_1}}{2}. \end{cases}$$

Let us notice that $\Phi_0, \Phi_1 \in C^0(\mathit{Aff}^+(\mathbb{R}^d), [0,1])$, since the functions $M \mapsto m_0(\mathcal{L}(M))$, $M \mapsto m_1(\mathcal{L}(M))$ are (locally Lipschitz) continuous on $GL(d,R)$, (see [9]). Finally we define

$$W(y, \mathcal{M}) := \Phi_0(\mathcal{M})\Phi_0(\mathcal{M})\Psi(y,\mathcal{M}) + (1 - \Phi_0(\mathcal{M})\Phi_1(\mathcal{M}))\,\mathrm{dist}^2(y, \mathcal{L}(\mathcal{M})).$$

By the choice of $\psi(\cdot,\cdot)$ and (A.1), (A.2) we have: $W(\cdot,\cdot) \in C^0(\mathbb{R}^d \times \mathit{Aff}^+(\mathbb{R}^d))$ and $W(\cdot,\cdot) = \Psi(\cdot,\cdot) \in C^2(\mathbb{R}^d \times \mathcal{E})$; for every $\mathcal{M} \in \mathcal{E}$ and $y \in \mathbb{R}^d$ such that $\mathrm{dist}(y, \mathcal{L}(\mathcal{M})) < \sigma m_0(\mathcal{L}(\mathcal{M}))/2$ we have $\Psi(y,\mathcal{M}) = \mathrm{dist}^2(y, \mathcal{L}(\mathcal{M}))$; there exist $0 < C_{W,0} \le C_{W,1}$ such that for every $(y, \mathcal{M}) \in \mathbb{R}^d \times \mathit{Aff}^+(\mathbb{R}^d)$ we have

$$C_{W,0}\,\mathrm{dist}^2(y, \mathcal{L}(\mathcal{M})) \le W(y,\mathcal{M}) \le C_{W,1}\,\mathrm{dist}^2(y, \mathcal{L}(\mathcal{M})).$$

Hence $W(\cdot,\cdot)$ satisfies the assumptions (P1) and (P3) (for $\beta_0 = \sigma\overline{m_0}/2$). Moreover, by construction, $W(\cdot,\cdot)$ verifies also the assumption (P2).

Other periodic potentials can be constructed using a structure similar to the one we used to define $W(\cdot,\cdot)$ as above. For example certain "anisotropies" can be introduced adapting the previous construction to the case where $|y - \mathcal{M}(z_k)|$ is replaced with $(D(y-\mathcal{M}(z_k))\cdot(y-\mathcal{M}(z_k)))^{1/2}$ in the argument of $\psi(\cdot,\cdot)$ ($D \in GL^+(d,\mathbb{R})$ being a positive definite matrix). In general, the only difficulty in producing explicit examples of periodic potentials verifying (P1)-(P3) is represented by the smoothness requirement coupled with the invariance with respect to the action of $GL^+(d,\mathbb{Z})$ (see [9] for the discussion of a related problem).

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Stephan Luckhaus, Mathematisches Institute der Universität Leipzig, Augustusplatz 10/11, D-04109 Leipzig, Germany

E-mail address: Stephan.Luckhaus@math.uni-leipzig.de

Luca Mugnai, Max Planck Institute for Mathematics in the Sciences, Inselstr. 22, D-04103 Leipzig, Germany

E-mail address: mugnai@mis.mpg.de,