Study of a Model for reference free plasticity

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Contents

Chapter 1

Introduction

1.1 Abstract:

In this thesis we investigate a Kac-type many particle model that allows a reference-free description of plastic deformation. We calculate an upper bound for the energy barrier of plastic relaxation. Furthermore, we construct local Lagrangian coordinates and use them to bound the energy-density from below.

1.2 Motivation

The basic of the theory of non linear elasticity The classical theory of elasticity is based on the concept of a reference configuration. The reference configuration is the fictive ground state of the deformed object. The ground state is assumed to have no external forces and no defects in the interior that create internal stresses. The reference configuration is given as a set $\tilde{\Omega} \subset \mathbb{R}^d$. Then one uses a differentiable map $\phi : \tilde{\Omega} \to \mathbb{R}^d$ to describe the deformation that turns the reference $\tilde{\Omega}$ into the deformed configuration $\Omega = \phi(\tilde{\Omega})$ The energy is assumed be a functional of the deformation ϕ. One assumes that the energy is translational invariant and local. Translational invariance means that it is actual only a functional of $\nabla\phi$. Locality means that the energy can be described as an integral over an energy density F that only depends on the local gradient $\nabla\phi(x)$. That means:

$$H := \int_{\tilde{\Omega}} \tilde{F}\left(\nabla\phi\left(z\right)\right) dz \quad . \tag{1.2.1}$$

where $\tilde{F}$ denotes the energy density function, $\tilde{F}\mathrm{GL_d}\left(\mathbb{R}\right) \to \mathbb{R}^+$ satisfying the following properties:

1) $\tilde{F}(RA) = F(A)$ for all $A \in \mathbb{R}^{d\times d}$ and all $R \in SO_3$ (Frame indifference)

2) $\tilde{F}(A) \geq 0$ for all $A \in \mathbb{R}^{d\times d}$ (Positivity)

3) $\tilde{F}(id) = 0$ (Reference configuration as a minimizer)

Frame indifference ensures that rigid motions do not change the energy. The other two conditions ensure that the reference configuration is really the ground state. The energy functional (1.2.1) determines the form some object will have under certain boundary conditions by a minimization of F over all ϕ that fulfill these boundary conditions. A detailed description of the theory of non-linear elasticity is found in [1].

Introduction of the model for reference-free plasticity If we deform a metal object with low stress, we get a elastic deformation that can be well described in the framework of the elasticity theory. The elastically deformed configuration is a global minimum of the energy functional. However, the elastically deformed configuration is not the lowest energy state in real physics. Between this minimizer and lower energy states there is an energy barrier. High pressure, high temperature or long time may allow the system to overcome this barrier and reach lower energy states. Since the elastically deformed configuration is already the global minimum of the elastic energy functional (1.2.1), this process can not be described within the framework of elasticity theory. The use of a reference configuration is fixing the local order. The plastic deformation includes a change of the local structure of the metal, reaching configurations, that are excluded in elasticity theory. To describe these processes we want to study a model which has the freedom to change the local order. Still we want to make use of elasticity theory. Hence, we use the elasticity theory and bring the model to a point, where we do not need a reference configuration anymore. We start with a map $\phi : \tilde{\Omega} \to \mathbb{R}^d$. Since we do not want to use a reference configuration, we transform from Lagrangian coordinates to Eulerian coordinates.

$$H = \int_\Omega F(\nabla\phi\left(\phi^{-1}(x)\right))dx \tag{1.2.2}$$

with $F(A) := \tilde{F}(A) \det A^{-1}$ and $\Omega := \phi(\tilde{\Omega})$. In this formulation we need the reference configuration for calculating $\nabla\phi\,(\phi^{-1}(x))$. This we want to substitute by information over the local lattice structure around the point x. To see the local order we will fill the reference $\tilde{\Omega}$ with an atom lattice $\mathbb{Z}^d$ This gives us atom positions $\phi(\mathbb{Z}^d)$ in the configuration Ω. The neighborhood of a point z produces to first order the configuration:

$$x_i := \phi(z_i) \approx \phi(z) + \nabla\phi(z)(z_i - z) \quad . \tag{1.2.3}$$

So in the neighborhood of the point $x \in \Omega$ the configuration looks like

$$x_i \approx \phi(z) + \nabla\phi(\phi^{-1}(x))(z_i - z) \quad . \tag{1.2.4}$$

This means that for an atom configuration in Ω and a lattice $G\left(\mathbb{Z}^d + \tau\right)$ fitted to it in a neighborhood around a point $x \in \Omega$, where $G \in Gl_d(\mathbb{R})$ and $\tau \in \mathbb{R}^d$, the

Eulerian energy functional (1.2.2) does only depend on G and there is no need to use a reference configuration.

1.3 Definition of the model

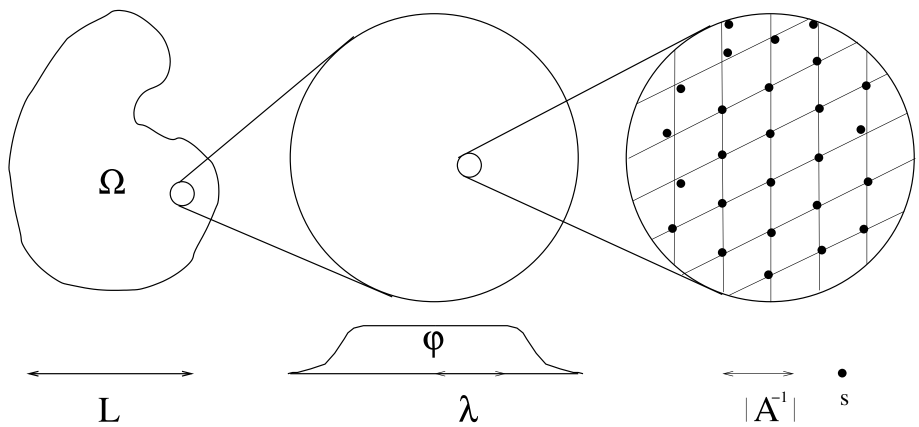

Figure 1.1: Multi-scale model with three different scales: Microscopic scale: $|A^{-1}|$ distance between atoms, macroscopic scale L size of the body , mesoscopic scale: λ the configuration looks like a lattice

In this section we will briefly present our model. In our model the actual state of the described body is given by a domain $\Omega \subset \mathbb{R}^d$ and a set $\chi = \{x_i \in B_{4\lambda}(\Omega) | i = 1...N\}$ of atom positions, where λ is the mesoscopic scale $\lambda << \mathrm{diam}(\Omega)$. Here d denotes the dimension. We will focus on dimension $d = 2$ and $d = 3$. The set of atoms χ fall consists of two subsets $\chi = \chi_I \cup \chi_S$. The internal atoms $\chi_I \subset \Omega$ can move freely inside a compact set $\Omega \subset \mathbb{R}^d$, but are not allowed to leave it. The boundary atoms $\chi_S \subset B_{4\lambda}(\Omega)/\Omega$ are fixed and serve as our boundary condition. We call the number of internal atoms $N_I = \sharp\chi_I$ and the number of boundary atoms $N_S = \sharp\chi_S$. The energy in our model is given by an integral over an energy density and an hardcore particle interaction V with radius s_0.

$$H_\lambda(\chi) := \int_{B_{2\lambda}(\Omega)} \hat{h}_\lambda(\chi, x) + \sum_{i,j} V(|x_i - x_j|)\,. \tag{1.3.1}$$

The main part of the model is the energy density $\hat{h}_\lambda(\chi, x)$ in Eulerian coordinates x. This density is determined by fitting a Bravais lattice. $\chi_{A,\tau} + x = A^{-1}(\mathbb{Z}^d - \tau) + x$ locally to the atom positions χ, where $A \in Gl_d(\mathbb{R})$ and $\tau \in \mathbb{R}^d$. We denote: $\mathcal{A} = (A, \tau)$. For every $\mathcal{A}$ one can calculate a pre-energy density $h_\lambda(\mathcal{A}, \chi x)$ at a given point The energy density $\hat{h}_\lambda(\chi, x)$ is then given by the infinum of this pre-energy densities.

$$\hat{h}_\lambda(\chi, x) := \inf_{\mathcal{A}} \{h_\lambda(\mathcal{A}, \chi, x)\} \quad . \tag{1.3.2}$$

The pre-energy density $h_\lambda(\mathcal{A}, \chi x)$ consists of three parts.

$$h_\lambda(\mathcal{A}, \chi x) := F(A) + J_\lambda(\mathcal{A}, \chi, x) + \nu_\lambda(\chi, A, x) \tag{1.3.3}$$

The first term F measures the elastic contribution to the energy and corresponds to the energy density in the classical theory. The second part $J_\lambda(\mathcal{A}, \chi, x)$ measures energy cost of deviations of the configuration χ from the fitted lattice . The last part $\nu_\lambda(\chi, A, x)$ assigns a cost to the vacancies, and introduces a chemical potential In the following we will explain the properties of the different parts of the energy density in more detail.

The elastic energy $F(A)$ is related to $\tilde{F}$ of the classical theory with the formula $F(G) = \tilde{F}(G^{-1})\det(G^{-1})$ for the transformation between Eulerian and Lagrangian coordinates. We want to consider F with the following properties for $C_1^{El}, C_2^{El} > 0$

- $F \in C_2(Gl_d(\mathbb{R}))$ (Regularity)
- $F(A) = F(AR)$, $\forall A \in Gl_d(\mathbb{R})$, $\forall R \in SO_d$ (Frame indifference)
- $\exists E \in Gl_d(\mathbb{R})$ with $F(E) = 0$ (Existence of minimizer)
- $F(A) \geq C_1^{El}(\det(E) - \det(A)))^2 + C_2^{El}\text{dist}^2(A, E\, SO_d)$ (Coercivity)

Here we use the euclidean norm to define the distance for two matrices $\text{dist}(A, E) = |X - Y|$.

The deviation energy $J_\lambda(\mathcal{A}, \chi, x)$ uses the affine transformation $\mathcal{A}(x) = Ax + \tau$ to map the atom positions in the λ-neighborhood of the position x into a periodic potential W with minima in $\mathbb{Z}^d$ and W is assumed to be locally convex around the minima. In this way J_λ is approximately the standard deviation of the configuration χ from the fitted lattice $\chi_{\mathcal{A}} + x$.

$$J_\lambda(\mathcal{A}, \chi, x) := \frac{\|A^{-1}\|^2}{C_\varphi \lambda^d} \sum_i W(A(x_i - x) + \tau)\varphi\left(\lambda^{-1}|x_i - x|\right) \tag{1.3.4}$$

where φ is a smooth and monotone decreasing cut-off function. It ensures that only atoms in the neighborhood of x contributes to the energy density in x, and has the following

- $\varphi \in C^\infty(\mathbb{R}^+)$
- $\varphi(x) = 1$ for $x \leq 1$
- $\varphi(x) = 0$ for $x \geq 2$

- $\partial_x \varphi \leq 0$

We use $C_\varphi := \int_{\mathbb{R}^d} \varphi(|x|)dx$ as a normalization constant. We also use the notation $\tilde{\varphi}(x) := \varphi(|x|)$

There are some constants $\Theta_W, c_\Theta^0, c_\Theta^1, C_0^W, C_1^W > 0$ such that the periodic potential W fulfills:

- $W \in C^2\left(\mathbb{R}^d\right)$ (Regularity)
- $W(z) = W(z + z_n)\ \forall z_n \in \mathbb{Z}^d \forall z \in \mathbb{R}^d$ (Periodicity)
- $c_\Theta^0 y^2 \leq y \nabla^2 W(x) y \leq c_\Theta^1 y^2\ \forall y \in R^d, x \in B_{\Theta_W}(Z^d)$ (Local convexity)
- W is infinitely times differentiable at all $x \in B_{\Theta_W}(Z^d)$
- $W(z) = W(-z)\ \forall \in \mathbb{R}^d$ (Symmetry)
- $C_0^W \operatorname{dist}^2(z, \mathbb{Z}^d) \leq W(z) \leq C_1^W \operatorname{dist}^2(z, \mathbb{Z}^d)$ (Coercivity)

Penalizing the vacancies The density of atoms in a lattice χ_A is $\det(A)$. We define the local density of a configuration χ by

$$\rho_\lambda(\chi, x) := \frac{1}{C_\varphi \lambda^d} \sum_i \varphi\left(\lambda^{-1} |x_i - x|\right) \tag{1.3.5}$$

Hence, we define :

$$\nu_\lambda(\chi, A, x) := \vartheta\left(\det A - \rho_\lambda(\chi, x)\right) \tag{1.3.6}$$

So the energy per vacancies is ϑ. This part also ensures that a lattice that is finer than necessary will not be fitted to the configuration because it would contain a big number of vacancies.

Hard core potential $V : \mathbb{R}^+ \to \{0, \infty\}$ is an hard core repulsion. It has the technical purpose, to prevent several atoms from sitting at the same lattice side.

$$V(x) := \begin{cases} 0 & \text{for} \quad x \geq s_0 \\ \infty & \text{for} \quad x < s_0. \end{cases} \tag{1.3.7}$$

The hard-core potential implies, that any configuration with finite energy smaller than $\rho_d^{max} + O(\lambda^{-1})$.

$$\rho_d^{max} = \frac{2^d}{w_d s_0^d} + O(s_o \lambda^{-1}) \tag{1.3.8}$$

Where w_d is the volume of the d-dimensional unit sphere[1]

[1] One can use the density of the closest sphere packing for an improvement

Integration domain and boundary values. We integrate the energy density over $B_{2\lambda}(\Omega)$ instead of Ω so that the effective chemical potential for atoms is not different at the boundary of Ω (see section 2.1.1). In our model boundary values are given by the atoms placed in $B_{4\lambda}(\Omega)/\Omega$. We define these atoms by $\chi_S := \chi \cap B_{2\lambda}(\Omega)$ and we consider them to have fixed positions. The atoms $\chi_I = \chi \cap \Omega$ can be moved but are forbidden to leave Ω. So for most cases we deal with fixed particle number.

Compatibility conditions The model has a large number of parameters and not in any combination of them it will work as intended. Therefore, we assume the following compatibility conditions.

1) The Compatibility condition for the hard core potential

$$C_0^W \frac{s_0^2}{2} > \vartheta \tag{1.3.9}$$

This condition guarantees that a configuration with one atom per potential valley of J_λ is of lower energy than one with two atoms per valley. This condition is primary used in theorem 2.4.3, which is used throughout the thesis.

2) Compatibility condition for elastic potential

$$\vartheta \leq C_1^{El} \det(E) \tag{1.3.10}$$

This compatibility condition ensures together with the coercivity condition for F that for low particle density only matrices A of a compact subset $Gl_d(\mathbb{R})$ have low pre-energy densities. This condition is only used in Lemma 2.2.6. But the result of Lemma 2.2.6 is used in many proofs.

Reparametrisation:

Definition 1.3.1. *We call a pair $\mathcal{B} = (B, z) \in Gl_d(\mathbb{Z}) \times \mathbb{Z}^d$ a reparametrisation. For $\mathcal{A} = (A, \tau) \in Gl_d(\mathbb{Z}) \times \mathbb{Z}^d$ we define the reparametrisation of $\mathcal{A}$ as*

$$\mathcal{B}\mathcal{A} = (BA_R, B\tau_R + t) \tag{1.3.11}$$

We note that

$$\begin{aligned} x \in \chi_{\mathcal{A}} &\Longleftrightarrow Ax + \tau \in \mathbb{Z}^d \\ &\Longleftrightarrow BAx + B\tau_R + t \in \mathbb{Z}^d \\ &\Longleftrightarrow x \in \chi_{\mathcal{B}\mathcal{A}} \quad . \end{aligned}$$

So Bravais-lattices are invariant under reparametrisations

1.4 Overview of the results

Our model is a modified version of the one that was proposed and studied by S.Luckhaus and L.Mugnai in [7]. The main difference is that a different J_λ is used for the same purpose. In that paper the authors have shown that for points with low energy density the approximation procedure leads to a uniquely defined fitted Bravais lattice $\chi_{\mathcal{A}} + x$. One can span the same lattice with different affine transformations $\mathcal{A}_{\mathcal{B}}$. Furthermore it is proved in [7] that the multivalued map $\mathcal{A}_{\mathcal{B}}(x)$ is differentiable and its gradients satisfies

$$\lambda \|\nabla A_{\mathcal{B}}(x)\| + \|A_{\mathcal{B}}(x) - \nabla \tau_{\mathcal{B}}(x)| \leq \frac{C_{\nabla}^{\mathcal{B}}}{\lambda} \quad . \tag{1.4.1}$$

Finally, the authors discuss the possibility to use $\tau_{\mathcal{B}}(x)$ to construct local Lagrangian coordinates and to define 'holonomy representation map', which can be used to identify topological defects as dislocations.

In Chapter 3 we study the properties of the model in the case, that the particle configuration is a Bravais lattice $\chi_{\mathcal{A}_R}$ or a elastically deformed state $\chi = \psi(\mathbb{Z}^d)$. As the first main result Theorem 3.1.5 states that, even in the case that the atom configuration is the Bravais lattice $\chi_{\mathcal{A}_R}$, the approximated lattice $\chi_{\mathcal{A}(x)} + x$ will not coincide with the prescribed particle configuration $\chi_{\mathcal{A}_R}$. The difference between A and A_R scales like λ^{-2}. Furthermore, we define the average effective elastic potential as the average energy density of the model in the case, that the configuration is a Bravais lattice, and calculate an upper bound for the energy of elastically deformed configurations $\chi = \psi(\mathbb{Z}^d)$. This way we get an estimate that also holds in the case $L \to \infty$ and fixed λ We apply this estimate to gain an upper bound for the energy barrier of plastic deformation for dimension two, considering the formation and movement of a pair of dislocations. This upper bound scales like λ^2(Theorem 3.3.2). One of the main technical difficulties is, that we allow reparametrisations. If we restrict A to one map of $Gl_d(\mathbb{R})/Gl_d(\mathbb{Z})$, many estimates become easier.

In Chapter 3 we explore the possibility to construct Lagrangian coordinates in the framework of our model. First we concentrate on a method to calculate discrete Lagrangian coordinates. We prove in Theorem 4.1.2 that for two points y_1 and y_2 satisfying some regularity condition and $|y_1 - y_2| \leq 1.5\lambda$ there is a reparametrisation $\mathcal{B} = (B, t) \in Gl(\mathbb{Z}) \times \mathbb{Z}^d$ such that

$$\|id - A^{-1}(y_1) B A(y_2)\| < C_J^A \frac{\sqrt{J_\lambda}}{\lambda} \quad ,$$

$$\left| B\tau(y_2) + t - \tau(y_1) - \frac{BA(y_2) + A(y_1)}{2} (y_2 - y_1) \right| < \|A_1\| \sqrt{J_\lambda} \quad .$$

This estimate is a discrete analogon to the estimate for the gradient (1.4.1). For a finite sequence of regular points $|y_i - y_{i+1}| \leq 1.5\lambda$ the product of the reparametrisations gained from Theorem 4.1.2 is a topological quantity (Theorem 4.1.8). Hence, one can use these sequences for homotopy-type arguments just as one would use a differentiable curve. The sequence of reparametrisations for such a chain, that comes back to its starting points, will allow us to define a generalized Burgers vector as the product of the reparametrisations in the sequence. Compared to the method, that is used in [7] to identify topological defects, our methods has the advantage, that we do not need a differentiable curve of low energy points for the homotopy argument but only some points so the homotopy class can be extended through areas of irregular points, provided the thickness of the area is maximal 1.5λ . This framework also allows to proof a lower bound for the energy of the core region of a dislocation scaling like λ^2.

In the second part of Chapter 4 we finally adapt the method of [7] for constructing Lagrangian coordinates to our model. Since, in our case, the global minimizer $\mathcal{A}(x)$ of $h_\lambda(\cdot, \chi, x)$ will not be differentiable we will use local minimizers instead. We prove that ,under some regularity assumptions, local minimizers of h_λ and of J_λ are differentiable functions of x and of the atom positions. (Theorem 4.2.5). Furthermore we improve the estimate (1.4.1) to

$$\lambda \|\nabla \tilde{A}_{\mathcal{B}}(x)\| + \|\tilde{A}_{\mathcal{B}}(x) - \nabla \tau_{\mathcal{B}}(x)\| \leq O\left(\frac{\sqrt{J_\lambda}}{\lambda}\right) \quad . \tag{1.4.2}$$

and calculate the corresponding estimate for the second derivatives of the minimizer $\mathcal{B}$ that it holds

$$\lambda \|\nabla^2 \tilde{A}_{\mathcal{B}}(x)\| + \|\nabla^2 \tilde{A}_{\mathcal{B}}(x) - \nabla \tau_{\mathcal{B}}(x)\| \leq \left(\frac{\sqrt{J_\lambda}}{\lambda^2}\right) \quad . \tag{1.4.3}$$

This improved estimates allow us to calculate in Theorem 4.2.5 a lower bound for the energy density as a functional of the Lagrangian coordinate $\tilde{\tau}_B$ in the form

$$\hat{h}_\lambda(\chi, y) \geq F_C\left(\nabla \tilde{\tau}_B(y)\right) + \frac{1}{5}\tilde{C}_\nabla \left(\frac{\rho_{2\lambda}}{\rho_\lambda}\right) \left\|\nabla \tilde{\tau}_B^{-1}(y)\right\|^2 \lambda^4 \|\nabla^2 \tilde{\tau}_B(y)\|^2 \det\left(\nabla \tilde{\tau}_B\right) \quad , \tag{1.4.4}$$

where F_C is a modified elastic potential satisfying

$$F_C\left(A\right) = \min\left\{F(BA) | B \in Gl_d(\mathbb{Z}^d)\right\} + O(\lambda^{-2}) \quad . \tag{1.4.5}$$

Chapter 2

Basic mathematical properties

2.1 General properties

The energy density is in our model

$$\hat{h}_\lambda(\chi, x) = \inf_{\mathcal{A}} \{F(A) + J_\lambda + \vartheta(\det A - \rho_\lambda)\} \quad . \tag{2.1.1}$$

Because $\rho_\lambda(\chi, x)$ does not depend on $\mathcal{A}$ we get

$$\hat{h}_\lambda(\chi, x) = \inf_{\mathcal{A}} \{F(A) + J_\lambda + \vartheta \det A\} - \vartheta\rho_\lambda \quad . \tag{2.1.2}$$

Hence, in the definition of the energy density appears the particle density $\rho_\lambda(\chi, x)$ as a linear contribution. We can integrate this density out and see that this term is depending on the particle number but not on the position of the inner atoms.

Lemma 2.1.1. *For all configuration χ holds*

$$\int_{B_{2\lambda}(\Omega)} \rho_\lambda(\chi, x)dx = N_I + \int_{B_{2\lambda}(\Omega)} \rho_\lambda(\chi_S, x)dx \quad , \tag{2.1.3}$$

where N_I is the number of inner atoms.

Proof. We have

$$\begin{aligned}
&\int_{B_{2\lambda}(\Omega)} \rho_\lambda(\chi, x)dx \\
&= \frac{1}{C_\varphi\lambda^d} \int_{B_{2\lambda}(\Omega)} \left(\sum_{x_i \in \chi_I} \varphi\left(\lambda^{-1}|x_i - x|\right) + \sum_{x_i \in \chi_I} \varphi\left(\lambda^{-1}|x_i - x|\right) \right) dx \\
=&\frac{1}{C_\varphi\lambda^d} \sum_{x_i \in \chi_I} \int_{B_{2\lambda}(\Omega)} \varphi\left(\lambda^{-1}|x_i - x|\right) dx + \int_{B_{2\lambda}(\Omega)} \rho_\lambda(\chi_S, x)dx \quad .
\end{aligned} \tag{2.1.4}$$

For $x_i \in \chi_I \subset \Omega$ and $x \notin B_2\lambda(\Omega)$ holds $\varphi\left(\lambda^{-1}|x_i - x|\right) = 0$. We calculate

$$\begin{aligned}\int_{B_{2\lambda}(\Omega)} \rho_\lambda(\chi, x)dx =& \frac{1}{C_\varphi \lambda^d} \sum_{x_i \in \chi_I} \int_{\mathbb{R}^d} \varphi\left(\lambda^{-1}|x_i - x|\right) dx + \int_{B_{2\lambda}(\Omega)} \rho_\lambda(\chi_S, x)dx \\ =& \frac{1}{C_\varphi} \sum_{x_i \in \chi_I} \int_{\mathbb{R}^d} \varphi(|y|)\, dy + \int_{B_{2\lambda}(\Omega)} \rho_\lambda(\chi_S, x)dx \\ =& N_I + \int_{B_{2\lambda}(\Omega)} \rho_\lambda(\chi_S, x)dxv \quad . \end{aligned} \tag{2.1.5}$$

□

This lemma implies

$$\forall x_i \in \chi_I \quad \partial_{x_i} \int_{B_{4\lambda}} \rho_\lambda(\chi, x)dx = 0 \quad . \tag{2.1.6}$$

Hence, atoms in the interior do not experience a force due to the chemical potential. An integration of the density over Ω instead of $B_{2\lambda}(\Omega)$ would make the contribution of the atoms near the boundary smaller. So the boundary would be repulsive for atoms. This would have the consequence that the ground state can not be a Bravais lattices.

Next we will prove a lemma that is technical very important for the further treatment of our model. If the configuration is a Bravais lattice $\chi_{\mathcal{A}_R}$, then for any function ψ that is infinitely times differentiable and has compact support the difference between the sum of the values of the function ψ and the integral of ψ times $\det A_R \sum_x \psi\left(\lambda^{-1}(x_i - x)\right)$ is bounded from above with $O(\lambda^m)$ for any m. In particular the particle density of the Bravais lattice is $\det A_R$ up to order $O(\lambda^m)$. This will be important in Section 3.1, where our configuration is a Bravais lattice, and in Section 3.2, where we deform a Bravais lattice. However the result is also used in many other sections where we only compare the configuration with a Bravais lattice.

Lemma 2.1.2. *For every $m \in \mathbb{N}$ there exists $C_m > 0$ such that for all $A_R \in Gl_d(\mathbb{R})$, $\tau_R \in \mathbb{R}^d$ and $\psi \in C_C^\infty(\mathbb{R}^d)$ with $supp(\psi) \subset B_2(0)$ it holds*

$$\begin{aligned}&\left| \frac{1}{\lambda^d} \sum_{x_i \in \chi_{\mathcal{A}_R}} \psi\left(\lambda^{-1}(x_i - x)\right) - \det A_R \int_{\mathbb{R}^d} \psi(y)dy \right| \\ \leq& C_m \frac{|A_R^{-1}|^m}{\lambda^m} \frac{\left(\lambda + |A_R^{-1}|\right)^d}{\lambda^d} \|\nabla^m \psi\|_\infty \det A_R \quad . \end{aligned} \tag{2.1.7}$$

In particular for $\psi = \tilde{\varphi}$ we have

$$\begin{aligned}&|\rho(\chi_{\mathcal{A}_R}, x) - \det A_R| \\ \leq& \frac{C_m}{C_\varphi} \frac{|A_R^{-1}|^m}{\lambda^m} \frac{\left(\lambda + |A_R^{-1}|\right)^d}{\lambda^d} \|\nabla^m \psi\|_\infty \det A_R \end{aligned} \tag{2.1.8}$$

Proof. We consider

$$\rho_\lambda(\chi_{(A_R,\tau_R)}, x) = \rho_\lambda(\chi_{(A_R,\tau_R - A_R x)}, 0) \quad . \tag{2.1.9}$$

This means that we can assume w.l.o.g $x = 0$. We calculate

$$\begin{aligned}\sum_{x_i \in \chi_{\mathcal{A}_R}} \det A_R^{-1}\, \psi\left(\lambda^{-1} x_i\right) &= \sum_{x_i \in \chi_{\mathcal{A}_R}} \int_{Q_i} dy \psi\left(\lambda^{-1} x_i\right) \\ &= \sum_{x_i \in \chi_{\mathcal{A}_R}} \int_{Q_i} \psi\left(\lambda^{-1} y\right) + \left(\psi\left(\lambda^{-1} x_i\right) - \psi\left(\lambda^{-1} y\right)\right) dy \quad .\end{aligned} \tag{2.1.10}$$

We have)

$$\begin{aligned}\sum_{x_i \in \chi_{\mathcal{A}_R}} \int_{Q_i} \psi\left(\lambda^{-1} y\right) dy = &\int_{\mathbb{R}^d} \psi\left(\lambda^{-1} y\right) dy \\ = &\lambda^d \int_{\mathbb{R}^d} \psi\left(\tilde{y}\right) d\tilde{y} \quad .\end{aligned} \tag{2.1.11}$$

Next we apply a Taylor expansion up to order m. We obtain

$$\begin{aligned}\psi\left(\lambda^{-1} y\right) = &\psi\left(\lambda^{-1} x_i\right) + \sum_{|\mathbf{j}|=\mathbf{1}}^{m} \frac{1}{\mathbf{j}!\lambda^{|\mathbf{j}|}} \left(\partial^{\mathbf{j}} \psi\right)\left(\lambda^{-1} x_i\right)(y - x_i)^{\mathbf{j}} \\ &+ O(\lambda^{-m-1}) \max_{t \in [0,1]} \|\nabla^{m+1} \psi(t x_i + (1-t) y)\| \, |x_i - y|^{m+1} \quad .\end{aligned} \tag{2.1.12}$$

We use this to calculate the second term in (2.1.10) and we get

$$\begin{aligned}&\sum_{x_i \in \chi_{\mathcal{A}_R}} \int_{Q_i} \left(\psi\left(\lambda^{-1} x_i\right) - \psi\left(\lambda^{-1} y\right)\right) dy \\ = &- \sum_{x_i \in \chi_{\mathcal{A}_R}} \int_{Q_i} \sum_{|\mathbf{j}|=1}^{m} \frac{1}{\mathbf{j}!\lambda^{|\mathbf{j}|}} \left(\partial^{\mathbf{j}} \psi\right)\left(\lambda^{-1} x_i\right)(y - x_i)^{\mathbf{j}}\, dy \\ &+ O(\lambda^{-m-1}) \sum_{x_i \in \chi_{\mathcal{A}_R}} \int_{Q_i} \max_{t \in [0,1]} \|\nabla^{m+1} \psi(t x_i + (1-t) y)\| \, |x_i - y|^{m+1}\, dy \quad .\end{aligned} \tag{2.1.13}$$

We estimate the error term of order $m+1$ in (2.1.13). The i only contributes to the sum if $Q_i \cap B_{2\lambda}(x)$ is none empty. Hence, $x_i \in B_{2\lambda + \sqrt{d}|A_R^{-1}|}(x)$ and $Q_i \subset$

$B_{2\lambda+2\sqrt{d}|A_R^{-1}|}(x)$

$$
\begin{aligned}
&O(\lambda^{-m-1})\sum_{x_i\in\chi\mathcal{A}_R}\int_{Q_i}\max_{t\in[0,1]}\left\|\nabla^{m+1}\psi\left(tx_i+(1-t)y\right)\right\||x_i-y|^{m+1}\,dy\\
\leq &O(\lambda^{-m-1})\frac{w_d}{d}(2\lambda+4|A_R^{-1}|)^d 2^{m+1}|A_R^{-1}|^{m+1}\|\nabla^{m+1}\psi\|_\infty \det A_R\\
\leq &O\left(\frac{|A_R^{-1}|^{m+1}}{\lambda^{m+1}}\right)(\lambda+|A_R^{-1}|)^d\|\nabla^{m+1}\psi\|_\infty \det A_R \quad . \qquad (2.1.14)
\end{aligned}
$$

Now we prove by induction that for every multi index $\mathbf{j}$ it holds

$$
\begin{aligned}
&\sum_{x_i\in\chi\mathcal{A}_R}\int_{Q_i}\lambda^{-|\mathbf{j}|}\left(\partial^{\mathbf{j}}\psi\right)\left(\lambda^{-1}x_i\right)\\
=&\sum_{|\mathbf{k}|=\mathbf{1}}^{m-\mathbf{j}-1}\sum_{x_i\in\chi\mathcal{A}_R}\int_{Q_i}\lambda^{-|\mathbf{j}+\mathbf{k}|}\left(\partial^{\mathbf{j}+\mathbf{k}}\psi\right)\left(\lambda^{-1}x_i\right)\\
&+O\left(\frac{|A_R^{-1}|^{m+1}}{\lambda^{m+1}}\right)(\lambda+|A_R^{-1}|)^d\|\nabla^{m+1}\psi\|_\infty \det A_R \quad . \qquad (2.1.15)
\end{aligned}
$$

Integrating directly $(y-x_i)^{\mathbf{j}}$ and making a change of coordinates, we get

$$
\begin{aligned}
&\sum_{x_i\in\chi\mathcal{A}_R}\int_{Q_i}\lambda^{-|\mathbf{j}|}\left(\partial_{\mathbf{j}}\psi\right)\left(\lambda^{-1}x_i\right)(y-x_i)^{\mathbf{j}}\,dy\\
=&\sum_{x_i\in\chi\mathcal{A}_R}\lambda^{-|\mathbf{j}|}\left(\partial_{\mathbf{j}}\psi\right)\left(\lambda^{-1}x_i\right)\int_{Q_i}(y-x_i)^{\mathbf{j}}\,dy\\
=&\sum_{x_i\in\chi\mathcal{A}_R}\lambda^{-|\mathbf{j}|}\left(\partial_{\mathbf{j}}\psi\right)\left(\lambda^{-1}x_i\right)\int_{Q_0}\tilde{y}^{\mathbf{j}}d\tilde{y} \quad . \qquad (2.1.16)
\end{aligned}
$$

If $|\mathbf{j}|$ is odd, then $\int_{Q_0}\tilde{y}^{\mathbf{j}}d\tilde{y}$ is zero, because it is an odd function integrate over an symmetric domain. If $|\mathbf{j}|$ is even, then $\int_{Q_0}\tilde{y}^{\mathbf{j}}d\tilde{y}$ may be not 0 but is still independent of i. This means, we can write the contribution of $\mathbf{j}$ as some constant times $\det A_R^{-1}$ times $\sum_{x_i\in\chi\mathcal{A}_R}|A_R^{-1}|^{|\mathbf{j}|}\lambda^{-|\mathbf{j}|}(\partial^{\mathbf{j}}\psi)(\lambda^{-1}x_i)$. Since ψ is an infinitely often differentiable function with compact support, so is $\partial^{\mathbf{j}}\psi$ Hence, the calculation above for ψ applies also to $\partial^{\mathbf{j}}\psi$. We can split the sum as follows

$$
\begin{aligned}
&\sum_{x_i\in\chi\mathcal{A}_R}\det A_R^{-1}\partial^{\mathbf{j}}\psi\left(\lambda^{-1}x_i\right)\\
=&\int\partial^{\mathbf{j}}\psi\left(\lambda^{-1}|y|\right)dy+\sum_{x_i\in\chi\mathcal{A}_R}\int_{Q_i}\partial^{\mathbf{j}}\psi\left(\lambda^{-1}x_i\right)-\partial^{\mathbf{j}}\psi\left(\lambda^{-1}y\right)dy \quad . \qquad (2.1.17)
\end{aligned}
$$

We have

$$\sum_{x_i \in \chi\mathcal{A}_R} \int_{Q_i} \partial^{\mathbf{j}} \psi \left(\lambda^{-1} (y - x)\right) dy = \lambda^d \int_{\mathbb{R}^d} \partial^{\mathbf{j}} \psi (\tilde{y})\, d\tilde{y} \quad . \tag{2.1.18}$$

Since $\partial^{\mathbf{j}}\psi$ is a derivative of a function with compact support its integral is zero. and the first term in (2.1.17) is zero too. To estimate the difference term (2.1.17) we again consider the Taylor expansion up to order $(m - |\mathbf{j}|)$.

$$\begin{aligned} &\sum_{x_i \in \chi\mathcal{A}_R} \int_{Q_i} \partial^{\mathbf{j}} \psi \left(\lambda^{-1} x_i\right) - \partial^{\mathbf{j}} \psi \left(\lambda^{-1} y\right) dy \\ &= - \sum_{x_i \in \chi\mathcal{A}_R} \sum_{|\mathbf{k}|=1}^{m-|\mathbf{j}|} \frac{1}{\mathbf{k}!} \lambda^{-|\mathbf{k}|} \left(\partial_{\mathbf{k}} \partial^{\mathbf{j}} \psi\right) \left(\lambda^{-1} x_i\right) (y - x_i)^{\mathbf{k}} \\ &\quad + O\left(\frac{|A_R^{-1}|^{m+1-|\mathbf{j}|}}{\lambda^{m+1-|\mathbf{j}}}\right) (\lambda + |A_R^{-1}|)^d \|\nabla^{m+1}\psi\|_\infty \det A_R \quad . \end{aligned} \tag{2.1.19}$$

We get together with the factor $|A_R^{-1}|^{|\mathbf{j}|}\lambda^{-|\mathbf{j}|}$,

$$\begin{aligned} &\sum_{x_i \in \chi\mathcal{A}_R} \int_{Q_i} \lambda^{|\mathbf{j}|} \left(\partial^{\mathbf{j}} \psi\right) \left(\lambda^{-1} x_i\right) \\ &= - \sum_{x_i \in \chi\mathcal{A}_R} \sum_{|\mathbf{k}|=1}^{m-|\mathbf{j}|} \frac{1}{\mathbf{k}!} \lambda^{-|\mathbf{k}|-|\mathbf{j}|} \left(\partial_{\mathbf{k}} \partial^{\mathbf{j}} \psi\right) \left(\lambda^{-1} x_i\right) \\ &\quad + O\left(\frac{|A_R^{-1}|^{m+1-|\mathbf{j}|}}{\lambda^{m+1-|\mathbf{j}|}}\right) (\lambda + |A_R^{-1}|)^d \|\nabla^{m+1}\psi\|_\infty \det A_R \quad . \end{aligned} \tag{2.1.20}$$

Now we iteratively increase the multi index $|\mathbf{j}|$ of the derivative on ψ and we only produce error terms of order $O\left(\frac{|A_R^{-1}|^{m+1}}{\lambda^{m+1}}\right) (\lambda + |A_R^{-1}|)^d \|\nabla^{m+1}\psi\|_\infty \det A_R$, Since, we need to increase the multi index only up to $|\mathbf{j}| = m$ this procedure terminates. Finally, this leads to

$$\det A_R^{-1} \sum_{x_i \in \chi\mathcal{A}_R} \psi \left(\lambda^{-1} x_i\right) = \lambda^d \int_{\mathbb{R}^d} \psi (y)\, dy + O\left(\frac{|A_R^{-1}|^{m+1}}{\lambda^{m+1}}\right) (\lambda + |A_R^{-1}|)^d \|\nabla^{m+1}\psi\|_\infty \quad . \tag{2.1.21}$$

□

We study the symmetries of the model and note that rotations and translations are not changing the energy density.

Lemma 2.1.3. *The energy functional is translational invariant. This means*

$$\forall y \in \mathbb{R}^d \quad \hat{h}_\lambda (\chi, x) = \hat{h}_\lambda (\chi + y, x + y) \quad . \tag{2.1.22}$$

Additionally the energy functional is frame indifferent. This means

$$\forall R \in SO_d \quad \hat{h}_\lambda(\chi, x) = \hat{h}_\lambda(R\chi, Rx) \quad . \tag{2.1.23}$$

Proof. The pre-energy density is

$$h_\lambda(\mathcal{A}, \chi, x) = F(A) + J_\lambda(x, \mathcal{A}, \chi) + \vartheta \det A - (\vartheta + \vartheta_2)\rho_\lambda \quad .$$

The configuration enters at two points into the pre-energy density, namely in J_λ and in ρ_λ.

$$\begin{aligned} J_\lambda(\mathcal{A}, \chi, x) =& \frac{\|A^{-1}\|^2}{C_\varphi \lambda^d} \sum_i W(A(x_i - x) + \tau)\varphi\left(\lambda^{-1}|x_i - x|\right) \\ \rho_\lambda(\chi, x) =& \frac{1}{C_\varphi \lambda^d} \sum_i \varphi\left(\lambda^{-1}|x_i - x|\right) \end{aligned} \tag{2.1.24}$$

In both cases x_i only appears as $x_i - x$ and we can add y to both x_i and x without changing J_λ and ρ_λ. We get for every $\mathcal{A}$

$$h_\lambda(\mathcal{A}, \chi, x) = h_\lambda(\mathcal{A}, \chi + y, x + y) \quad . \tag{2.1.25}$$

This proves the translation invariance. If we apply a rotation matrix R to both χ and x, then ρ_λ is not changing at all.

$$\begin{aligned} \rho_\lambda(R\chi, Rx) =& \frac{1}{C_\varphi \lambda^d} \sum_i \varphi\left(\lambda^{-1}|Rx_i - Rx|\right) \\ =& \frac{1}{C_\varphi \lambda^d} \sum_i \varphi\left(\lambda^{-1}|x_i - x|\right) = \rho_\lambda(\chi, x). \end{aligned} \tag{2.1.26}$$

Furthermore, because a rotation is not changing the norm of a matrix, we similarly obtain

$$\begin{aligned} J_\lambda(A, \tau, R\chi, Rx) =& \frac{\|A^{-1}\|^2}{C_\varphi \lambda^d} \sum_i W(A(Rx_i - Rx) + \tau)\varphi\left(\lambda^{-1}|Rx_i - Rx|\right) \\ =& \frac{\|(AR)^{-1}\|^2}{C_\varphi \lambda^d} \sum_i W(AR(x_i - x) + \tau)\varphi\left(\lambda^{-1}|x_i - x|\right) \\ =& J_\lambda(AR, \tau, \chi, x) \quad . \end{aligned} \tag{2.1.27}$$

Finally, also the determinant is invariant under rotations and the frame invariance of F leads to

$$h_\lambda(A, \tau, R\chi, Rx) = h_\lambda(AR, \tau, \chi, Rx) \quad . \tag{2.1.28}$$

Since the energy density $\hat{h}_\lambda$ is the infimum over all A, we finally get

$$\hat{h}_\lambda(\chi, x) = \hat{h}_\lambda(R\chi, Rx) \quad . \tag{2.1.29}$$

□

2.2 Existence and properties of the minimizing $\mathcal{A}$

The energy density of our model is defined as

$$\hat{h}_\lambda(\chi, x) := \inf_{\mathcal{A}} \{h_\lambda(\mathcal{A}, \chi, x)\} \quad .$$

In this section will prove that there exists a minimizer $\hat{\mathcal{A}} \in Gl_d(\mathbb{R}^d) \times \mathbb{R}^d$ such that

$$h_\lambda\left(\hat{\mathcal{A}}, \chi, x\right) = \hat{h}_\lambda(\chi, x) \quad . \tag{2.2.1}$$

First we will prove that $J_\lambda(\mathcal{A}, \chi, x)$ can be estimated form below and above with the mean square distance between the atoms and the Bravais lattice $\chi_{\mathcal{A}} + x$. We can use this to show that there is a general upper bound for the energy of a configuration only depending on the particle density ρ_λ. Then we proof that there is a compact subset of $Gl_d(\mathbb{R}^d)$ such that all $\mathcal{A}$ with low enough pre- energy has to be in this compact subset. If we combine this with the continuity of $h_\lambda(\mathcal{A}, \chi, x)$ in the first argument, we get the existence of a minimizer, and some bounds on its norms and determinate. Finally we use the existence of the minimizers to define the effective particle potential.

$J_\lambda(\mathcal{A}, \chi, x)$ acts like a standard deviation of the atom position J and the lattice $\chi_{\mathcal{A}} + x$

Lemma 2.2.1. *For all $A \in GL_d(\mathbb{R})$, all $\tau \in R^d$, all positions x and configurations χ it holds*

$$\begin{aligned} J_\lambda(\mathcal{A}, \chi, x) \geq& \frac{C_0^W}{C_\varphi \lambda^d} \sum_i \operatorname{dist}^2(x_i, \chi_{\mathcal{A}} + x) \varphi\left(\lambda^{-1}|x_i - x|\right) \quad , \\ J_\lambda(\mathcal{A}, \chi, x) \leq& \frac{C_1^W \|A\|^2 \|A^{-1}\|^2}{C_\varphi \lambda^d} \sum_i \operatorname{dist}^2(x_i, \chi_{\mathcal{A}} + x) \varphi\left(\lambda^{-1}|x_i - x|\right) \quad . \end{aligned} \tag{2.2.2}$$

This implies in particular

$$0 < J_\lambda(\mathcal{A}, \chi, x) < dC_1^W \|A\|^2 \left\|A^{-1}\right\|^4 \rho_\lambda(\chi, x) \quad . \tag{2.2.3}$$

Proof. On the one hand we have

$$\begin{aligned}
& C_\varphi \lambda^d J_\lambda(\mathcal{A},\chi,x) \\
= & \left\|A^{-1}\right\|^2 \sum_i W(A(x_i-x)+\tau)\varphi\left(\lambda^{-1}|x_i-x|\right) \\
\leq & C_1^W \left\|A^{-1}\right\|^2 \sum_i \operatorname{dist}^2(A(x_i-x)+\tau,\mathbb{Z}^d)\varphi\left(\lambda^{-1}|x_i-x|\right) \\
\leq & C_1^W \left\|A^{-1}\right\|^2 \sum_i \operatorname{dist}^2(A(x_i-x),\mathbb{Z}^d-\tau)^2\varphi\left(\lambda^{-1}|x_i-x|\right) \\
\leq & C_1^W \left\|A^{-1}\right\|^2 \sum_i \|A\|^2 \operatorname{dist}^2((x_i-x),A^{-1}(\mathbb{Z}^d-\tau))\varphi\left(\lambda^{-1}|x_i-x|\right) \\
\leq & C_1^W \left\|A^{-1}\right\|^2 \|A\|^2 \sum_i \operatorname{dist}^2(x_i,\chi_{\mathcal{A}}+x)\varphi\left(\lambda^{-1}|x_i-x|\right) \quad . \qquad (2.2.4)
\end{aligned}$$

On the other hand we have

$$\begin{aligned}
& C_\varphi \lambda^d J_\lambda(\mathcal{A},\chi,x) \\
= & \left\|A^{-1}\right\|^2 \sum_i W(A(x_i-x)+\tau)\varphi\left(\lambda^{-1}|x_i-x|\right) \\
\geq & C_0^W \left\|A^{-1}\right\|^2 \sum_i \operatorname{dist}^2(A(x_i-x)+\tau,\mathbb{Z}^d)\varphi\left(\lambda^{-1}|x_i-x|\right) \\
\geq & C_0^W \left\|A^{-1}\right\|^2 \sum_i \operatorname{dist}^2(A(x_i-x),\mathbb{Z}^d-\tau)^2\varphi\left(\lambda^{-1}|x_i-x|\right) \\
\geq & C_0^W \sum_i \operatorname{dist}^2((x_i-x),A^{-1}(\mathbb{Z}^d-\tau))\varphi\left(\lambda^{-1}|x_i-x|\right) \\
\geq & C_0^W \sum_i \operatorname{dist}^2(x_i,\chi_{\mathcal{A}}+x)\varphi\left(\lambda^{-1}|x_i-x|\right) \quad . \qquad (2.2.5)
\end{aligned}$$

□

We introduce a corollary that is not important for the main line of thoughts of this section. However it will be important in Section 4.2. Since $J_\lambda(\mathcal{A},\chi,x)$ can be estimate with the mean square distance between the configuration χ and the Bravais lattice $\chi_{\mathcal{A}}+x$ And a reparametrisation of $\mathcal{BA}$ has the same Bravais lattice. We can estimate $J_\lambda(\mathcal{A},\chi,x)$ with $J_\lambda(\widetilde{\mathcal{A}}\mathcal{A},\chi,x)$.

Corollary 2.2.2. *For all $\mathcal{A}\in Gl_d(\mathbb{R})\times\mathbb{R}^d$ and $\mathcal{B}\in Gl_d(\mathbb{Z})\times\mathbb{Z}^d$ fulfill*

$$\begin{aligned}
J_\lambda(x,\mathcal{A},\chi) \leq & \frac{C_1^W \|A\|^2 \left\|A^{-1}\right\|^2}{C_\varphi \lambda^d} \sum_i \operatorname{dist}^2(x_i,\chi_{A,\tau}+x)\varphi\left(\lambda^{-1}|x_i-x|\right) \\
\leq & \frac{C_1^W \|A\|^2 \left\|A^{-1}\right\|^2}{C_\varphi \lambda^d} \sum_i \operatorname{dist}^2(x_i,\chi_{BA,B\tau+z}+x)\varphi\left(\lambda^{-1}|x_i-x|\right) \\
\leq & \frac{C_1^W \|A\|^2 \left\|A^{-1}\right\|^2}{C_0^W} J_\lambda(x,(BA,B\tau+z),\chi) \quad . \qquad (2.2.6)
\end{aligned}$$

Since the infimum in the energy density $\hat{h}_\lambda$ is smaller equal the pre-energy for every τ, J_λ is always smaller than the average over W. No matter how irregular the configuration is. Hence, we get a general upper bound for the energy density.

Lemma 2.2.3. *For any configuration χ with finite energy we have*

$$\hat{h}_\lambda(\chi, x) \le \inf_A \left\{ F(A) + \vartheta \det A - \vartheta\rho_\lambda + \left\|A^{-1}\right\|^2 \left(\int_{[0,1]^d} W(\tau) d\tau \right) \rho_\lambda(\chi, x) \right\} \quad . \tag{2.2.7}$$

In particular we get

$$\hat{h}_\lambda(x, \chi) \le \vartheta \det E - \vartheta\rho_\lambda + \left\|E^{-1}\right\|^2 \left(\int_{[0,1]^d} W(\tau) d\tau \right) \rho_\lambda \quad . \tag{2.2.8}$$

Proof. We calculate

$$\begin{aligned} \hat{h}_\lambda(x, \chi) &= \inf_{\mathcal{A}} \{ h_\lambda(\mathcal{A}, \chi, x) \} \\ &= \inf_{\mathcal{A}} \{ F(A) + J_\lambda(\mathcal{A}, \chi, x) + \nu_\lambda(A, \chi, x) \} \\ &= \inf_A \left\{ F(A) + \nu_\lambda(\chi, A, x) + \inf_\tau \{ J_\lambda(\mathcal{A}, \chi, x) \} \right\} \quad . \end{aligned} \tag{2.2.9}$$

We will study $\inf_\tau \{J_\lambda(\mathcal{A}, \chi, x)\}$ in more detail. We use that the infimum is less or equal than the average.

$$\begin{aligned} \inf_\tau \{ J_\lambda(\mathcal{A}, \chi, x) \} &\le \int_{[0,1]^d} \{ J_\lambda(\mathcal{A}, \chi, x) \} d\tau \\ &\le \int_{[0,1]^d} \frac{\|A^{-1}\|^2}{C_\varphi \lambda^d} \sum_i W(A(x_i - x) + \tau) \varphi\left(\lambda^{-1} |x_i - x|\right) d\tau \\ &\le \frac{\|A^{-1}\|^2}{C_\varphi \lambda^d} \sum_i \left(\int_{[0,1]^d} W(A(x_i - x) + \tau) d\tau \right) \varphi\left(\lambda^{-1} |x_i - x|\right) \quad . \end{aligned} \tag{2.2.10}$$

The periodicity of W leads to the conclusion

$$\inf_\tau \{ J_\lambda(\mathcal{A}, \chi, x) \} \le \left\|A^{-1}\right\|^2 \left(\int_{[0,1]^d} W(\tau) d\tau \right) \rho_\lambda \quad . \tag{2.2.11}$$

□

We introduce the definition of regular and irregular atoms.

Definition 2.2.4. *For an atom configuration χ and lattice parameters $A \in Gl_d(\mathbb{R})$, $\tau \in \mathbb{R}^d$, and a position x and a distance $\beta > 0$, we define*

- *the* $(\mathcal{A}, \beta, x)$*-regular atoms*

$$\chi^{reg}_{\mathcal{A},\beta,x} := \{x_i \in \chi | dist(x_i, \chi_{\mathcal{A}} + x) \leq \beta\}, \tag{2.2.12}$$

- *and the irregular atoms*

$$\chi^{irr}_{\mathcal{A},\beta,x} := \{x_i \in \chi | dist(x_i, \chi_{\mathcal{A}} + x) > \beta\}, \tag{2.2.13}$$

- *and the densities of regular atoms and irregular atoms*

$$\rho^{reg}_{\mathcal{A},\beta}(x) := \rho_\lambda(\chi^{reg}_{\mathcal{A},\beta,x}, x) = \frac{1}{C_\varphi \lambda^d} \sum_{x_i \in \chi^{reg}_{\mathcal{A},\beta,x}} \varphi\left(\lambda^{-1} |x_i - x|\right) \quad , \tag{2.2.14}$$

$$\rho^{irr}_{\mathcal{A},\beta}(x) := \rho_\lambda(\chi^{irr}_{\mathcal{A},\beta,x}, x) = \frac{1}{C_\varphi \lambda^d} \sum_{x_i \in \chi^{irr}_{\mathcal{A},\beta,x}} \varphi\left(\lambda^{-1} |x_i - x|\right) \quad . \tag{2.2.15}$$

We proof simple estimate on the density of regular and irregular atoms depending on J_λ.

Lemma 2.2.5. *If* $x \in B_{2\lambda}(\Omega)$ *and* $\mathcal{A} \in Gl_d(\mathbb{R}) \times \mathbb{R}^d$*, we have*

$$\begin{aligned} \rho^{irr}_{\mathcal{A},\beta}(x) \leq & \frac{1}{C^W_0 \beta^2} J_\lambda(\mathcal{A}, \chi, x) \quad , \\ \rho^{reg}_{\mathcal{A},\beta}(x) \geq & \rho_\lambda(\chi, x) - \frac{1}{C^W_0 \beta^2} J_\lambda(\mathcal{A}, \chi, x) \quad . \end{aligned} \tag{2.2.16}$$

Proof. We use equation (2.2.2) to get

$$\begin{aligned} J_\lambda\left(\mathcal{A}, \chi_{\mathcal{A}_R}, x\right) \geq & \frac{C^W_0}{C_\varphi \lambda^d} \sum_{i \in \chi} \mathrm{dist}^2(x_i, \chi_{\mathcal{A}} + x) \varphi\left(\lambda^{-1} |x_i - x|\right) \\ \geq & \frac{C^W_0}{C_\varphi \lambda^d} \sum_{x_i \in \chi^{irr}_{\mathcal{A},\beta,x}} \mathrm{dist}^2(x_i, \chi_{\mathcal{A}} + x) \varphi\left(\lambda^{-1} |x_i - x|\right) \\ \geq & \frac{C^W_0}{C_\varphi \lambda^d} \sum_{x_i \in \chi^{irr}_{\mathcal{A},\beta,x}} \beta^2 \varphi\left(\lambda^{-1} |x_i - x|\right) \\ \geq & C^W_0 \beta^2 \rho^{irr}_{\mathcal{A},\beta} \quad . \end{aligned} \tag{2.2.17}$$

Because it holds $\rho_\lambda = \rho^{irr}_{\mathcal{A},\beta} + \rho^{reg}_{\mathcal{A},\beta}$, we obtain

$$\begin{aligned} \rho^{irr}_{\mathcal{A},\beta}(x) \leq & \frac{1}{C^W_0 \beta^2} J_\lambda\left(\mathcal{A}, \chi_{\mathcal{A}_R}, x\right) \quad , \\ \rho^{reg}_{\mathcal{A},\beta}(x) \geq & (\rho - \frac{1}{C^W_0 \beta^2} J_\lambda\left(\mathcal{A}, \chi_{\mathcal{A}_R}, x\right)) \quad . \end{aligned} \tag{2.2.18}$$

□

We want to prove that all A with pre-energy below our general upper bound are elements of a compact subset of $Gl_d(\mathbb{R})^d$. Due to the coercivity condition on $F(A$ we directly get that $\det A$ and $|A|$ are bounded from above. However $Gl_d(\mathbb{R})^d$ itself is not a compact subset of $\mathbb{R}^{d\times d}$. Therefore, we also need to find a lower bound for $|A|$ If the particle density is sufficiently small, we get this bound from the coercivity condition. If, in contrast, there is a particle density that is not vanishing, then an A with a small determinant can not offer enough low energy positions for all the atoms. In this way we get a lower bound for $\det A$ and we can derive from it bounds for $|A|$ and $|A^{-1}|$.

Lemma 2.2.6. *There exists $\hat{\lambda} \in \mathbb{R}$ and $c_1, c_2, c_3, c_4, c_5, c_6 > 0$ such that for all $\lambda > \hat{\lambda}$, for all positions x, and all configurations χ, and all $\mathcal{A} \in Gl_d\mathbb{R} \times \mathbb{R}^d$ with*

$$h(\mathcal{A}, \chi, x) \leq \vartheta \det E - \vartheta \rho_\lambda + \left\|E^{-1}\right\|^2 \left(\int_{[0,1]^d} W(\tau) d\tau \right) \rho_\lambda \tag{2.2.19}$$

it holds

$$\begin{aligned} c_1 \leq \det A \leq c_2 \quad , \\ c_3 \leq \|A^{-1}\| \leq c_4 \quad , \\ c_5 \leq \|A\| \leq c_6 \quad . \end{aligned} \tag{2.2.20}$$

Proof. **Step 1: Upper Bound for $\det A$ and $|A|$:** With the upper bound (2.2.19) on the pre-energy density and the coercivity condition on $F(A)$ we directly get

$$\begin{aligned} h_\lambda(\mathcal{A}, \chi, x) \leq & \vartheta \det E - \vartheta \rho_\lambda + \left\|E^{-1}\right\|^2 \left(\int_{[0,1]^d} W(\tau) d\tau \right) \rho_\lambda \\ \leq & J_\lambda(\mathcal{A}, \chi, x) + F(A) + \vartheta \det A \\ \leq & \vartheta \det E + \left\|E^{-1}\right\|^2 \left(\int_{[0,1]^d} W(\tau) d\tau \right) \rho_\lambda \,. \end{aligned} \tag{2.2.21}$$

We will use the abbreviation $X := \|E^{-1}\|^2 \int_{[0,1]^d} W(\tau) d\tau$ Because $J_\lambda \geq 0$ we get with the coercivity condition for $F(A)$ the estimates

$$\begin{aligned} C_1^{El} \left(\det(E) - \det(A)\right)^2 + \vartheta \det A + C_2^{El} \mathrm{dist}^2\left(A, ESO_d\right) \leq \vartheta \det E + X\rho_\lambda \quad , \\ C_1^{El} \left(\det(A) - \det(E) + \frac{\vartheta}{2C_1^{El}} \right)^2 + C_2^{El} \mathrm{dist}^2\left(A, ESO_d\right) \leq \frac{\vartheta^2}{4C_1^{El}} + X\rho_\lambda \quad . \end{aligned} \tag{2.2.22}$$

Hence, we get an upper bound for $\det(A)$.

$$\det(A) \leq \det(E) - \frac{\vartheta}{2C_1^{El}} + (C_1^{El})^{-\frac{1}{2}} \left(\frac{\vartheta^2}{4C_1^{El}} + X\rho_\lambda \right)^{\frac{1}{2}} \quad . \tag{2.2.23}$$

Since the density is bounded from above by ρ_d^{max} for any configuration with finite energy we have

$$\det(A) \leq \det(E) - \frac{\vartheta}{2C_1^{El}} + (C_1^{El})^{-\frac{1}{2}} \left(\frac{\vartheta^2}{4C_1^{El}} + X\rho_d^{max} \right)^{\frac{1}{2}} \quad . \tag{2.2.24}$$

Finally because of dist $(A, ESO_d) \geq ||E| - |A||$ we get the upper bound

$$|A| \leq |E| + (C_2^{El})^{-\frac{1}{2}} \left(\frac{\vartheta^2}{4C_1^{El}} + X\rho_d^{max} \right)^{\frac{1}{2}} \quad . \tag{2.2.25}$$

Step 2: Lower Bound in case of low density: It holds the compatibility condition (2)

$$\vartheta \leq C_1^{El} \det(E) \quad .$$

Hence, we have the estimate

$$\rho_\lambda \leq \frac{C_1^{El} \det(E)^2 - \vartheta \det E}{4 \|E^{-1}\|^2 X}. \tag{2.2.26}$$

For $\rho_\lambda \leq \hat{\rho}$ the estimates (2.2.22) leads to

$$\begin{aligned}
\det(A) &\geq \det(E) - \frac{\vartheta}{2C_1^{El}} - (C_1^{El})^{-\frac{1}{2}} \left(\frac{\vartheta^2}{4C_1^{El}} + X\rho_\lambda \right)^{\frac{1}{2}} \\
&\geq \det(E) - \frac{\vartheta}{2C_1^{El}} - (C_1^{El})^{-\frac{1}{2}} \left(\frac{\vartheta^2}{4C_1^{El}} + 1/4C_1^{El} \det(E)^2 - 1/4\vartheta \det E \right)^{\frac{1}{2}} \\
&\geq \det(E) - \frac{\vartheta}{2C_1^{El}} - \frac{1}{2} \left(\left(\det(E) - \frac{\vartheta}{2C_1^{El}} \right)^2 + 3/4 \frac{\vartheta^2}{4C_1^{El}} \right)^{\frac{1}{2}} \\
&\geq \frac{1}{2} \det(E) - \frac{1 + \sqrt(3)}{4} \frac{\vartheta}{C_1^{El}} > 0 \quad .
\end{aligned} \tag{2.2.27}$$

Because of $|A|^d \geq \det A$. This also implies a lower bound for $|A|$.

Step 3: Lower bound in case of higher density: We only need to search a lower bound for $\det A$ in case of a density

$$\rho_\lambda \geq \frac{C_1^{El} \det(E)^2 - \vartheta \det E}{4 \|E^{-1}\|^2 X} \quad . \tag{2.2.28}$$

We use $F(A) \geq 0$, $\det A > 0$ and the lower bound (2.2.21) for J_λ to get

$$\begin{aligned}
h_\lambda(\mathcal{A}, \chi, x) =& J_\lambda(\mathcal{A}, \chi, x) + F(A) + \vartheta \det A \\
\geq& \vartheta \det E + \left\|E^{-1}\right\|^2 \left(\int_{[0,1]^d} W(\tau) d\tau \right) \rho_\lambda
\end{aligned} \tag{2.2.29}$$

With Lemma 2.2.1 we get

$$\frac{C_0^W}{C_\varphi \lambda^d} \sum_i \mathrm{dist}^2(x_i, \chi_{\mathcal{A}}+x)\varphi\left(\lambda^{-1}\left|x_i - x\right|\right) \leq \vartheta \det E + \left\|E^{-1}\right\|^2 \left(\int_{[0,1]^d} W(\tau)d\tau\right)\rho_\lambda \tag{2.2.30}$$

We consider the set of regular points $\rho^{reg}_{\mathcal{A},\beta}(x)$ with β given by

$$\beta = \frac{1}{2}\left(C_0^W\right)^{-\frac{1}{2}}\left(\vartheta\frac{\det E}{\rho_\lambda} + \left\|E^{-1}\right\|^2 \int_{[0,1]^d} W(\tau)d\tau\right)^{\frac{1}{2}} \tag{2.2.31}$$

According to Lemma 2.2.5, the density of regular atoms satisfies

$$\rho^{reg}_{\mathcal{A},\beta}(x) \geq \frac{3}{4}\rho_\lambda\left(\chi\right) \quad . \tag{2.2.32}$$

On the other hand each atom in $\rho^{reg}_{\mathcal{A},\beta}$ is taking a volume of $w_d d\left(\frac{s_0}{2}\right)^d$. All this space has a maximal distance of $s_0/2 + \beta$ to a lattice point. On the other hand, there is only $w_d d\left(\beta + \frac{s_0}{2}\right)^d$ space near this point Therefore, the number of atoms nearby one lattice point can be maximal

$$N \leq \frac{w_d d\left(\beta + s_0/2\right)^d}{w_d d\left(\frac{s_0}{2}\right)^d} = \left(\frac{2\beta}{s_0} + 1\right)^d \quad . \tag{2.2.33}$$

Since β is not growing with λ and $\frac{d}{dx}\varphi(\frac{|x-x_i|}{\lambda})$ is scaling like $O(1/\lambda)$, all this atoms have the same weight as the lattice point up to $O(\beta/\lambda)$. Therefore, we get for large enough λ

$$\rho_\lambda(\chi_{\mathcal{A}}) \geq \rho_\lambda(\chi)/N \geq \left(\frac{2\beta}{s_0} + 1\right)^{-d}\rho_\lambda \quad . \tag{2.2.34}$$

Furthermore, we know from Lemma 2.1.2 that for any $B \in Gl_d(\mathbb{Z}^d)$ it holds

$$\rho_\lambda(\chi_{\mathcal{A}}) = \det A \pm C_m \frac{|A^{-1}|^m}{\lambda^m}\frac{\left(\lambda + |A^{-1}|\right)^d}{\lambda^d}\|\nabla^m\psi\|_\infty \det A \quad . \tag{2.2.35}$$

We note that in this equation the error term is the only term depending on the parametrization. This allows us to re-parametrize the lattice in the sense of Definition 1.3.1 to arrive at the estimate We can choose $B \in Gl_d(\mathbb{Z})$ to make the error minimal. We define

$$X := \min_{B\in Gl_d(\mathbb{Z})} \max_{j=1\ldots d} |A^{-1}B^{-1}e_j| \quad . \tag{2.2.36}$$

We have for the minimizing B

$$\|A^{-1}B^{-1}\|^2 = \sum_j e_j|A^{-1}B^{-1}e_j|^2 \geq dX^2 \quad . \tag{2.2.37}$$

Hence, it holds

$$|A^{-1}B^{-1}| \leq \|A^{-1}B^{-1}\| \leq \sqrt{d}X \quad . \tag{2.2.38}$$

We apply this on the estimate 2.2.35 and get:

$$\rho_\lambda(\chi_{\mathcal{A}}, x) = \det A \pm C_m \frac{\left(\sqrt{d}X\right)^m}{\lambda^m} \frac{\left(\lambda + \sqrt{d}X\right)^d}{\lambda^d} \|\nabla^m \psi\|_\infty \det A \quad . \tag{2.2.39}$$

We get from the inequality (2.2.34) and the equation (2.2.39) a lower bound for $\det A$ provided X/λ is small enough.

$$\det A \geq \rho_\lambda(\chi_{\mathcal{A}}, x) - O\left(\frac{X^m}{\lambda^m}\right)\left(\frac{2\beta}{s_0} + 1\right)^{-d} \rho_\lambda(\chi, x) - O\left(\frac{X^m}{\lambda^m}\right) \quad . \tag{2.2.40}$$

We still need to treat the case that $X\lambda^{-1}$ is not small. The d dimensional lattice is spanned by d vectors $A^{-1}B^{-1}e_j$ each have a length smaller equal X. And at least one $A^{-1}B^{-1}e_k$ has a length equal to X. The to other vectors are spanning a plain. If we project $A^{-1}B^{-1}e_k$ on this plain the distance p between the projected point and the next lattice position and the distance δ_p between $A^{-1}B^{-1}e_k$ and the plain fulfill

$$\delta_p^2 + p^2 = X^2 \quad . \tag{2.2.41}$$

Since it holds $p^2 \leq \frac{d+1}{4}X^2$, we get

$$\delta p \geq 1/2\,(5-d)^{1/2}\,X \quad . \tag{2.2.42}$$

At least in one direction the layers of the lattice have a distance larger than δp. There are maximal $(2\lambda\delta p^{-1})+1$ layers that intersect $B_{2\lambda}(x)$. In the neighborhood of these layers there is less than $w_d\lambda^{d-1}2\beta((2\lambda\delta p^{-1}+1)$ space for regular atoms. But we know that regular atoms have a density $\rho^{reg}_{\mathcal{A},\beta} \geq 3/4\rho_\lambda\left(\chi\right)$. Hence, they are filling, up to order λ^{-1}, a volume of at least $\frac{w_d}{d}(s_0/2)^d 3/4\rho_\lambda\left(\chi\right)C_\varphi\lambda^d$. We get

$$\begin{aligned} \frac{w_d}{d}\left(\frac{s_o}{2}\right)^d \frac{3}{4}\rho_\lambda\left(\chi\right)C_\varphi\lambda^d <& w_d\lambda^{d-1}2\beta\left(\left(2\lambda\delta p^{-1}\right)+1\right) \\ \delta p \leq& \frac{2\sqrt{d}\lambda}{\frac{3s_0^dC_\varphi\rho_\lambda(\chi)\lambda}{d2^{d+3}\beta} - 1} \quad . \end{aligned} \tag{2.2.43}$$

If we combine this with (2.2.42), we obtain

$$X \leq 2\,(5-d)^{-1/2}\,\frac{2\sqrt{d}\lambda}{\frac{3s_0^dC_\varphi\rho_\lambda(\chi)\lambda}{d2^{d+3}\beta} - 1} \quad . \tag{2.2.44}$$

Hence, we have an upper bound for X provided that

$$\rho_\lambda\left(\chi\right) \geq \frac{d2^{d+3}\beta}{3s_0^dC_\varphi\lambda} \quad . \tag{2.2.45}$$

Therefore, we have an lower bound for $\det A$ for sufficiently large ρ_λ. If λ is large enough one of the conditions (2.2.45) or (2.2.26) will be always fulfiled. So both bounds together gives a bound for any density. Furthermore, we know from Lemma B.2.2 that it holds

$$|A^{-1}| \leq |A|^{d-1} \det A^{-1} \leq c_4 \quad . \tag{2.2.46}$$

So with the lower bound for $\det A$ and the upper bound for $|A|$ we get also an upper bound for $|A^{-1}|$. We convert the upper bound of $|A^{-1}|$ in a lower bound for $|A|$

$$\begin{aligned} 1 =& |id| \leq |A^{-1}||A| \leq c_4(\rho)|A| \quad , \\ \frac{1}{c_4} \leq& |A| \quad . \end{aligned} \tag{2.2.47}$$

And the same way we get from the upper bound of $|A|$ a lower bound of $|A|^{-1}$. □

With the compactness of the set of $\mathcal{A}$ with low pre energy density we can finally proof that there exists an $\hat{\mathcal{A}}$ such that $\hat{h}_\lambda(\chi, x) = h_\lambda(\hat{\mathcal{A}}, \chi, x)$ Furthermore, we get upper an lower bounds on $\det \hat{A}$, $\left|\hat{A}^{-1}\right|$ and $|\hat{A}|$.

Lemma 2.2.7. *There exists$\hat{\lambda}$ and $c_1, c_2, c_3, c_4, c_5, c_6 > 0$ such that for all $\lambda > \hat{\lambda}$, positions x, and configurations χ there exists $\hat{A} \in Gl_d(\mathbb{R})$ and $\hat{\tau} \in \mathbb{Z}^d$ such that*

$$h\left(\hat{\mathcal{A}}, x, \chi\right) = \hat{h}\left(x, \chi\right) \quad . \tag{2.2.48}$$

Additionally the minimizer $\hat{A}$ satisfies

$$\begin{aligned} &c_1 \leq \det \hat{A} \leq c_2 \quad , \\ &c_3 \leq \|\hat{A}^{-1}\| \leq c_4 \quad , \\ &c_5 \leq \|\hat{A}\| \leq c_6 \quad . \end{aligned} \tag{2.2.49}$$

Proof. From Lemma 2.2.3 we know that there exists an $\tilde{A} \in Gl_d(\mathbb{R})$ and $\tilde{\tau} \in R^d$ such that

$$h\left(\tilde{A}, \tilde{\tau}x, \chi\right) \leq \vartheta \det E - \vartheta\rho_\lambda + \left\|E^{-1}\right\|^2 \left(\int_{[0,1]^d} W(\tau)d\tau\right)\rho_\lambda \quad . \tag{2.2.50}$$

So, we can conclude that

$$\inf_{A,\tau} h\left(A, \tau, x, \chi\right) \leq \vartheta \det E - \vartheta\rho_\lambda + \left\|E^{-1}\right\|^2 \left(\int_{[0,1]^d} W(\tau)d\tau\right)\rho_\lambda \quad . \tag{2.2.51}$$

If the equality holds in (2.2.51) then $(\tilde{A}\tilde{\tau})$ is the minimizer and satisfies the conditions according to Lemma 2.2.6 the conditions (2.2.49). If $\inf_{A,\tau} h\left(A, \tau x, \chi\right)$

is smaller it is still bounded from below by $-\vartheta\rho$, so there exists a minimizing sequence (A_n, τ_n). Therefore, for all n large enough it holds

$$h\left(A_n, \tau_n, x, \chi\right) \leq \vartheta \det E - \vartheta\rho_\lambda + \left\|E^{-1}\right\|^2 \left(\int_{[0,1]^d} W(\tau) d\tau\right) \rho_\lambda \quad . \tag{2.2.52}$$

Hence, for n large enough (A_n, τ_n) satisfies the conditions of Lemma (2.2.6). Therefore, A_n satisfies the bonds (2.2.49). τ_n can be selected to be confined in $[0,1]^d$ because of the periodicity of $h_\lambda(A, \tau, \chi, x)$- Therefore, (A_n, τ_n) is confined in a compact subset of $Gl_d(\mathbb{R}) \times \mathbb{R}^d$ and converges to some $(\hat{A}, \hat{\tau})$ also satisfying the bonds (2.2.49). The conclusion follows from the continuity of $h_\lambda(\mathcal{A}, \chi, x)$ in A and τ. □

Since we now know that there exists a $\hat{\mathcal{A}}$ minimizing $h_\lambda(\cdot, \chi, x)$ we use this to define the effective particle potential.

Definition 2.2.8. *Let $\mathcal{A}(\chi) : \Omega \to Gl_d(\mathbb{R}) \times \mathbb{R}^d$ be such that for all x holds $\hat{h}_\lambda(\chi, x) = \hat{h}_\lambda(\hat{\mathcal{A}}(x), \chi, x)$. We define the effective particle potential*

$$V_{\mathcal{A}(\chi)}(y) := \int_{B_{2\lambda}(\Omega)} \frac{\left\|\hat{A}^{-1}(x)\right\|^2}{C_\varphi \lambda^d} W(\hat{A}(x)\left(y - x\right) + \hat{\tau}(x)) \varphi\left(\lambda^{-1}\left|y - x\right|\right) \quad . \tag{2.2.53}$$

To motivate this definition reformulate the model using the definition If the hard core condition is fulfilled our model has the following form

$$H_\lambda(\chi) \int_{B_{2\lambda}(\Omega)} = \inf_{\mathcal{A}} \left(F\left(A\right) + J_\lambda\left(\mathcal{A}, \chi, x\right) + \vartheta_1 \det A - \left(\vartheta_1 + \vartheta_2\right)\rho_\lambda\right) dx \quad . \tag{2.2.54}$$

According to Lemma 2.2.7 the infimum is actually a minimum. We introduce (not necessary unique) $\hat{\mathcal{A}}(x)$ minimizing $F\left(A\right) + J_\lambda\left(x, \mathcal{A}, \chi\right) + \nu_\lambda\left(\chi, A, x\right)$ for the configuration χ in the point x. Next we look at our energy functional for given $\mathcal{A}(x)$ $F(A)$ and $\det A$ are immediately determined by $A(x)$. Changes of the atom positions will not influence $\int_{B_{2\lambda}(\Omega)} \left(\vartheta_1 + \vartheta_2\right)\rho_\lambda dx$ as shown in Lemma 2.1.1. We reformulate

$$\begin{aligned}
H_\lambda(\chi) = & \int_{B_{2\lambda}(\Omega)} F(A(x)) + \vartheta_1 \det A(x) + \left(\vartheta_1 + \vartheta_2\right)\rho_\lambda dx \\
& + \sum_i \int_{B_{2\lambda}(\Omega)} \frac{\left\|A^{-1}(x)\right\|^2}{C_\varphi \lambda^d} W(A(x)\left(x_i - x\right) + \tau(x)) \varphi\left(\lambda^{-1}\left|x_i - x\right|\right) \\
= & \int_{B_{2\lambda}(\Omega)} F(A(x)) + \vartheta_1 \det A(x) dx + N_I + \int_{B_{4\lambda}} \rho_\lambda(\chi_B, x) dx \\
& + \sum_{x_i \in \chi} V_{\mathcal{A}(\chi)}(x_i) \quad .
\end{aligned} \tag{2.2.55}$$

The effective can be used to estimate the energy difference between two configurations. The idea is that if we changing the configuration without changing the $\mathcal{A}$ the resulting energy will be higher than if we adapting the $\mathcal{A}$ to the new configuration.

Lemma 2.2.9. *For two configurations χ and $\tilde{\chi}$ it holds*

$$H_\lambda(\tilde{\chi}) \leq H_\lambda(\chi) + \sum_i V_{\mathcal{A}(\chi)}(\tilde{x}_i) - \sum_i V_{\mathcal{A}(\chi)}(x_i) \quad . \tag{2.2.56}$$

Proof. For all $\mathcal{A}_\chi(x) = \arg\min_{\mathcal{A}\in(Gl_d(\mathbb{R}),\mathbb{R}^d)} h_\lambda(A,\tau,\chi,x)dx$ it holds

$$\begin{aligned} H_\lambda(\tilde{\chi}) =& \int \min_{\tilde{A},\tilde{\tau}} h_\lambda(\tilde{A},\tilde{\tau},\tilde{\chi})dx \\ \leq& \int h_\lambda(\mathcal{A}_\chi(x),\tilde{x})dx \\ =& \int_{B_{2\lambda}(\Omega)} F(A(x)) + \vartheta_1 \det A(x)dx + N_I + \int_{B_{4\lambda}} \rho_\lambda(\chi_B,x)dx + \sum_i V_{\mathcal{A}}(\tilde{x}_i) \\ =& \int_{B_{2\lambda}(\Omega)} F(A(x)) + \vartheta_1 \det A(x)dx + N_I + \int_{B_{4\lambda}} \rho_\lambda(\chi_B,x)dx + \sum_i V_{\mathcal{A}}(x_i) \\ &+ \sum_i V_{\mathcal{A}(\chi)}(\tilde{x}_i) - \sum_i V_{\mathcal{A}(\chi)}(x_i) \\ =& H_\lambda(\chi) + \sum_i V_{\mathcal{A}(\chi)}(\tilde{x}_i) - \sum_i V_{\mathcal{A}(\chi)}(x_i) \quad . \end{aligned} \tag{2.2.57}$$

□

There are two possible applications for this. If the atoms of a configuration does do not sit in the local minima we can move them to the local minima. This will lead to a new configuration $\tilde{\chi}$ with lower energy and with a smaller number of defects. The second way is to calculate bounds for perturbations of configurations. If we have an idea of how $\mathcal{A}(x)$ of a configuration looks like we can get upper bound for the energy difference between this and other configurations with lemma 2.2.9.

2.3 Regular and irregular points

In this section we introduce the notation of regular points

Definition 2.3.1. *Let $\mathcal{A} = (A,\tau) \in Gl_d(\mathbb{R}) \times \mathbb{R}^d$ and $\epsilon_\rho, \epsilon_J, C_A \in \mathbb{R}$ and let χ be the configuration then we say that $x \in B_{2\lambda}(\Omega)$ is $(\epsilon_\rho, \epsilon_J, C_A)$-regular with $\mathcal{A}$, if the following conditions are fulfilled*

1. $\|A^{-1}\| < C_A$,

2. $|\rho_\lambda(\chi, x) - \det A| < \epsilon_\rho \det A$,

3. $J_\lambda(\mathcal{A}, \chi, x) < \epsilon_J \rho_\lambda(\chi, x)$,

4. $|x_i - x_j| > s_o$ *for all* i, j .

Remark 2.3.2. The definition above implies an upper for $|A|$ since

$$|A| \leq |A^{-1}|^{d-1} \det A \leq |A^{-1}|^{d-1} \frac{1}{1+\epsilon_\rho} \rho \leq \frac{C_A^{d-1}}{1-\epsilon_\rho} \rho_d^{max}. \tag{2.3.1}$$

For $\epsilon_\rho = 1/8$ we get

$$|A| \leq C_{|A|} := \frac{8 C_A^d}{7} \rho_d^{max} \quad . \tag{2.3.2}$$

If the point x is regular with $\mathcal{A}$ this means that the configuration looks like the lattice $\chi_\mathcal{A} + x$ in the $B_{2\lambda}(x)$. A reparametrisation of $\mathcal{A}$ creates the same lattice. Therefore, if x is a regular with $\mathcal{A}$, it is also regular with reparametrisations of $\mathcal{BA}$ (See Corollary 2.2.2). The main goal of this section is to proof for small enough ϵ_ρ and ϵ_J that, if x is $(\epsilon_\rho, \epsilon_J, C_A)$-regular with two $\mathcal{A}_1$ and $\mathcal{A}_2$, then $\mathcal{A}_2$ has to be a reparametrisation of $\mathcal{A}_1$ up to a small difference controlled by $\sqrt{J_\lambda}$. We will proof that in three steps. Lemma 2.3.3 has primary a technical purpose. It deals with a very specific case that the configuration is locally a subset of a Bravais lattice $\chi_{\mathcal{A}_R}$ and the mean square difference of these atoms to an other Bravais lattice $\chi_\mathcal{A}$ is small. Lemma 2.3.4 deals with the same case but improves the estimates. The final theorem 2.3.5 generalizes the result to general regular configurations. A similar result is obtained in Lemma 5.12 from [7]. However the estimate in [7] is not using all atoms in the 2λ-ball but just the ones in a smaller cube. Hence, it needs much higher density to be true. Furthermore, we will explicitly calculate the coefficient for the estimate of the difference between $\mathcal{A}_1$ and $\mathcal{A}_2$.

Lemma 2.3.3. *For all* $C_A > s_0$ *there exists* $\hat{\lambda} \in \mathbb{R}$ *and* $\hat{\epsilon}_J > 0$ *such that for all* $\lambda > \hat{\lambda}$, $\epsilon_J^* < \hat{\epsilon}_J$, $A, A_R \in Gl_d(\mathbb{R})$ *and* $\tau, \tau_R \in \mathbb{R}^d$ *satisfying*

1) $\|A^{-1}\| < C_A$ *and* $\|A_R^{-1}\| < C_A$,

2) $\chi \cap B_{2\lambda}(0) \subseteq \chi_{\mathcal{A}_R}$,

3) $\frac{1}{2} \det A < \frac{3}{4} \det A_R < \rho_\lambda(\chi, 0)$,

4) $|x_i - x_j| > s_o$ *for all* i, j,

5)

$$\epsilon_J^* \rho_\lambda(\chi, 0) > \frac{C_0^W}{C_\varphi \lambda^d} \sum_{x_i \in \chi} \operatorname{dist}^2(x_i, \chi_\mathcal{A}) \varphi\left(\lambda^{-1} |x_i|\right) \quad , \tag{2.3.3}$$

the following holds:

1) There exists a reparametrisation $B \in \mathrm{GL_d}(\mathbb{Z})$ and $t \in \mathbb{Z}^d$ such that

$$\|A_R^{-1}B^{-1} - A^{-1}\| \leq O\left(\frac{\sqrt{\epsilon_J^*}}{\lambda}\right) \quad , \tag{2.3.4}$$

$$|B\tau_R + t - \tau| \leq O(\sqrt{\epsilon_J^*}) \quad , \tag{2.3.5}$$

2) if additionally $x_j \in \chi_{\mathcal{A}_R}$ and $\tilde{x}_j \in \chi_{\mathcal{A}}$ such that

$$\mathrm{dist}(x_j, \chi_{\mathcal{A}}) = \mathrm{dist}(x_j, \tilde{x}_j) \quad , \tag{2.3.6}$$

then for all $z \in \mathbb{Z}^d$ with $x_i + A_R^{-1}B^{-1}z \in B_{2\lambda}(0)$ it holds

$$\mathrm{dist}(x_j + A_R^{-1}B^{-1}z, \chi) = \mathrm{dist}(x_j + A_R^{-1}B^{-1}z, x_j + A^{-1}z) \quad . \tag{2.3.7}$$

Proof. Due to remark 2.3.2 $\|A\|^{-1}$ can be bounded from below uniformly Because of equation (2.2.5) we get for $\beta = 2\sqrt{\frac{\epsilon_J^*}{C_0^W}} < 1/10\|A\|^{-1}$

$$\rho_{\mathcal{A},\beta,0}^{reg} \geq 3/4\rho_\lambda \geq 9/16 \det A_R \quad . \tag{2.3.8}$$

Hence, we know that at least at 9/16 of all points of $\chi_{\mathcal{A}_R}$ there is a regular atom. Now lets consider $A_R^{-1}e_j$. Because of $\|A^{-1}\| < C_A$ we know that up to order $O(\lambda^{-1})$, x_i and $x_i + A_R^{-1}e_j$ have the same contribution to ρ_λ. That means there have to exist $x_{i_j} \in \chi_{\mathcal{A},\beta,0}^{reg}$ and $x_{i_j} + A_R^{-1}e_j \in \chi_{\mathcal{A},\beta,0}^{reg}$. By contradiction argument, if there would not exist such a x_{i_j}, for each regular point there would be a irregular point. Hence, it would hold $\rho_{\mathcal{A},\beta,0}^{reg} < \frac{1}{2}\det A_R + O(\lambda^{-1})$, which contradicts $\rho_{\mathcal{A},\beta,x}^{reg} > 9/16 \det A_R$. Therefore, there exists x_{ij} such that both x_{ij} and $x_{ij} + A_R^{-1}e_j \in \chi_{\mathcal{A},\beta,0}^{reg}$ and there also have to exists $\tilde{x}_{ij}^1, \tilde{x}_{ij}^2 \in \chi_{\mathcal{A}}$ with $\left|x_{ij} - \tilde{x}_{ij}^1\right| < \beta$ and $\left|x_{ij} + A_R^{-1}e_j - \tilde{x}_{ij}^2\right| < \beta$. Hence, we get

$$\begin{aligned} \left|A^{-1}\tilde{e}_j - A_R^{-1}e_j\right| &= \left|(\tilde{x}_{ij}^2 - \tilde{x}_{ij}^1) - (x_{ij} + A_R^{-1}e_j - x_{ij})\right| \\ &= \left|(\tilde{x}_{ij}^2 - x_{ij} - A_R^{-1}e_j) - (\tilde{x}_{ij}^1 - x_{ij})\right| \\ &= \left|\tilde{x}_{ij}^2 - x_{ij} - A_R^{-1}e_j\right| + \left|\tilde{x}_{ij}^1 - x_{ij}\right| \\ &\leq 2\beta \quad . \end{aligned} \tag{2.3.9}$$

We get one $\tilde{e}_j$ for every dimension basis vector e_j. This vectors form a matrix B

with entries in $\mathbb{Z}$ such that $\tilde{e}_j = Be_j$. Furthermore, we obtain

$$\begin{aligned} \|A^{-1}B - A_R^{-1}\| \leq & \sum_{j=1}^{d} \left|(A^{-1}B - A_R^{-1})e_j\right| \\ = & \sum_{j=1}^{d} \left|A^{-1}\tilde{e}_j - A_R^{-1}e_j\right| \\ \leq & 2d\beta \leq 4d\sqrt{\frac{\epsilon_J^*}{C_0^W}} \quad . \end{aligned} \tag{2.3.10}$$

Now we look at a regular point $x_i \in \chi_{\mathcal{A}_R}$ and the corresponding $\tilde{x}_i \in \chi_{\mathcal{A}}$ with $\|x_i - \tilde{x}_i\| < \beta$ Let assign additionally $x_i + A_R^{-1}ne_j$ that is regular for a $n \in \mathbb{Z}$. There are two cases. In Case one $\tilde{x}_i + A^{-1}Bne_j$ is the closest point to $x_i + A_R^{-1}ne_j$ in $\chi_{\mathcal{A}}$. In case two an other point $\tilde{x}_i + A^{-1}Bne_j + A^{-1}\delta z \in \chi_{\mathcal{A}}$ is closer. In case one we estimate

$$\begin{aligned} \left|x_i + A_R^{-1}ne_j - \tilde{x}_i - A^{-1}Bne_j\right| < \beta \quad , \\ \|(A_R^{-1} - A^{-1}B)ne_j\| - \|x_i - \tilde{x}_i\| < \beta \quad , \\ n < 2\frac{\beta}{\left|(A_R^{-1} - A^{-1}B)e_j\right|} \quad . \end{aligned} \tag{2.3.11}$$

In the second case the closes point in χ_A is $\tilde{x}_i + A^{-1}Bne_j + A^{-1}\delta z$ and we get

$$\begin{aligned} \left|x_i + A_R^{-1}ne_j - \left(\tilde{x}_i + A^{-1}Bne_j + A^{-1}\delta z\right)\right| < \beta \quad , \\ \left|A^{-1}\delta z\right| - \left|(A_R^{-1} - A^{-1}B)ne_j\right| - |x_i - \tilde{x}_i| < \beta \quad , \\ \frac{\|A\|^{-1} - 2\beta}{\left|(A_R^{-1} - A^{-1}B)e_j\right|} < n \quad . \end{aligned} \tag{2.3.12}$$

This means that in a line next to a regular atoms there are maximal $Z_1 := 2\frac{\beta}{\left|(A_R^{-1} - A^{-1}B)e_j\right|}$ other regular atoms. And then there comes a minimum of $Z_2 := \frac{\|A\|^{-1} - 2\beta}{\left|(A_R^{-1} - A^{-1}B)e_j\right|}$ positions of χ_{A_R} before there can be regular atoms again in this line. Since $\beta < \frac{1}{10}\|A_R\|^{-1}$, we know

$$\frac{Z_1}{Z_2} = 2\frac{\beta}{\|A\|^{-1} - 2\beta} > \frac{1}{4} \quad . \tag{2.3.13}$$

Therefore, there are at least 4-times more irregular than regular atoms. Hence, the regular atoms need to have in average a higher weight φ than the irregular atoms. The highest weight can be found in the middle of every line (see Figure 2.3). We define $\rho_{k,j,1}$ as the contribution to the density atoms from the finite series closest to the middle of the line k and $\rho_{k,j,2}$ as the contribution to the density of

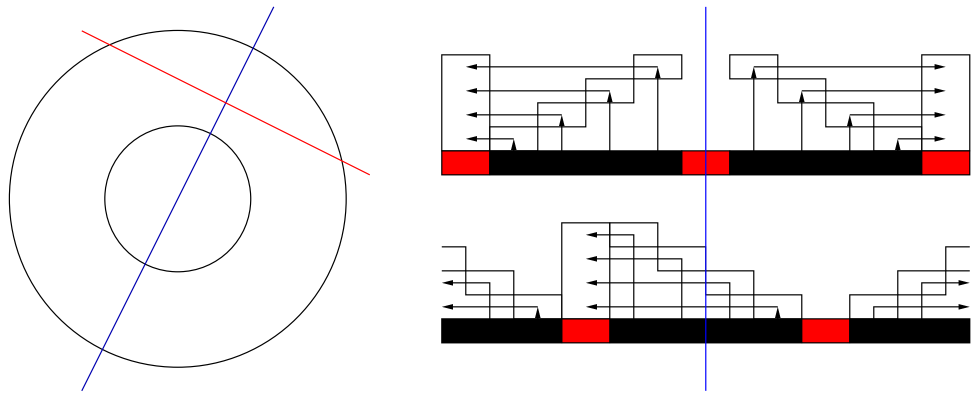

Figure 2.1: The left picture shows a line of atoms(red) going through the 2λ-Ball around x The point where the red line intersects with the blue line is the middle of the line of atoms. The right picture shows how to compare the irregular positions(black) with the regular positions (red) to see that except of one central sequence the weight of the irregular parts are four times higher.

all other series of regular positions in the line k. For every finite series of regular position but the closest to the middle there exists at least 4 times as many irregular atoms that has at least the same weight since φ is monotone decreasing(see Figure 2.3). For the contribution to the density of irregular position in $\chi_{\mathcal{A}_R}$ in the line k, we get $\rho^{irr}_{k,j} > 4\rho_{k,j,2}$. The density of irregular atoms consists of the contributions of every line and is at least four times bigger than the contribution of regular atoms from the outer series.

$$\rho^{irr}_{\mathcal{A},\beta}(0) = \sum_k \rho^{irr}_{k,j} \geq 4 \sum_k \rho_{kj2} = 4 \sum_k \rho_{k,j,2} \quad . \tag{2.3.14}$$

On the other hand the density of regular points and of irregular positions together are given asymptotically by $\det A_R$ to $O(\lambda^{-k})$. Hence, we have

$$7/16 \det A_R + O(\lambda^{-2}) > \rho^{irr}_{\mathcal{A},\beta}(x) > 4 \sum_k \rho_{k,j,2} \quad . \tag{2.3.15}$$

Furthermore, we have $9/16 \det A_R$ density of the regular points. These consists of the regular points from the inner series plus the contribution from the outer series.

$$\sum_k \rho_{k,j,1} + \sum_k \rho_{k,j,2} = \rho^{reg}_{\mathcal{A},\beta}(x) > 9/16 \det A_R \quad . \tag{2.3.16}$$

Putting the estimates (2.3.15) and (2.3.16) together, we get

$$\sum_k \rho_{kj1} > \frac{29}{64} \det A_R \quad . \tag{2.3.17}$$

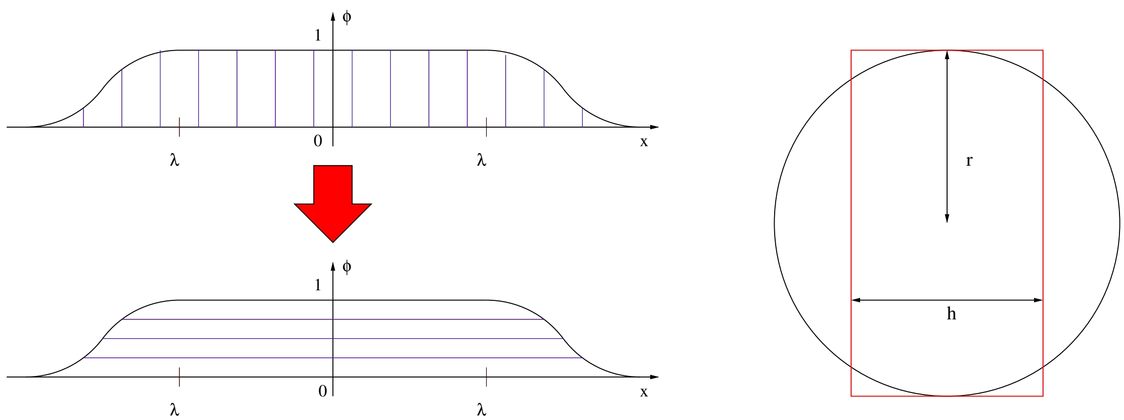

Figure 2.2: The left picture shows the change in equation (2.3.18) from vertical slights to horizontal slights using with Fubinis theorem. The right picture show how we cover the parts of a circle with radius r, that have a distance from the middle line less than h, with a rectangle. For dimension three we have to cover a sphere instead of the circle an cover it with a cylinder instead of rectangle

Hence,the contribution to the density of the regular atoms in the series closest to the middle of each line is at least $\frac{29}{64}\det A_R$. On the other hand we know that those series consists at most of Z_1 atoms, which implies a length of at most $h = Z_1 \left|A_R^{-1} e_j\right|$. Since the inner regular series cover 29/64 of the total density, we can calculate a lower bound for h. The maximum contribution, that one can reach with a given h, is obtained, if the series is centered in the middle. We notice that we can rewrite(see Figure 2.3)

$$\int \varphi(x/\lambda)dx = \int_0^1 \left|B_{(\lambda\varphi^{-1}(y))}(0)\right| dy \quad . \tag{2.3.18}$$

All spheres $B_{(\varphi^{-1}(y))}(0)$ have a radius of at least λ. Hence, it is sufficient to study how much of a sphere with radius $r > \lambda$ can be filled for a given h.

Case 2D: The filled part of the circle can be estimated from above by a rectangle with one side $2r$ and the other h. The circle itself has an area πr^2. If the rectangle is supposed to be bigger than 29/64 of the circle we need

$$\begin{aligned} \frac{2rh}{\pi r^2} &> \frac{29}{64} \quad , \\ h &> \frac{29\pi}{128} r > 0.7\lambda \quad . \end{aligned} \tag{2.3.19}$$

Case 3D: The filled part of the sphere can be estimated from above by an cylinder with radius r and the height h. The sphere itself has an volume $4/3\pi r^3$.

If the cylinder is supposed to be bigger than 29/64 parts of the sphere we need

$$\begin{aligned} \frac{\pi r^2 h}{4/3\pi r^3} > & \frac{29}{64} \quad , \\ h > & \frac{29}{48} r > 0.6\lambda \quad . \end{aligned} \tag{2.3.20}$$

We get for both cases $2D$ and $3D$ that

$$\begin{aligned} h > & 0.6\lambda \quad , \\ Z_1 > & 0.6\|A_r^{-1}e_j\|^{-1}\lambda \quad , \\ \|(A_R^{-1} - A^{-1}B)e_j\| < & \frac{10\|A_R^{-1}\|\beta}{3\lambda} \quad , \\ \|(A_R^{-1} - A^{-1}B)\| < & \frac{10\sqrt{d}\|A_R^{-1}\|}{3}\frac{\beta}{\lambda} \quad . \end{aligned} \tag{2.3.21}$$

Therefore, as B has entries in $\mathbb{Z}$, the determinant of B is an integer. Since we know $|A_R^{-1} - A^{-1}B\| \leq O(\beta/\lambda)$, $\det B$ can not be zero. Due to $3/2 \det A_R > \det A$, $\det B$ can not be bigger than 1. So, $\det B = 1$ and $B \in Gl_d\mathbb{Z}$.

$$\begin{aligned} \|A_R{}^{-1}B^{-1} - A^{-1}\| \leq & \frac{10\sqrt{d}\|A_R^{-1}\|\|B\|}{3}\frac{\beta}{\lambda} \quad , \\ \|A_R{}^{-1}B^{-1} - A^{-1}\| \leq & O\left(\frac{\sqrt{\epsilon_J^*}}{\lambda}\right) \quad . \end{aligned} \tag{2.3.22}$$

Further more we know that there exist a regular point with $\|x_i - \tilde{x}_i\| < \beta$ and we have

$$\begin{aligned} \left|x_i - A^{-1}(z_j - \tau)\right| \leq & O(\sqrt{\epsilon_J^*}) \quad , \\ |Ax_i - (z_j - \tau)| \quad , \leq & O(\sqrt{\epsilon_J^*}) \\ |BA_R x_i - (z_j - \tau| - \left|(B^{-1}A_R - A)x_i\right| \quad , & \\ |BA_R x_i - (z_j - \tau)| \leq & O(\sqrt{\epsilon_J^*}) \quad , \\ \left|BA_R A_R^{-1}(z_i - \tau_R) + \tau - z_j\right| \leq & O(\sqrt{\epsilon_J^*}) \quad , \\ |\tau - B\tau_R + (z_j - Bz_i)| \leq & O(\sqrt{\epsilon_J^*}) \quad , \\ |\tau - B\tau_R + (z_j - Bz_i)| \leq & O(\sqrt{\epsilon_J^*}) \quad . \end{aligned} \tag{2.3.23}$$

Finally we assume that $x_i \in \chi \cap B_{2\lambda}(0)$ is regular. And that $\tilde{x}_i$ is the clossest point to it in χ. Now we consider $z_k \in \mathbb{Z}^d$ satisfying $x_i + A_R^{-1}B^{-1}z_k \in B_{2\lambda}(0)$. We calculate

$$\begin{aligned} \left|(x_i + A_R^{-1}B^{-1}z_k) - (\tilde{x}_i + A^{-1}z_k)\right| = & |x_i - \tilde{x}_i| + \left|(A_R^{-1}B^{-1} - A^{-1})z_k)\right| \\ = & \beta + \left|A_R^{-1}B^{-1} - A_R^{-1}\right| |z_k| \quad . \end{aligned} \tag{2.3.24}$$

Because of $x_i \in B_{2\lambda}(x)$ and $x_i + A_R^{-1}B^{-1}z_k \in B_{2\lambda}(x)$. z_k is maximal of order λ. It holds

$$\left|(x_i + A_R^{-1}B^{-1}z_k) - (\tilde{x}_i + A^{-1}z_k)\right| = O(\epsilon_J^*) \quad . \tag{2.3.25}$$

Hence, for sufficiently small ϵ_J^* it holds

$$\left|(x_i + A_R^{-1}B^{-1}z_k) - (\tilde{x}_i + A^{-1}z_k)\right| \leq \frac{1}{2\,|A|} \quad . \tag{2.3.26}$$

Hence, $(\tilde{x}_i + A^{-1}z_k)$ is the element in $\chi_{\mathcal{A}}$ that is closest to $(x_i + A_R^{-1}B^{-1}z_k)$. □

The next lemma improves the estimate (2.3.4) for the difference of the lattice parameters in Lemma 2.3.3. According to Lemma 2.3.3 there is a reparametrisation of $\mathcal{A}_R$ close enough too $\mathcal{A}$, such that, if $x_i \in \chi_{\mathcal{A}_R}$ is the nearest neighbor to $y_i \in \chi_{\mathcal{A}}$, then $x_i + A_R^{-1}z$ is the nearest neighbor to $x_i + A^{-1}B^{-1}z$. Therefore, we just need to distribute atoms on positions that contributes to J_λ in a quadratic potential. If we fill up the positions with the lowest contribution, we get a lower bound for J_λ, that can be transformed to an upper bound for the difference between $\mathcal{A}_R$ and $\mathcal{B}\mathcal{A}$.

Lemma 2.3.4. *For all $C_A > s_0$ there exists $\hat{\lambda} \in \mathbb{R}$ and $\hat{\epsilon}_J > 0$ such that for all $\lambda > \hat{\lambda}$, $\epsilon_J^* < \hat{\epsilon}_J$, $A, A_R \in Gl_d(\mathbb{R})$ and $\tau, \tau_R \in \mathbb{R}^d$ satisfying*

1) $\|A^{-1}\| < C_A$ *and* $\|A_R^{-1}\| < C_A$,

2) $\chi \cap B_{2\lambda}(0) \subseteq \chi_{\mathcal{A}_R}$,

3) $\frac{1}{2}\det A < \frac{3}{4}\det A_R < \rho_\lambda(\chi, 0)$,

4) $|x_i - x_j| > s_o$ *for all* i, j ,

5)

$$\epsilon_J^* \rho_\lambda(\chi, 0) > \frac{C_0^W}{C_\varphi \lambda^d} \sum_{x_i \in \chi} \operatorname{dist}^2(x_i, \chi_{\mathcal{A}}) \varphi\left(\lambda^{-1}|x_i|\right) \quad , \tag{2.3.27}$$

the following holds: There exists an reparametrisation $B \in \mathrm{GL_d}(\mathbb{Z})$ and $t \in \mathbb{Z}^d$ such that

$$\begin{aligned} \|1 - A^{-1}BA_R\| &< \left(\frac{C_0^W C_{\varphi 2}}{dC_\varphi}\det A_R - 8C_0^W(\det A_R - \rho_\lambda)\right)^{-\frac{1}{2}} \frac{\sqrt{\epsilon_J^* \rho_\lambda}}{\lambda} \quad , \\ \|B\tau_R - \tau + t\| &< \|A\| \left(C_0^W(2\rho_\lambda - \det A_R)\right)^{-\frac{1}{2}} \sqrt{\epsilon_J^* \rho_\lambda} \quad . \end{aligned} \tag{2.3.28}$$

Proof. We use the abbreviations

$$\begin{aligned} X :=& \frac{C_0^W}{C_\varphi \lambda^d} \sum_{x_i \in \chi_{A_R}} \mathrm{dist}^2(x_i, \chi_{\mathcal{A}}) \varphi\left(\lambda^{-1}|x_i|\right) \quad , \\ Y :=& \sup_{x_i \in \chi_{\mathcal{A}_R} \cap B_{2\lambda}(0)} \mathrm{dist}^2(x_i, \chi_{\mathcal{A}}) \end{aligned} \tag{2.3.29}$$

and estimate

$$\begin{aligned} \epsilon_J^* \rho_\lambda >& \frac{C_0^W}{C_\varphi \lambda^d} \sum_{x_i \in \chi} \mathrm{dist}^2(x_i, \chi_{\mathcal{A}}) \varphi\left(\lambda^{-1}|x_i|\right) \\ =& X - \frac{C_0^W}{C_\varphi \lambda^d} \sum_{x_i \in \chi_{A_R}/\chi} \mathrm{dist}^2(x_i, \chi_{\mathcal{A}}) \varphi\left(\lambda^{-1}|x_i|\right) \\ =& X - \frac{C_0^W}{C_\varphi \lambda^d} \sum_{x_i \in \chi_{A_R}/\chi} \varphi\left(\lambda^{-1}|x_i|\right) \sup_{x_i \in \chi_{\mathcal{A}_R} \cap B_{2\lambda}(0)} \mathrm{dist}^2(x_i, \chi_{\mathcal{A}}) \\ =& X - (\det A_R - \rho_\lambda) \sup_{x_i \in \chi_{\mathcal{A}_R} \cap B_{2\lambda}(0)} \mathrm{dist}^2(x_i, \chi_{\mathcal{A}}) \\ =& X - (\det A_R - \rho_\lambda) y \quad . \end{aligned} \tag{2.3.30}$$

Next, we calculate $\mathrm{dist}^2(x_i, \chi_{\mathcal{A}})$. According to Lemma 2.3.3 for sufficiently high λ and low ϵ_J^* there exists an reparametrisation $\mathcal{B} = (B, t) \in \mathrm{GL_d}(\mathbb{Z}) \times \in \mathbb{Z}^{\mathrm{d}}$ such that the closest point to $x_i = A_R^{-1} B^{-1}(z_i - B\tau_R - t)$ in $\chi_{\mathcal{A}}$ will be $A^{-1}(z_i - \tau)$. Hence, we get

$$\begin{aligned} \mathrm{dist}^2(x_i, \chi_{\mathcal{A}}) =& (x_i - A^{-1}(z_i - \tau))^2 \\ =& (x_i - A^{-1}(BA_R x_i + B\tau_R + t - \tau))^2 \\ =& (1 - A^{-1}BA_R)x_i + A^{-1}(B\tau_R + t - \tau)))^2 \quad . \end{aligned} \tag{2.3.31}$$

We set

$$\begin{aligned} \delta_A =& 1 - A^{-1}BA_R \quad , \\ \delta_\tau =& A^{-1}(B\tau_R + t - \tau) \quad , \end{aligned} \tag{2.3.32}$$

and obtain

$$\begin{aligned} Y =& \sup_{x_i \in \chi_{\mathcal{A}_R} \cap B_{2\lambda}(0)} (\delta_A x_i + \delta_\tau)^2 \\ <& (\|\delta_A\| 2\lambda + |\delta_\tau|)^2 \\ <& 8\lambda^2 (\|\delta_A\|)^2 + 2|\delta_\tau|^2 \quad . \end{aligned} \tag{2.3.33}$$

Using (2.3.31) we get

$$X = \frac{C_0^W}{C_\varphi \lambda^d} \sum_{x_i \in \chi_{A_R}} (\delta_A x_i + \delta_\tau)^2 \varphi\left(\lambda^{-1}|x_i|\right) \quad . \tag{2.3.34}$$

Next, we estimate the sum in equation 2.3.34 by an integral using Lemma 2.1.2 with $m = 2$ and get

$$X > \frac{C_0^W}{C_\varphi \lambda^d} \sum_{x_i \in \chi \mathcal{A}_R} (\delta_A \tilde{y} + \delta_\tau)^2 \varphi\left(\lambda^{-1} |\tilde{y}|\right) \det A_R d\tilde{y} + O\left(\frac{\|\delta_\mathcal{A}\|_\lambda^2}{\lambda^2}\right) \quad . \tag{2.3.35}$$

We substitute $y = \frac{\tilde{y}}{\lambda}$ and obtain

$$X > \frac{C_0^W}{C_\varphi} \sum_{x_i \in \chi \mathcal{A}_R} (\delta_A \lambda y + \delta_\tau)^2 \varphi\left(|y|\right) \det A_R dy + O\left(\frac{\|\delta_\mathcal{A}\|_\lambda^2}{\lambda^2}\right) \quad . \tag{2.3.36}$$

The integral of an odd function over an even area is zero. So the mixed term vanishes

$$X > \frac{C_0^W}{C_\varphi \lambda^d} \int \left((\delta_A y)^2 + (\delta_\tau)^2\right) \varphi\left(\lambda^{-1} |y|\right) dz + O\left(\frac{\|\delta_\mathcal{A}\|_\lambda^2}{\lambda^2}\right) \quad . \tag{2.3.37}$$

The symmetric matrix $\delta_A^+ \delta_A$ has d eigenvalues $a_1..a_d$ In the eigensystem of $(\delta_A^+ \delta_A)$ we get

$$\begin{aligned}
\int (\delta_A y)^2 \varphi\left(\lambda^{-1} |y|\right) &= \int \sum_{k=1}^{d} a_k y_k^2 \varphi\left(\lambda^{-1} |y|\right) dz \\
&= \sum_{k=1}^{d} a_k \int y_k^2 \varphi\left(\lambda^{-1} |y|\right) dz \\
&= Tr(\delta_A^+ \delta_A) \frac{1}{d} \lambda^d \int \lambda^2 y^2 \varphi\left(|y|\right) dz \\
&= \frac{C_{\varphi 2}}{d} \lambda^{d+2} \|\delta_A\|^2 \quad .
\end{aligned} \tag{2.3.38}$$

We obtain

$$X > \left(\frac{C_{\varphi 2} C_0^W}{d C_\varphi} \lambda^2 \|\delta_A\|^2 + \|\delta_\tau\|^2\right) \det A_R + O\left(\frac{\|\delta_\mathcal{A}\|_\lambda^2}{\lambda^2}\right) \quad . \tag{2.3.39}$$

We apply our estimates for X and Y to (2.3.30), and get

$$\begin{aligned}
\epsilon_J^* \rho_\lambda > & \left(\frac{C_0^W C_{\varphi 2}}{d C_\varphi} \lambda^2 \|\delta_A\|^2 + C_0^W \|\delta_\tau\|^2\right) \det A_R \\
& - C_0^W (\det A_R - \rho_\lambda)(8\lambda^2 (\|\delta_A\|)^2 + 2\|\delta_\tau\|^2) \quad .
\end{aligned} \tag{2.3.40}$$

We resubstitute δ_A, and δ_τ with equation 2.3.32 and obtain

$$\begin{aligned}
\|1 - A^{-1} B A_R\|^2 &< \left(\frac{C_0^W C_{\varphi 2}}{d C_\varphi} det A_R - 8 C_0^W (\det A_R - \rho_\lambda)\right)^{-1} \frac{\epsilon_J^* \rho_\lambda}{\lambda^2}, \\
\|1 - A^{-1} B A_R^{-1}\| &< \left(\frac{C_0^W C_{\varphi 2}}{d C_\varphi} \det A_R - 8 C_0^W (\det A_R - \rho_\lambda)\right)^{-\frac{1}{2}} \frac{\sqrt{\epsilon_J^* \rho_\lambda}}{\lambda}.
\end{aligned} \tag{2.3.41}$$

Hence, we get

$$\begin{aligned}\|A^{-1}(B\tau_R + t - \tau)\|^2 <& \left(C_0^W(2\rho_\lambda - \det A_R)\right)^{-1} \epsilon_J^* \rho_\lambda \quad , \\ \|(B\tau_R + t - \tau)\| <& \|A_1\| \left(C_0^W(2\rho_\lambda - \det A_R)\right)^{\frac{1}{2}} \sqrt{\epsilon_J^* \rho_\lambda} \quad . \end{aligned} \tag{2.3.42}$$

□

In Theorem 2.3.5 we apply the specfic Lemma 2.3.4 to get a more general result. If the configuration χ in one point is regular with two different lattice parameters $\mathcal{A}_1$ and $\mathcal{A}_2$, there exists a number of atoms regular with both lattices. If we take the lattice points of one of theses lattices, that are close to theses points, then we get a set fulfilling the conditions of Lemma 2.3.4. Hence, we get the the same estimate as we did in the specific case.

Theorem 2.3.5. *For all $C_A > s_0$ exists $\hat{\lambda} \in \mathbb{R}$ and ϵ_J such that for all $\lambda > \hat{\lambda}$, $\mathcal{A}_1 = (A_1, \tau_1), \mathcal{A}_1 = (A_1, \tau_1) \in Gl_d(\mathbb{Z}^d) \times \mathbb{Z}^d$ and $x \in B_{2\lambda}(\Omega)$, that are $(1/28, \epsilon_J, C_A)$-regular with $\mathcal{A}_1$ and with $\mathcal{A}_2$, we have*

$$\begin{aligned}\|id - A_1^{-1}BA_2\| <& \left(\frac{C_0^W C_{\varphi 2}}{8dC_\varphi} \det A_2\right)^{-\frac{1}{2}} \frac{\sqrt{J_{max}}}{\lambda} \quad , \\ \|B(\tau_1 + t) - \tau_2\| <& \|A_1\| \left(\frac{1}{10} C_0^W \det A_2\right)^{-\frac{1}{2}} \sqrt{J_{max}} \quad , \end{aligned} \tag{2.3.43}$$

where

$$J_{max} = \max J_\lambda(\mathcal{A}_1, \chi, x), J_\lambda(\mathcal{A}_2, \chi, x) \quad . \tag{2.3.44}$$

Proof. We have $\|A_2^{-1}\|, \|A_2^{-1}\| < C_A$. Using equation (2.2.5) and $\beta = 4\sqrt{\frac{\epsilon_J^*}{C_0^W}} < \min\left\{s_o/2, \frac{1-\epsilon_\rho}{2C_A^{d-1}} \left(\rho_d^{max}\right)^{-1}\right\}$ we get the estimate $\rho_{\mathcal{A}_j,\beta,x}^{reg} \geq 15/16\rho_\lambda$. Hence, we have that at least a density of $7/8\rho_\lambda$ atoms, that are regular for $\mathcal{A}_1$ and $\mathcal{A}_2$. We call the set of this atoms χ_{reg}. Because of $\beta < s_0/2$, two different regular atoms can not belong to the same lattice point. Furthermore, if $\beta \leq \frac{1-\epsilon_\rho}{2C_A^{d-1}} \left(\rho_d^{max}\right)^{-1} \leq \frac{1}{2}\|A_j\|^{-1}$ a lattice point can not belong to two different atoms. Therefore, there is a bijection between the atoms of χ_{reg} and the corresponding points in the lattices $\chi_{\mathcal{A}_i}$. For every $x_i \in \chi_{reg}$ we denote by x_{ij} the corresponding element in $\chi_{\mathcal{A}_j}$. We denote by $\chi_{\mathcal{A}_j}^{reg}$ the set of these regular lattice points. We get

$$\begin{aligned}2J_{max} >& \frac{C_0^W}{C_\varphi \lambda^d} \sum_{x_i \in \chi_{reg}} (\mathrm{dist}^2(x_i, \chi_{\mathcal{A}_1} + x) + \mathrm{dist}^2(x_i, \chi_{\mathcal{A}_1} + x))\varphi\left(\lambda^{-1}|x_i - x|\right) \\ =& \frac{C_0^W}{C_\varphi \lambda^d} \sum_{x_i \in \chi_{reg}} ((x_i - x_{i1} - x)^2 + (x_i - x_{i2} - x)^2)\varphi\left(\lambda^{-1}|x_i - x|\right) \quad . \end{aligned} \tag{2.3.45}$$

Using $a^2+b^2=\frac{1}{2}(a-b)^2+\frac{1}{2}(a+b)^2$ one gets

$$\begin{aligned}4J_{max} >&\frac{C_0^W}{C_\varphi\lambda^d}\sum_{x_i\in\chi_{reg}}((x_{i1}-x_{i2})^2+(2x_i-x_{i1}-x_{i2}-2x)^2)\varphi\left(\lambda^{-1}\left|x_i-x\right|\right)\\ >&\frac{C_0^W}{C_\varphi\lambda^d}\sum_{x_i\in\chi_{reg}}(x_{i1}-x_{i2})^2\varphi\left(\lambda^{-1}\left|x_i-x\right|\right) \quad .\end{aligned} \tag{2.3.46}$$

We can count the x_{i2} instead of the x_i due to the one to one correspondence between them and change the argument of φ from $(\lambda^{-1}|x_i-x|)$ to $(\lambda^{-1}|x_{i2}|)$ paying with an error term as follows:

$$\begin{aligned}4J_{max} >&\frac{C_0^W}{C_\varphi\lambda^d}\sum_{x_{i1}\in\chi^{reg}_{\mathcal{A}_2}} dist(x_{i2},\chi_{\mathcal{A}_1})^2\varphi\left(\lambda^{-1}\left|x_{i2}\right|\right)\\ &+\frac{C_0^W}{C_\varphi\lambda^d}\sum_{x_{i2}\in\chi^{reg}_{\mathcal{A}_2}} dist^2(x_{i2},\chi_{\mathcal{A}_1})\left(\varphi\left(\lambda^{-1}\left|x_{i2}\right|\right)-\varphi\left(\lambda^{-1}\left|x_i-x\right|\right)\right).\end{aligned} \tag{2.3.47}$$

Next, we estimate the error term. We use $\mathrm{dist}(x_{i1},\chi_{\mathcal{A}_2})^2<4\beta^2$.

$$\begin{aligned}&\frac{C_0^W}{C_\varphi\lambda^d}\sum_{x_{i2}\in\chi^{reg}_{\mathcal{A}_2}}4\beta^2\left(\varphi\left(\lambda^{-1}\left|x_{i2}\right|\right)-\varphi\left(\lambda^{-1}\left|x_i-x\right|\right)\right)\\ <&4\beta^2\frac{C_0^W}{C_\varphi\lambda^d}\sum_{x_{i2}\in\chi^{reg}_{\mathcal{A}_2}}\frac{\|\nabla\varphi\|}{\lambda}\left|x_{i2}+x-x_i\right|\\ <&4\frac{C_0^W w_d d}{C_\varphi}\frac{\|\nabla\varphi\|}{\lambda}\det A_2\beta^3\\ <&\left(256\frac{w_d d}{C_\varphi}\frac{\|\nabla\varphi\|}{\lambda}\det A_1 2\left(\frac{\epsilon_J^*}{C_0^W}\right)^{\frac{1}{2}}\right)\epsilon_J.\end{aligned} \tag{2.3.48}$$

The error will be negligible for small enough ϵ_J. The density of $\chi^{reg}_{\mathcal{A}_1}$ fulfills $\rho_\lambda(\chi^{reg}_{\mathcal{A}_1},x)\leq 7/9\rho_\lambda(\chi,x)+O(\lambda^{-1})>3/4\det A_1$. Hence $\chi^{reg}_{\mathcal{A}_1}$ fulfills with the fitted $\mathcal{A}_2$ the conditions for Lemma 2.3.4 with density $7/9\rho_\lambda$ and $\epsilon_J^*\rho_\lambda=5J_{max}$, $A_R=A_2$, $\tau_R=\tau_2$, $A=A_1$ and $\tau=\tau_1$. Therefore, there exists $\mathcal{B}=(B,\tau)\in Gl_d(\mathbb{Z}^d)\times\mathbb{Z}^d$ satisfying

$$\begin{aligned}\|Id-A_1^{-1}BA_2\|<&\left(\frac{C_0^W C_{\varphi 2}}{4dC_\varphi}\det A_2-2C_0^W(\det A_2-7/9\rho_\lambda)\right)^{-\frac{1}{2}}\frac{\sqrt{J_{max}}}{\lambda} \quad ,\\ \|B(\tau_1+t)-\tau_2\|<&\|A_1\|\left(\frac{1}{5}C_0^W(7/4\rho_\lambda-\det A_2)\right)^{-\frac{1}{2}}\sqrt{J_{max}} \quad .\end{aligned} \tag{2.3.49}$$

For $\epsilon_\rho<1/28$ we have $(\det A_2-7/9\rho_\lambda)<\frac{C_{\varphi 2}}{16dC_\varphi}\det A_2$ and $\det A_2<5/4\rho_\lambda$ and we get 2.3.43. □

2.4 Regularity of low energy states

In Section 2.3 we proved some properties of regular points. Even more properties of regular points will be studied in Chapter 4. In this section we prove that points with low energy density are regular, and that we can control the coefficient ϵ_J and ϵ_ρ with the energy density. The main difficulty here is, that in the definition of the pre-energy density the particle density enters with a negative sign. Therefore, we first calculate an lower bound for J_λ depending on the matrix A and the particle density ρ_λ. If we combine this estimate with the coercivity condition on $F(A)$ we get a lower bound for $h_\lambda(\mathcal{A}, \chi x)$. Once we have this lower bound the regularity follows, since we constructed the model to penalize configurations that are not close to a lattice.

First we calculate a lower bound for J_λ depending on $\det A$ and ρ_λ in the case that there are no irregular atoms in the configuration.

Lemma 2.4.1. *For all $C_A > 0$ there exists $\hat{\lambda} \in \mathbb{R}$ such that for all $\lambda > \hat{\lambda}$, $\mathcal{A} = (A, \tau) \in Gl_d(\mathbb{R}) \times \mathbb{R}^d$ such that $|A^{-1}| < C_A$ and configurations χ satisfying $\rho_\lambda(\chi)(\chi, x) > \det A$ and $\chi = \chi^{reg}_{\mathcal{A},\beta,x}$ where $\beta = \min\{s_o/2, |A|\}$ it holds*

$$J_\lambda(\mathcal{A}, \chi, x) \geq \left(C^W_\phi + O(\lambda^{-1})\right) \det A^{-1} \lambda^2 \left(\rho_\lambda - \det A + O(\lambda^{-m})\right)^2 \quad , \tag{2.4.1}$$

where

$$C^W_\phi := \left(\frac{1}{C^W_0 C_\varphi} \int_{\mathbb{R}^d} \frac{\varphi'^2}{\varphi}(|y|)\, dy\right)^{-1} \quad . \tag{2.4.2}$$

Proof. Without lose of generality we can restrict ourself to $x = 0$. As proven in Lemma 2.1.2 the density of a lattice fulfills for any $m \in \mathbb{N}$.

$$\rho_\lambda(\chi_\mathcal{A}) = \det A + O(\lambda^{-m}) \quad . \tag{2.4.3}$$

According to Lemma 2.2.1 we have the estimates (2.2.2)

$$J_\lambda(\mathcal{A}, \chi, x) \geq \frac{C^W_0}{C_\varphi \lambda^d} \sum_i \operatorname{dist}^2(x_i, \chi_\mathcal{A}) \varphi\left(\lambda^{-1} |x_i - x|\right) \quad , \tag{2.4.4}$$

The configuration $\chi_\mathcal{A}$ with $\rho_\lambda(\chi_\mathcal{A}) = \det A_R$ has $J_\lambda = 0$. If we increase the density by moving the atoms, we automatically increase J_λ. We denote $y_i := A^{-1}(z_i - \tau)$ and $\delta x_i := x_i - y_i$

$$J_\lambda(\mathcal{A}, \chi, x) \geq \tilde{J}_\lambda(x, \mathcal{A}, \chi) = \frac{C^W_0}{C_\varphi \lambda^d} \sum_i \delta x_i^2 \varphi\left(\lambda^{-1} |y_i + \delta x_i|\right) \quad . \tag{2.4.5}$$

We will now minimize $\tilde{J}_\lambda$ for constant $\rho_\lambda(x,\chi) = \tilde{\rho} \in \mathbb{R}$. Hence, we consider the Lagrange function

$$\tilde{L} := \tilde{J}_\lambda(x, \mathcal{A}, \chi) - \mu \left(\frac{1}{C_\varphi \lambda^d} \sum_i \varphi\left(\lambda^{-1} |y_i - \delta x_i|\right) - \tilde{\rho} \right) . \tag{2.4.6}$$

For the minimizing δx_i it holds

$$\begin{aligned} \partial_{\delta x_i} \rho_\lambda(\delta x_i, x) =& \partial_{\delta x_i} \tilde{J}_\lambda(x, \mathcal{A}, \delta x_i) \quad , \\ \mu \partial_{\delta_{x_i}} \varphi\left(\lambda^{-1} |y_i + \delta x_i|\right) =& 2C_0^W \delta x_i \varphi\left(\lambda^{-1} |y_i + \delta x_i|\right) \\ &+ C_0^W \delta x_i^2 \partial_{\delta_{x_i}} \varphi\left(\lambda^{-1} |y_i + \delta x_i|\right) . \end{aligned} \tag{2.4.7}$$

Since δx_i^2 penalizes increases of δx_i isotropically, the minimizing δx_i will be parallel to $\nabla\varphi(\lambda^{-1}|y_i|)$ that means anti parallel to y_i. Furthermore, the term on the left side of equation 2.4.6 balances the two terms on the right side. If the left side would have to balance only one of the terms on the right side $|x_i|$ would be larger. Hence, we get two upper bounds

$$|\delta x_i| < \frac{\mu}{2C_0^W \lambda} \frac{|\varphi''|}{\varphi} \left(\lambda^{-1} |y_i + \delta x_i|\right) \quad , \tag{2.4.8}$$

$$|\delta x_i| < \sqrt{\frac{\mu}{2C_0^W}} \quad . \tag{2.4.9}$$

Due to the upper bound (2.4.8) and mean value theorem there exists $\delta\tilde{x}_i := \nu \delta x_i$ with $\nu \in [0,1]$ such that

$$\varphi\left(\frac{|y_i + \delta x_i|}{\lambda}\right) - \varphi\left(\frac{|y_i|}{\lambda}\right) < \frac{\mu}{2C_0^W \lambda^2} \frac{|\varphi'|}{\varphi} \left(\lambda^{-1} |y_i + \delta x_i|\right) |\varphi'| \left(\lambda^{-1} |y_i + \delta\tilde{x}_i|\right) . \tag{2.4.10}$$

We have two cases. In the first case it holds

$$|\varphi'| \left(\lambda^{-1} \left|y_i + \delta\tilde{x}_i\right|\right) \geq |\varphi'| \left(\lambda^{-1} \left|y_i + \delta\tilde{x}_i\right|\right) \tag{2.4.11}$$

. Then, we have

$$\varphi\left(\frac{|y_i + \delta x_i|}{\lambda}\right) - \varphi\left(\frac{|y_i|}{\lambda}\right) < \frac{\mu}{2C_0^W \lambda^2} \frac{\varphi'^2}{\varphi} \left(\lambda^{-1} |y_i + \delta x_i|\right) \quad . \tag{2.4.12}$$

In the second case it holds

$$|\varphi'| \left(\lambda^{-1} \left|y_i + \delta\tilde{x}_i\right|\right) \leq |\varphi'| \left(\lambda^{-1} \left|y_i + \delta\tilde{x}_i\right|\right) \tag{2.4.13}$$

Then, we get

$$\varphi\left(\frac{|y_i + \delta x_i|}{\lambda}\right) - \varphi\left(\frac{|y_i|}{\lambda}\right) \leq \frac{\mu}{2C_0^W \lambda^2} \frac{1}{\varphi} \left(\lambda^{-1} |y_i + \delta x_i|\right) |\varphi'|^2 \left(\lambda^{-1} \left|y_i + \delta\tilde{x}_i\right|\right) \quad . \tag{2.4.14}$$

Since φ is monotone decreasing, we have

$$\varphi\left(\frac{|y_i+\delta x_i|}{\lambda}\right)-\varphi\left(\frac{|y_i|}{\lambda}\right)<\frac{\mu}{2C_0^W\lambda^2}\frac{|\varphi'|^2}{\varphi}\left(\lambda^{-1}\left|y_i+\delta\tilde{x}_i\right|\right) \quad . \tag{2.4.15}$$

In both cases, we obtain

$$\begin{aligned}&\varphi\left(\frac{|y_i+\delta x_i|}{\lambda}\right)-\varphi\left(\frac{|y_i|}{\lambda}\right)\\ \leq&\max\left\{\frac{\mu}{2C_0^W\lambda^2}\frac{|\varphi'|^2}{\varphi}\left(\frac{|y_i|-\delta x_i}{\lambda}\right)|\delta x_i\in\left[0,\frac{\mu}{2C_0^W}\right]\right\}.\end{aligned} \tag{2.4.16}$$

We now look closer at $\frac{|\varphi'|^2}{\varphi}(x)$. Since φ is continuous, monotone decreasing and fulfills $\varphi(2)=0$, there has to exists $x_0\in[1,2]$ such that $\varphi(z)>0$ for $z<x_0$ and $\varphi(z)=0$ for $z\geq x_0$ Since φ is continuously differentiable $\lim_{x\to x_0}\varphi'=0$ Applying L' Hospital we get:

$$\lim_{x\to x_0}\frac{\varphi'^2}{\varphi}(x)=\lim_{x\to x_0}\frac{2\varphi'\varphi''}{\varphi'}(x)=\lim_{x\to x_0}\nabla\varphi'=0 \quad . \tag{2.4.17}$$

Therefore, $\frac{\varphi'^2}{\varphi}(x)$ is bounded in a neighborhood of x_0 and therefore bounded everywhere, since is a continuous function on a compact set. Hence, we get

$$\begin{aligned}\delta\rho:=&\frac{1}{C_\varphi\lambda^d}\sum_i\varphi\left(\frac{|y_i+\delta x_i|}{\lambda}\right)-\varphi\left(\frac{|y_i|}{\lambda}\right)\\ \leq&\frac{\mu}{\lambda^2}\frac{1}{2C_0^WC_\varphi\lambda^d}\sum_i\max\left\{\frac{\varphi'^2}{\varphi}\left(\lambda^{-1}(|y_i|-\delta x_i)\right)|\delta x_i\in\left[0,\frac{\mu}{2C_0^W}\right]\right\} \quad .\end{aligned} \tag{2.4.18}$$

where

$$\tilde{C}_\phi^W:=\left(\frac{1}{2C_0^WC_\varphi\lambda^d}\sum_i\max\left\{\frac{\varphi'^2}{\varphi}\left(\lambda^{-1}(|y_i|-\delta x_i)\right)|\delta x_i\in\left[0,\frac{\mu}{2C_0^W}\right]\right\}\right)^{-1} \quad , \tag{2.4.19}$$

and obtain

$$\mu\geq 2C_\phi^W\lambda^2\delta\rho \quad . \tag{2.4.20}$$

Due to equation (B.1.31) we get $\mu=\frac{\partial J}{\partial\delta\rho}$ and therefore

$$J_\lambda(\delta\rho)\geq\int_0^{\delta\rho}\mu(\delta\rho)d\tilde{\delta\rho}\geq\tilde{C}_\phi^W\lambda^2\delta\rho^2 \quad . \tag{2.4.21}$$

Finally, we estimate

$$\begin{aligned}\tilde{C}_\phi^W &= \left(\frac{1}{C_0^W C_\varphi \lambda^d}\sum_i \max\left\{\frac{\varphi'^2}{\varphi}\left(\lambda^{-1}(|y_i|-\delta x_i)\right)|\delta x_i \in \left[0,\frac{\mu}{C_0^W}\right]\right\}\right)^{-1}\\ &= \left(\frac{1}{C_0^W C_\varphi \lambda^d}\sum_i \frac{\varphi'^2}{\varphi}\left(\lambda^{-1}(|y_i|\right)\right)^{-1} + O(\lambda^{-1})\\ &= \left(\frac{1}{C_0^W C_\varphi \lambda^d}\int_{\mathbb{R}^d} \frac{\varphi'^2}{\varphi}\left(\lambda^{-1}(|y|\right)dy\right)^{-1} + O(\lambda^{-1})\\ &= \left(\frac{1}{C_0^W C_\varphi}\int_{\mathbb{R}^d} \frac{\varphi'^2}{\varphi}\left((|y|\right)dy\right)^{-1} + O(\lambda^{-1}) \quad .\end{aligned} \tag{2.4.22}$$

Hence, we get the conclusion. □

Next, we calculate a general lower bound for J_λ for given A and ρ_λ. There are two ways to increase the density. First, one can move exiting atoms to positions of higher φ second one can add additional atoms. As show in Lemma 2.4.1 J_λ increases quadratically, if we move the atoms. In contrast if we add atoms it will increase linearly. Hence, our lower bound has a quadratically grow up to a certain threshold and grows linear from there

Lemma 2.4.2. *For all $C_A \in \mathbb{R}$ there exists $\hat{\lambda} \in \mathbb{R}$ such that for all $\lambda > \hat{\lambda}$ and $\mathcal{A} \in Gl_d(\mathbb{R})$ such that $|A^{-1}| < C_A$ the following estimates hold:*

1) For $\rho_\lambda(\chi, x) \le \rho_\lambda(\chi_{\mathcal{A}}, 0)$ it holds

$$J_\lambda(\mathcal{A}, \chi, x) \ge 0 \quad . \tag{2.4.23}$$

2) For $\rho_\lambda(\chi_{\mathcal{A}}, 0) \le \rho_\lambda(\chi, x) \le \rho_\lambda(\chi_{\mathcal{A}}, 0) < \rho_1$ it holds

$$\frac{C_\phi^W}{\det A}\lambda^2(\rho_\lambda - \rho_\lambda(\chi_{\mathcal{A}}, 0))^2 \quad . \tag{2.4.24}$$

3) For $\rho_1 \le \rho_\lambda$ it holds

$$J_\lambda \ge \frac{\mu_1^2 \det A}{4C_\phi^W \lambda^2} + \mu_1(\rho_\lambda - \rho_1) \quad . \tag{2.4.25}$$

where

$$\begin{aligned} C_\phi^W &:= \left(\frac{1}{C_0^W C_\varphi}\int_{\mathbb{R}^d}\frac{\varphi'^2}{\varphi}(|y|)\,dy\right)^{-1} \quad ,\\ \mu_1 &= C_0^W \frac{s_0^2}{2} - \frac{C_0^W s_0^4 \|\varphi'^2\|_\infty}{16\varphi\lambda^2} \quad ,\\ \rho_1 &= \left(1\frac{\mu_1}{2C_\phi^W \lambda^2}\right)\det A \quad .\end{aligned} \tag{2.4.26}$$

Proof. Since, by construction it holds $J_\lambda \geq 0$, no prove is needed for first statement. Instead, we note that we note $J_\lambda = 0$ for $\chi \subset \chi_{\mathcal{A}}$. Hence, the trivial bound is optimal in this generality. We minimize J_λ with the constrain of fixed density $\rho_\lambda(\chi, x) = \tilde{\rho}$. Therefore, we consider the Lagrange function

$$\tilde{L} := J_\lambda\left(\mathcal{A}, \chi, x\right) - \mu\left(\rho_\lambda\left(\chi, x\right) - \tilde{\rho}\right) \tag{2.4.27}$$

The function is minimized by the configuration. This means the particle position and the particle number can change. In Lemma 2.4.1 we calculated a lower bound in the case of constant particle number. Now we study the change of particle numbers.

Step 1: More than one atom per valley in the center With energy valley we mean for any point $y_i \in \chi_{\mathcal{A}}$ the sphere $B_{|A|^{-1}/2}(y_i)$ For K atoms in one energy valley, we get

$$\begin{aligned}\delta J_\lambda(K) \geq & \sum_{i=1}^{K} C_0^W \delta x_i^2 \geq \frac{C_0^W}{N} \sum_{i=1}^{K}\sum_{j=1}^{K} \delta x_i^2 = \frac{C_0^W}{2K}\sum_{i=1}^{K}\sum_{j=1}^{K}(\delta x_i^2 + \delta x_j^2) \\ = & \frac{C_0^W}{2K}\sum_{i=1}^{K}\sum_{j=1}^{K}(\delta x_i^2 - 2\delta x_i \delta x_j + \delta x_j^2) + \frac{C_0^W}{K}\sum_{i=1}^{K} x_i \sum_{j=1}^{K} x_j \\ = & \frac{C_0^W}{2K}\sum_{i=1}^{K}\sum_{j=1}^{K}(x_i - x_j)^2 + C_0^W K \left(\frac{\sum_{i=1}^{K} x_i}{K}\right)^2 \quad .\end{aligned} \tag{2.4.28}$$

Since the second term of in the last line of (2.4.28) is a square,, it is always larger equal zero. The first sum contains K^2 terms. The K-terms with $i = j$ are 0. The remaining $K^2 - K$ terms has to be at least $C_0^W s_o^2$. Hence, we get

$$\delta J_\lambda(K) \geq C_0^W s_0^2/2\,(K-1) \quad . \tag{2.4.29}$$

Hence, added atoms has to cost at least $C_0^W s_0^2/2$. Every two $s_0/2$ spheres has to touch each other to reach this minimal cost. In d dimensions this can be fulfilled by maximal $d+1$ spheres. Then the density of atoms can potentially be increased up to $d + 1 \det A$ without further change of μ. If we move the atoms in the potential valleys the chemical potential increases when it reaches $C_0^W s_0^2/2$ it becomes more favorable to add more atoms then to move the existing ones. Therefore, adding of additional atoms in the center starts when μ reaches $C_0^W s_0^2/2$

Step 2: More than one atom per valley at the boundary If $\mu \neq 0$, the atoms are already moved out of the positions of $\chi_{\mathcal{A}}$ in the area where $\nabla\varphi \neq 0$. Hence, the transition to more than one atoms happens there at a lower μ than

$C_0^W s_0^2/2$ For the contribution of one potential valley in that area we will consider for one atom.

$$\delta L_i(1) := C_0^W \delta x_i^2 \varphi(\lambda^{-1}|y_i|) + \frac{\mu}{\lambda}\varphi'(\lambda^{-1}|y_i|)\delta x_i \quad . \tag{2.4.30}$$

That basically neglects changes of φ in the first part and changes of φ' in the second part. Minimizing L we get

$$\begin{aligned} 0 =& 2C_0^W \delta x_i \varphi(\lambda^{-1}|y_i|) + \frac{\mu}{\lambda}\varphi'(\lambda^{-1}|y_i|) \quad , \\ \delta x_i =& -\frac{\mu}{2C_0^W\lambda}\frac{\varphi'}{\varphi}(\lambda^{-1}|y_i|) \quad , \\ \delta L(1) =& -\frac{\mu^2}{4C_0^W\lambda^2}\frac{\varphi'^2}{\varphi}(\lambda^{-1}|y_i|) \quad . \end{aligned} \tag{2.4.31}$$

If we denote with δx_i the difference between the i minimum and the center of math of the atoms in the i-valley, we get analogous to (2.4.28):

$$\begin{aligned} \delta L_i(K) :=& (K-1)C_0^W \frac{s_o^2}{2}\varphi(\lambda^{-1}|y_i|) + KC_0^W \delta x_i^2 \varphi(\lambda^{-1}|y_i|) \\ &+ K\delta x_i \frac{\mu}{\lambda}\varphi'(\lambda^{-1}|y_i|) - (K-1)\mu\varphi(\lambda^{-1}|y_i|) \quad . \end{aligned} \tag{2.4.32}$$

Hence, the minimizing δ_i fulfills:

$$\begin{aligned} 0 =& KC_0^W \delta x_i \varphi(\lambda^{-1}|y_i|) + K\frac{\mu}{\lambda}\varphi'(\lambda^{-1}|y_i|) \quad , \\ \delta x_i =& \frac{\mu}{2\lambda}\varphi\frac{|\varphi'|}{\varphi}(\lambda^{-1}|y_i|) \quad , \\ \delta L(K) =& -K\frac{\mu^2 \nabla\varphi^2}{4C_0^W \varphi\lambda^2} + (K-1)\left(C_0^W \frac{s_0^2}{2} - \mu\right)\varphi \quad . \end{aligned} \tag{2.4.33}$$

The transition from one atom to K atoms only reduces the Lagrange function, if $\delta J(K) \leq \delta J(1)$. This leads to

$$\begin{aligned} -N\frac{\mu^2\nabla\varphi^2}{4C_0^W\varphi\lambda^2} + (K-1)\left(C_0^W s_0^2/2 - \mu\right) \leq& -\frac{\mu_0^2\nabla\varphi^2}{4C_0^W\varphi\lambda^2} \quad , \\ \mu \geq& C_0^W\frac{s_0^2}{2} - \frac{\mu^2\nabla\varphi^2(y_i)}{C_0^W\varphi(y_i)\lambda^2} \quad , \\ \geq& \mu_1 := C_0^W\frac{s_0^2}{2} - \frac{C_0^W s_0^4}{16\lambda^2}\|\frac{\varphi'^2}{\varphi}\|_\infty \quad . \end{aligned} \tag{2.4.34}$$

Hence for $\mu \leq \mu_1$ the minimal J_λ the atom number is fixed. The atoms are just moving in the valleys and the lower bound is given by Lemma 2.4.1.

$$J_\lambda = \frac{C_\phi^W}{\det A}\lambda^2(\rho_\lambda - \det A)^2 \quad . \tag{2.4.35}$$

This leads to the chemical potential

$$\mu = \frac{\partial J_\lambda}{\partial \rho} \geq 2\frac{C_\phi^W}{\det A}\lambda^2(\rho_\lambda - \det A) \quad . \tag{2.4.36}$$

Until the $\mu = \frac{\partial J_\lambda}{\partial \rho}$ reaches μ_1. For $\mu > \mu_1$. For higher densities we use a constant $\mu = \mu_1$ to estimate the increase of the lower bound for J_λ □

The next theorem shows that every state with sufficiently low energy has to be regular. Furthermore, ϵ_J is bounded from above by a term of the form $A\epsilon + B\lambda^{-2}$. Hence, we can apply all our results for regular points on points with low energy density.

Theorem 2.4.3. *There exists $\hat{\lambda} \in R$ and $\hat{\epsilon} > 0$ such that for all $\lambda > \hat{\lambda}$, $\epsilon \leq \hat{\epsilon}$, $A \in Gl_d R$, $\tau \in \mathbb{R}^d$ and $x \in \Omega$ such that $h_\lambda(\mathcal{A}, \chi, x) < \epsilon$ the points x is $(\epsilon_\rho, \epsilon_J, C_A)$-regular with $\mathcal{A}$ and the coefficients satisfies*

$$\begin{aligned} C_A =& 2\sqrt{d}\,(2\,|E|)^{d-1}\det E^{-1} \quad , \\ \epsilon_\rho =& 2\det E^{-1} max\left\{(\mu_1 - \vartheta)^{-1}, \vartheta^{-1}\right\}\epsilon + \frac{\mu_1^2}{4C_\phi^W(\mu_1 - \vartheta)\lambda^2} \quad , \\ \epsilon_J =& 4\frac{\mu_1}{\mu_1 - \vartheta}\det E^{-1}\epsilon + \frac{\vartheta\mu_1^2}{2(\mu_1 - \vartheta)C_\phi^W\lambda^2} \quad . \end{aligned} \tag{2.4.37}$$

Furthermore we have

$$\left|\det(A) - \det(E) - \frac{\vartheta^2}{8C_\phi^W C_1^{El}\lambda^2}\right| \leq \frac{1}{\sqrt{C_1^{El}}}\sqrt{\epsilon - \epsilon_{min}} \quad , \tag{2.4.38}$$

$$J_\lambda \leq \epsilon + \frac{\vartheta}{\mu_1 - \vartheta}\left(\epsilon + \frac{\mu_1^2}{4C_\phi^W\lambda^2}\det A\right) \quad . \tag{2.4.39}$$

where

$$\begin{aligned} C_\phi^W :=& \left(\frac{1}{C_0^W C_\varphi}\int_{\mathbb{R}^d}\frac{\varphi'^2}{\varphi}(y)\,(|y|)\right)^{-1} \quad , \\ \mu_1 =& C_0^W\frac{s_0^2}{2} - \frac{C_0^W s_0^4\|\varphi'^2\|_\infty}{16\varphi\lambda^2} \quad , \\ \rho_1 =& \left(1\frac{\mu_1}{2C_\phi^W\lambda^2}\right)\det A \quad . \end{aligned} \tag{2.4.40}$$

Proof. Due to the assumptions of the theorem it holds

$$\epsilon > \hat{h}_\lambda(x, \chi) > F(A) + J_\lambda(x, \mathcal{A}, \chi) + \vartheta(\det A - \rho_\lambda) \quad . \tag{2.4.41}$$

According to Lemma 2.2.6 $|A^{-1}|$ is bounded by a finite constant independent of λ. Therefore, for large enough λ we can use Lemma 2.4.2 to get lower bounds for J_λ depending on $\det A$ and ρ_λ. The lower bound $\vartheta\left(\det A-\rho_\lambda\right)+J_\lambda$ is monoton decreasing for $\rho_\lambda(\chi,x)\leq\rho_\lambda(\chi_{\mathcal{A}},0)$ and monotone increasing for $\rho_\lambda(\chi,x)\geq\rho_1$. Therefore, the minimum of the lower bound is between $\rho_\lambda(\chi_{\mathcal{A}},0)$ and ρ_1. For $\rho_\lambda(\chi_{\mathcal{A}},0)\leq\rho_\lambda(\chi,x)\leq\rho_1$ we have due to the lower bound (2.4.24) from Lemma 2.4.2

$$\begin{aligned}J_\lambda+\vartheta\left(\det A-\rho_\lambda\right)\geq&\frac{C_\phi^W}{\det A}\lambda^2(\rho_\lambda-\det A)^2+\vartheta\left(\det A-\rho_\lambda\right)+O\left(\lambda^{-m}\right)\\ \geq&\frac{C_\phi^W}{\det A}\lambda^2\left(\rho_\lambda-\det A+O\left(\lambda^{-m}\right)+\frac{\vartheta}{2C_\phi^W\lambda^2}\det A\right)^2\\ &-\frac{\vartheta^2}{4C_\phi^W\lambda^2}\det A+O(\lambda^{-m})\\ \geq&-\frac{\vartheta^2}{4C_\phi^W\lambda^2}\det A+\vartheta\left(\det A-\rho_0\right)\quad.\end{aligned}\tag{2.4.42}$$

Due to the coercivity condition for F it holds

$$\begin{aligned}h_\lambda(\mathcal{A},\chi,x)\geq&F\left(A\right)-\frac{\vartheta^2}{4C_\phi^W\lambda^2}\det A+O(\lambda^{-m})\\ \geq&C_1^{El}\left(\det(E)-\det(A)\right)^2+C_2^{El}\mathrm{dist}^2\left(A,ESO_d\right)-\frac{\vartheta^2}{4C_\phi^W\lambda^2}\det A\\ \geq&\epsilon_{min}+C_1^{El}\left(\det(A)-\det(E)-\frac{\vartheta^2}{8C_\phi^WC_1^{El}\lambda^2}+O(\lambda^{-m})\right)^2\quad,\end{aligned}\tag{2.4.43}$$

where

$$\epsilon_{min}:=-\frac{\vartheta^4}{64\left(C_\phi^WC_1^{El}\right)^2\lambda^4}-\frac{\vartheta^2}{4C_\phi^W\lambda^2}\det E+O(\lambda^{-m})\quad.\tag{2.4.44}$$

Therefore, we have $h_\lambda(\mathcal{A},\chi,x)\geq\epsilon_{min}$ for all particle densities. Due to the estimate 2.4.43 and the coercivity condition on F, we get upper bounds for the difference between $\det E$ and $\det A$ and an other one for the difference between $|A|$ and $|E|$.

$$\begin{aligned}\left|\det(A)-\det(E)-\frac{\vartheta^2}{8C_\phi^WC_1^{El}\lambda^2}\right|\leq&\frac{1}{\sqrt{C_1^{El}}}\sqrt{\epsilon-\epsilon_{min}}\quad,\\ ||A|-|E||\leq&\frac{1}{\sqrt{C_2^{El}}}\sqrt{\epsilon-\epsilon_{min}}\quad.\end{aligned}\tag{2.4.45}$$

with these estimates and Lemma B.2.2 we get an upper bound for $\|A^{-1}\|$

$$\begin{aligned}\|A^{-1}\| <&\sqrt{d}|A^{-1}| \leq \sqrt{d}|A|^{d-1}\det A^{-1}\\ \leq&\sqrt{d}\left(|E| + \frac{1}{\sqrt{C_2^{El}}}\sqrt{\epsilon-\epsilon_{min}}\right)^{d-1}\\ &\times\left(\det E + \frac{\vartheta^2}{8C_\phi^W C_1^{El}\lambda^2} - \frac{1}{\sqrt{C_1^{El}}}\sqrt{\epsilon-\epsilon_{min}}\right)^{-1} \quad .\end{aligned} \tag{2.4.46}$$

Hence, for large enough λ and small enough ϵ it holds

$$|A^{-1}| \leq C_A := 2\sqrt{d}\,(2\,|E|)^{d-1}\det E^{-1} \quad . \tag{2.4.47}$$

Next, we derive the estimate for the density. Inequality (2.4.41) gives us together with $F > 0$ and $J > 0$ a lower bound for ρ_λ.

$$\frac{\epsilon}{\varphi_1} \geq \det A - \rho_\lambda \quad . \tag{2.4.48}$$

Just with $F > 0$ we get

$$\epsilon \geq \vartheta\,(\det A - \rho_\lambda) + J_\lambda \quad . \tag{2.4.49}$$

We use the estimate (2.4.25) from Lemma 2.4.2 to obtain

$$\begin{aligned}J_\lambda + \vartheta(\det A - \rho_\lambda) \geq& \frac{\mu_1^2}{4C_\phi^W\lambda^2}\det A + \mu_1\,(\rho_\lambda - \rho_1) + \vartheta(\det A - \rho_\lambda) \quad ,\\ \epsilon >& (\mu_1 - \vartheta)\,(\rho_\lambda - \det A) - \frac{\mu_1^2}{4C_\phi^W\lambda^2}\det A \quad .\end{aligned} \tag{2.4.50}$$

Summarizing the inequalities (2.4.48) and (2.4.50) we get

$$|\rho_\lambda - \det A| \leq \max\left\{(\mu_1-\vartheta)^{-1}\epsilon + \frac{\mu_1^2}{4C_\phi^W\,(\mu_1-\vartheta)\,\lambda^2}\det A, \frac{\epsilon}{\vartheta}\right\}. \tag{2.4.51}$$

. We apply the lower bound on $\det A$ of inequality (2.4.45) and get

$$|\rho_\lambda - \det A| < \epsilon_\rho \det A \tag{2.4.52}$$

where

$$\begin{aligned}\epsilon_\rho =: &\left(\det(E) - \frac{\vartheta^2}{8C_\phi^W C_1^{El}\lambda^2} - \frac{1}{\sqrt{C_1^{El}}}\sqrt{\epsilon-\epsilon_{min}}\right)^{-1}\max\left\{(\mu_1-\vartheta)^{-1}, \vartheta^{-1}\right\}\epsilon\\ &+ \frac{\mu_1^2}{4C_\phi^W\,(\mu_1-\vartheta)\,\lambda^2} \quad .\end{aligned} \tag{2.4.53}$$

For large enough λ and sufficiently small ϵ one gets

$$\epsilon_\rho \leq 2 \det E^{-1} \max\left\{(\mu_1-\vartheta)^{-1}, \vartheta^{-1}\right\}\epsilon + \frac{\mu_1^2}{4C_\phi^W(\mu_1-\vartheta)\lambda^2} \quad . \tag{2.4.54}$$

We also use the estimate (2.4.50) to get an upper bound on J

$$\begin{aligned} \epsilon \geq& \vartheta(\det A - \rho_\lambda) + J_\lambda \\ \geq& -\frac{\vartheta}{\mu_1-\vartheta}\left(\epsilon + \frac{\mu_1^2}{4C_\phi^W\lambda^2}\det A\right) \quad , \\ J_\lambda \leq& \epsilon + \frac{\vartheta}{\mu_1-\vartheta}\left(\epsilon + \frac{\mu_1^2}{4C_\phi^W\lambda^2}\det A\right) \quad . \end{aligned} \tag{2.4.55}$$

Furthermore, we use the lower bound for $\det A$ from inequality (2.4.45) to get

$$\begin{aligned} J_\lambda \leq& \frac{\mu_1}{\mu_1-\vartheta}\left(\det(E) - \frac{\vartheta^2}{8C_\phi^W C_1^{El}\lambda^2} - \frac{1}{\sqrt{C_1^{El}}}\sqrt{\epsilon-\epsilon_{min}}\right)^{-1}\epsilon\det A \\ &+ \frac{\vartheta\mu_1^2}{4(\mu_1-\vartheta)C_\phi^W\lambda^2}\det A \quad . \end{aligned} \tag{2.4.56}$$

Now, we need to estimate $\det A$ from above with ρ_λ. We use the estimates (2.4.48) and (2.4.45) to get

$$\begin{aligned} \rho_\lambda \geq& \det A - \frac{\epsilon}{\varphi_1} \\ \geq& \left(1 - \frac{\epsilon}{\varphi_1}\left(\det(E) - \frac{\vartheta^2}{8C_\phi^W C_1^{El}\lambda^2} - \frac{1}{\sqrt{C_1^{El}}}\sqrt{\epsilon-\epsilon_{min}}\right)^{-1}\right)\det A \quad . \end{aligned} \tag{2.4.57}$$

Hence, for large enough λ and small enough ϵ we have $2\rho_\lambda \geq \det A$ and get

$$\epsilon_J = 4\frac{\mu_1}{\mu_1-\vartheta}\det E^{-1}\epsilon + \frac{\vartheta\mu_1^2}{2(\mu_1-\vartheta)C_\phi^W\lambda^2} \quad . \tag{2.4.58}$$

□

Perspective 2.4.4. In Theorem 2.4.3 we have proven that all positions with low energy per volume density are regular. A alternative and probably better approach would be to use low energy per particle number instead low energy per volume as a criteria for regularity. Sadly this approach is not working for the model as it is written. To illustrate this we will reformulate this into two related questions

- How does configurations looks like that have minimal energy for a fixed particle density?
- What kind of implication does this have on our model?

Low density We define

$$\tilde{E} := \underset{A \in GL_d(\mathbb{R})}{\arg\min} \left(F(A) + \vartheta \det A \right) \quad . \tag{2.4.59}$$

Due to the compatibility condition on the compressibility $\det \tilde{E} > 0$. For any density $\rho_\lambda \leq \det \tilde{E}$ we consider a configuration satisfying $\chi \subset \tilde{E}^{-1}\mathbb{Z}^d$. We get for all x in Ω

$$\begin{aligned} \hat{h}_\lambda(\chi, x) =& \inf_{\mathcal{A}} \left\{ F\left(A\right) + J_\lambda\left(\mathcal{A}, \chi, x\right) + \vartheta \det A - \vartheta \rho_\lambda \right\} \\ =& F\left(\tilde{E}\right) + \vartheta \det \tilde{E} - \vartheta \rho_\lambda(\chi, x) \quad . \end{aligned} \tag{2.4.60}$$

We realize that this atoms sit on a lattice but they are no lattice. ρ_λ does not have to be anywhere near to $\det A = \det \tilde{E}$. Furthermore, with Lemma 2.1.1 we calculate

$$\begin{aligned} H_\lambda(\chi) =& \int_{B_{2\lambda}(\Omega)} \rho_\lambda(\chi, x) dx \\ =& |B_{2\lambda}\left(\Omega\right)| \left(F\left(\tilde{E}\right) + \vartheta \det \tilde{E} \right) - \vartheta \left(N_I - \int_{B_{4\lambda}(\Omega)} \rho_\lambda(\chi_S, x) dx \right) \end{aligned} \tag{2.4.61}$$

Hence, if the particle number fulfills $\frac{N}{|\Omega|} \leq \det \tilde{E}$, all configurations $\chi \subset \hat{E}^{-1}\mathbb{Z}^d$ have the same energy. They may form a solid crystal at some point and leave the rest of the set open or they may have a more or less homogeneous density, or anything between, and this does not make any difference in energy. Therefore, our model shows no crystallization for low density, and we not use it for overall densities $\frac{N}{|\Omega|} \leq \det \tilde{E}$. We need the term $\vartheta\left(\det A - \rho_\lambda\right)$ in our model is to separate the regime $\rho_\lambda < \det \hat{E}$, where the model doe not work, from the regime $\rho_\lambda \approx \det \hat{E}$, where we want to study the model.

Medium density With upper and lower bound on the particle density the energy per particle and energy per volume is essential the same. Hence, Theorem 2.4.3 proves that in this case all low energy configurations are close to lattices.

High density: We remember the coercivity condition for F

$$F(A) + \vartheta \det A > C_1^{El} \left(\det(E) - \det(A) \right)^2 + \vartheta \det A \quad .$$

For high ρ_λ the cost of increasing $\det A$ to this ρ_λ increases quadratically with ρ_λ. On the other hand, the cost of more than one atom per valley is $\frac{1}{2} C_W (s_o^2)$ per atom for a big range of atoms.

$$J_\lambda \approx \frac{1}{2} C_W s_o^2 \left(\rho_\lambda - \det(A) \right) \quad . \tag{2.4.62}$$

If we add this estimates and minimize them we get that for $\rho_\lambda \geq \frac{4\det E C_1^{El} + C_W s_o^2}{4C_1^{El}}$ the lower bound is actually reached by keeping $\det A = \frac{4\det E C_1^{El} + C_W s_o^2}{4C_1^{El}}$ constant and putting more atoms in each potential valley. The hard core potential may prevent that this actually happens (depending on the growth of F). But, if it happens, then we can not expect low energy configurations to be regular for high densities.

Chapter 3

Specific configurations

3.1 The Bravais-lattice as an atom configuration

In this section we want to discuss the behavior of the model when the atoms are arranged to form exactly a Bravais-lattice $\chi_{\mathcal{A}_R} = A^{-1}(\mathbb{Z}^d - \tau_R)$. There are two reasons for this. Firstly the model shows some unexpected technical difficulties that we want to treat in the easiest case they occur. Secondly we will use lattices as starting points for pertubative calculations in Section 3.2. For this we introduce the effective elastic potential. As the integral of the energy density of the Bravais lattice integrated over one periodic cell. We want to find out as much as possible about the properties of the effective elastic potential.

In Lemma 3.1.4 we show that even if the configuration is a Bravais lattice $\chi_{\mathcal{A}_R}$, the in terms of the energy best fitting lattice will not coincide with it in most cases. Near every reparametrisation of $\mathcal{A}_R$ there is a local minimizer $\tilde{\mathcal{A}}$ of the pre-energy density $h_\lambda(\mathcal{A}, \chi_{\mathcal{A}_R}, x)$ for fixed $\mathcal{A}_R$ and x. However the minimizer is not exactly the re-parametrized $\mathcal{A}_R$, but differs from it by a small $\delta\mathcal{A} = (\delta A, \delta\tau)$ this is due to the fact that the elastic energy contribution $F(A)$ and the term $\nu_\lambda(A, \chi, x)$ have a non vanishing derivative in A for most A_R. The difference between the re-parametrized A_R and the minimizing A will scale like $O(\lambda^{-2})$, and the pre-energy of the local minimizer will be $O(\lambda^{-2})$ lower than the pre-energy of the re-parametrized A_R. On the other hand the difference in τ can be estimated from above with any order $O(\lambda^{-k})$. Furthermore Lemma 3.1.6 shows that even $\delta\tau$ does not have to be zero and will still depends on x for the special case of locally quadratic W.

In Lemma 3.1.5 we prove that under reasonable assumptions on A_R one of the local minimizers described in Lemma 3.1.4 is actually the global minimizer of the pre-energy density $h_\lambda(\mathcal{A}, \chi_{\mathcal{A}_R}, x)$ and therefore determines the effective elastic potential. Finally, we will study the symmetries of the minimizers $\mathcal{A}$ (see Lemma 3.1.8) and of the effective elastic potential in Lemma (see 3.1.9).

First, we introduce the definition of the effective elastic potential.

Definition 3.1.1. *Let $G \in Gl_d(\mathbb{R})$ and $z \in \mathbb{R}^d$. We define the local effective elastic energy density by*

$$F_\lambda(G,z) := \hat{h}_\lambda\left(G\left(\mathbb{Z}^d - z\right), 0\right) \quad , \tag{3.1.1}$$

and the average effective elastic energy density by

$$F_\lambda(G) := \int_{[0,1]^d} F_\lambda(G,z)dz \quad . \tag{3.1.2}$$

When we discussing a Bravais lattice $\chi_{\mathcal{A}_R}$ it is convenient to use the difference between $\mathcal{A}$ and the closest reparamertisation of $\mathcal{A}_R$ as a variable.

Definition 3.1.2. *Let $A_R, A \in Gl_d(\mathbb{R})$, $\tau_R, \tau \in \mathbb{R}^d$ and let $B \in Gl_d(\mathbb{Z})$ and $t \in \mathbb{Z}^d$ then we define $\delta\mathcal{A} := (\delta A, \delta\tau)$*

$$\begin{aligned} \delta A :=& A - BA_R \quad , \\ \delta\tau :=& \tau - B\tau_R - BA_R x - t \quad . \end{aligned} \tag{3.1.3}$$

If the configuration χ is a Bravais-lattice $\chi_{\mathcal{A}_R}$ and $\mathcal{A} = (A,\tau)$ is close to a reparametrisation of $\mathcal{A}_R = (A_R, \tau_R)$, then we can rewrite J_λ in terms of $\delta\mathcal{A}$.

Lemma 3.1.3. *Let $A_R, A \in Gl_d(\mathbb{R})$, $\tau_R, \tau \in R^d$, $B \in Gl_d(\mathbb{Z})$ and $t \in \mathbb{Z}^d$. If the atom configuration is the Bravais lattice*

$$\chi_{\mathcal{A}_R} = A_R^{-1}\left(\mathbb{Z}^d - \tau_R\right) \quad , \tag{3.1.4}$$

then the following holds

$$\begin{aligned} W(A(x_i - x) + \tau) =& W(\delta A(x_i - x) + \delta\tau) \\ \nabla W(A(x_i - x) + \tau) =& \nabla W(\delta A(x_i - x) + \delta\tau) \\ \nabla^2 W(A(x_i - x) + \tau) =& \nabla^2 W(\delta A(x_i - x) + \delta\tau). \end{aligned} \tag{3.1.5}$$

Proof. Since $B \in Gl_d(\mathbb{Z})$ and $t \in \mathbb{Z}^d$ there is a numeration of $\mathbb{Z}^d$ such that

$$x_i = A_R^{-1}B^{-1}(z_i - B\tau_R - t) \quad . \tag{3.1.6}$$

This means

$$W(A(x_i - x) + \tau) = W(A\left(A_R^{-1}B^{-1}(z_i - B\tau_R - t) - x\right) + \tau) \quad . \tag{3.1.7}$$

By the periodicity of W we have

$$W(A(x_i - x) + \tau) = W(A\left(A_R^{-1}B^{-1}(z_i - B\tau_R - t) - x\right) + \tau - z_i) \quad . \tag{3.1.8}$$

Now we use $1 = BA_R(BA_R)^{-1}$.

$$\begin{aligned}
& W(A\,(x_i - x) + \tau) \\
=& W(A\left(A_R^{-1}B^{-1}(z_i - B\tau_R - t) - x\right) + \tau - BA_R(BA_R)^{-1}z_i) \\
=& W((A - BA_R)\left(B^{-1}A_R^{-1}(z_i - B\tau_R - t) - x\right) - B\tau_R - BA_Rx - t + \tau) \\
=& W((A - BA_R)\,(x_i - x) - B\tau_R - BA_Rx - t + \tau) \quad .
\end{aligned} \tag{3.1.9}$$

Finally, we substitute with δA and $\delta\tau$ and get

$$W(A\,(x_i - x) + \tau) = W(\delta A\,(x_i - x) + \delta\tau) \quad . \tag{3.1.10}$$

Since ∇W and $\nabla^2 W$ have the same argument and show the same periodicity, the same calculation can be used to prove (3.1.5). □

Now we study the local minimizers of h_λ in case that the configuration is a Bravais lattice. We will proof that there exists a unique local minimizer $\tilde{\mathcal{A}} = (\tilde{A}, \tilde{\tau})$ close to each reparametrisation of $\mathcal{A}_R$. The distance between $\tilde{A}$ and the re-parametrized A_R scales like λ^{-2}. The distance between $\tilde{\tau}$ and the the re-parametrized τ_R scales smaller than λ^{-k} for any natural number k. The difference between the pre-energy of the local minimum and that of the re-parametrized lattice scales like λ^{-2} Finally the local minimizers $\mathcal{A}$ are differentiable functions of $\mathcal{A}_R$.

Lemma 3.1.4. *For all $C_A > 0$, $n \in \mathbb{N}$ exists a $\lambda^* \in \mathbb{R}$ such that for all $\lambda \geq \lambda^*$, $A_R \in Gl_d(\mathbb{R})$, $\tau_R \in R^d$, $B \in Gl_d(\mathbb{Z})$ and all $t \in \mathbb{Z}^d$ with $|(BA_R)^{-1}| \leq C_A$ holds, there exists a unique local minimizer*

$$\delta\hat{\mathcal{A}} = \min\left\{ h_\lambda(\tilde{\mathcal{A}}(\delta\mathcal{A}), \chi_{\mathcal{A}_R}, x) \,\middle|\, |\delta A| \leq \frac{\Theta_W}{3\lambda}, |\delta\tau| \leq \frac{\Theta_W}{3\lambda} \right\}, \tag{3.1.11}$$

where

$$\begin{aligned}
\tilde{A}(\delta\mathcal{A}) =& BA_R + \delta A \\
\tilde{\tau}(\delta\mathcal{A}) =& B\tau_R + BA_Rx + t + \delta\tau
\end{aligned} \tag{3.1.12}$$

Moreover, the local minimizer satisfies

$$\begin{aligned}
\delta\hat{A} =& -\frac{1}{\lambda^2\left\|A_R^{-1}B^{-1}\right\|^2}\frac{C_\varphi d}{C_{\varphi 2}}(c_\Theta^0)^{-1}M_0 + O(\lambda^{-3}) \\
|\delta\hat{\tau}| \leq& O(\lambda^{-m}) \quad .
\end{aligned} \tag{3.1.13}$$

Moreover for the minima, we have

$$\begin{aligned}
& h_\lambda\left(BA_R + \delta\hat{A}_B, B\tau_R + BA_Rx + t + \delta\hat{\tau}, \chi_{\mathcal{A}_R}\right) \\
=& F\left(BA_R\right) - \frac{1}{2\lambda^2\left\|A_R^{-1}B^{-1}\right\|^2}\frac{C_\varphi d}{C_{\varphi 2}}Tr\left(M_0^T(\nabla^2 W(0))^{-1}M_0\right) \pm O\left(\lambda^{-4}\right) \quad .
\end{aligned} \tag{3.1.14}$$

where the matrix $M_0 \in \mathbb{R}^{d\times d}$ *is defined by its scalar product*[1] *with any test matrix* $M \in \mathbb{R}^{d\times d}$ *is*

$$< M_0, M >:= ((\partial_A F)(BA_R) + \vartheta(\partial_A \det)(BA_R))\,[M] \quad . \tag{3.1.15}$$

Finally, the local minimizer $\delta\hat{\mathcal{A}}$ *is a differentiable function of the lattice parameters* $\mathcal{A}_R$ *and we have*

$$\|\partial_{\mathcal{A}_R}\delta\hat{\mathcal{A}}[M]\|_\lambda \leq O(\lambda^{-2})\|\mathcal{M}\|_\lambda \quad . \tag{3.1.16}$$

Proof. We will prove the statement in three steps. In the first step we will just proof that the local minimizer exists. And give a upper bound for their distance to the reparametrisation of $\mathcal{A}_R$. In the second step we will improve the estimates and also give a lower bound for the distance. In the third step we will prove that the local minimizers $\mathcal{A}$ are differentiable functions of $\mathcal{A}_R$.

Step 1 Upper bound for the difference Our pre-energy density is

$$\begin{aligned}\tilde{h}_\lambda(\delta\mathcal{A}, \chi_{\mathcal{A}_R}, x) :=& h_\lambda\left(BA_R + \delta\hat{A}_B, B\tau_R + BA_R x + t + \delta\hat{\tau}_B, \chi_{\mathcal{A}_R}\right) \\ & \frac{\|(BA_R+\delta A)^{-1}\|^2}{C_\varphi\lambda^d}\sum_i W(\delta A(x_i - x) + \delta\tau)\,\varphi\left(\frac{|x_i - x|}{\lambda}\right) \\ & + F(BA_R + \delta A) + \vartheta\det(BA_R+\delta A) - \vartheta\rho_\lambda \quad .\end{aligned} \tag{3.1.17}$$

We estimate the first derivative of $\tilde{h}_\lambda(\delta\mathcal{A}, \chi_{\mathcal{A}_R}, x)$ in direction $\delta\mathcal{A}$ for the point $\delta\mathcal{A} = 0$ and the second derivative for $\delta A \leq \frac{\Theta_W}{3\lambda}$ and $|\delta\tau| \leq \frac{\Theta_W}{3\lambda}$ This will give us an estimate for the local minima according to Lemma B.1.1 from the appendix. We compute the derivatives of $\tilde{h}_\lambda(\delta\mathcal{A}, \chi_{\mathcal{A}_R}, x)$ in direction $\delta\mathcal{A}$ applied on a test matrix $\mathcal{M} = (M, \mu)$ with $M \in \mathbb{R}^{d\times d}(\mathbb{R})$ and $\mu \in \mathbb{R}^d$. [2]

$$\begin{aligned}\partial_{\delta\mathcal{A}}\tilde{h}_\lambda[\mathcal{M}] =& \frac{\|(BA_R+\delta A)^{-1}\|^2}{C_\varphi\lambda^d}\sum_i \langle\nabla W(\delta A(x_i - x) + \delta\tau), M(x_i - x) + \mu\rangle\,\varphi \\ & + \frac{\partial_{\delta\mathcal{A}}\|(BA_R+\delta A)^{-1}\|^2[M]}{C_\varphi\lambda^d}\sum_i W(\delta A(x_i - x) + \delta\tau)\,\varphi \\ & + (\partial_A F)(BA_R+\delta A)[M] + \vartheta(\partial_A\det)(BA_R+\delta A)[M] \quad .\end{aligned} \tag{3.1.18}$$

At the position $\delta\mathcal{A} = 0$ both $W(\delta A(x_i - x) + \delta\tau)$ and $\nabla W(\delta A(x_i - x) + \delta\tau)$ are zero, so we get

$$\partial_{\delta\mathcal{A}}\tilde{h}_\lambda(0, \chi_{\mathcal{A}_R}, x)[\mathcal{M}] = (\partial_A F)(BA_R)[M] + \vartheta(\partial_A\det)(BA_R)[M] = \langle M_0, M\rangle \quad . \tag{3.1.19}$$

[1] The scalar product belonging to the Frobenius norm

[2] In what follows, we will omit the arguments of W and φ.

Now, we calculate the second derivative multiplied with the test matrix $\mathcal{M}$ from both sides.

$$\begin{aligned}\partial^2_{\delta\mathcal{A}}\tilde{h}_\lambda[\mathcal{M}] =& \frac{\left\|(BA_R+\delta A)^{-1}\right\|^2}{C_\varphi\lambda^d}\sum_i \nabla^2 W\left[M\left(x_i-x\right)+\mu\right]\varphi \\ &+\frac{2}{C_\varphi\lambda^d}\partial_{\delta A}\left\|(BA_R+\delta A)^{-1}\right\|^2[M]\sum_i\left\langle\nabla W, M\left(x_i-x\right)+\mu\right\rangle\varphi \\ &+\frac{1}{C_\varphi\lambda^d}M\partial^2_{\delta A}\left\|(BA_R+\delta A)^{-1}\right\|^2[M]\sum_i W\varphi \\ &+\left(\partial^2_A F\right)\left(BA_R+\delta A\right)[M]+\vartheta(\partial^2_A\det)(BA_R+\delta A)[M] \quad . \end{aligned} \tag{3.1.20}$$

We estimate the last line of (3.1.20). Since $\delta A \leq O(\lambda^{-1})$, we know that $\partial^2_A F$ and $\det A$ are $O(1)$. We produce a factor λ^{-2} by passing from $\|M\|^2$ to $\|\mathcal{M}\|^2_\lambda$. Therefore, the contribution of the last line of (3.1.20) is

$$\left|M(\partial^2_A F)\left(BA_R+\delta A\right)M+\vartheta M(\partial^2_A\det)(BA_R+\delta A)M\right| \leq O(\lambda^{-2}\|\mathcal{M}\|^2_\lambda) \quad . \tag{3.1.21}$$

Now we look at the other terms in (3.1.20). Since $|\delta A| < \frac{\Theta_W}{3\lambda}$ and $|\delta\tau| < \frac{\Theta_W}{3}$, we get

$$|\delta A\left(x_i-x\right)+\delta\tau)| \leq |\delta A||x_i-x|+|\delta\tau| \leq \Theta_W \quad . \tag{3.1.22}$$

Therefore, the argument of W does not leave the area of local convexity. Additionally we have $W(0)=0$ and $\nabla W(0)=0$, and so

$$\begin{aligned}|\nabla^2 W(\delta A\left(x_i-x\right)+\delta\tau)| \leq& |c^1_\Theta| \quad , \\ |\nabla W(\delta A\left(x_i-x\right)+\delta\tau)| \leq& |c^1_\Theta|(2\lambda|\delta A|+|\delta\tau|) \quad , \\ W(\delta A\left(x_i-x\right)+\delta\tau) \leq& \frac{1}{2}|c^1_\Theta|(2\lambda|\delta A|+|\delta\tau|)^2 \quad . \end{aligned} \tag{3.1.23}$$

We apply (3.1.23) on the parts of equation (3.1.20) and get

$$\begin{aligned}&\frac{1}{\lambda^d}\partial_A\left\|(BA_R+\delta A)^{-1}\right\|^2[M]\sum_i\left\langle\nabla W, M\left(x_i-x\right)+\mu\right\rangle\varphi \\ &\leq O\left(\lambda^{-2}\|\delta\mathcal{A}\|_\lambda\|\mathcal{M}\|^2_\lambda\right) \quad . \end{aligned} \tag{3.1.24}$$

$$\frac{1}{C_\varphi\lambda^d}\partial^2_{\delta A}\left\|(BA_R+\delta A)^{-1}\right\|^2[M] \leq \sum_i W\varphi \leq O\left(\lambda^{-2}\|\delta\mathcal{A}\|_\lambda\|\mathcal{M}\|^2_\lambda\right) \quad . \tag{3.1.25}$$

The contribution of the last term can be written as

$$QJ := \frac{\left\|(BA_R+\delta A)^{-1}\right\|^2}{C_\varphi\lambda^d}\sum_i\nabla^2 W\left[M\left(x_i-x\right)+\mu\right]\varphi \quad . \tag{3.1.26}$$

We can estimate this last term from below by using the strict convexity of W around $\mathbb{Z}^d$. In fact

$$QJ \geq c_\Theta^0 \frac{\|(BA_R+\delta A)^{-1}\|^2}{C_\varphi \lambda^d} \sum_i \left(M\left(x_i-x\right)+\mu\right)^2 \varphi\left(\frac{|x_i-x|}{\lambda}\right) \quad . \tag{3.1.27}$$

Next we want to pass from the discrete sum to a continuum measure using Lemma 2.1.2. To this aim we define

$$\psi(X) := \left(MX+\mu\right)^2 \varphi\left(X\right). \tag{3.1.28}$$

Since $\psi \in C_C^\infty(\mathbb{R}^d)$, we get

$$\left|\lambda^{-d} \sum_{x_i \in \chi_{\mathcal{A}_R}} \psi\left(\lambda^{-1}\left(x_i-x\right)\right) - \int_{\mathbb{R}^d} \psi(y)dy \det A_R\right| \leq C_m \lambda^{-m} \left\|\nabla^m \psi\right\|_\infty \det A_R \quad , \tag{3.1.29}$$

and we can conclude that

$$\begin{aligned} QJ \geq & c_\Theta^0 \frac{\lambda^2 \|(BA_R+\delta A)^{-1}\|^2}{C_\varphi} \int_{\mathbb{R}^d} \left(My+\mu\right)^2 \varphi\left(|y|\right) \det BA_R dy - O(\lambda^{-m})\|\mathcal{M}\|_\lambda^2 \\ = & c_\Theta^0 \frac{\lambda^2 \|(BA_R+\delta A)^{-1}\|^2}{C_\varphi} \int_{\mathbb{R}^d} \left((My)^2+2\mu My+\mu^2\right)^2 \varphi\left(|y|\right) \det BA_R dy \\ & - O(\lambda^{-m})\|\mathcal{M}\|_\lambda^2 \quad . \end{aligned} \tag{3.1.30}$$

Since $\varphi\left(|y|\right) = \varphi\left(|-y|\right)$ we have $\int y\varphi\left(|y|\right)dy = 0$ and

$$\begin{aligned} QJ \geq & c_\Theta^0 \frac{\lambda^2 \|(BA_R+\delta A)^{-1}\|^2}{C_\varphi} \int_{\mathbb{R}^d} \left((My)^2+\mu^2\right)^2 \varphi\left(|y|\right) \det BA_R dy \\ & - O(\lambda^{-m})\|\mathcal{M}\|_\lambda^2 \quad . \end{aligned} \tag{3.1.31}$$

We calculate the integral $\int_{\mathbb{R}^d} y\left(M^TM\right)y\varphi\left(y\right)dy$ in the eigensystem of the positive definite symmetric matrix M^TM we get

$$\begin{aligned} \int_{\mathbb{R}^d} y\left(M^TM\right)y\varphi\left(y\right)dy = & \int_{\mathbb{R}^d} \sum_{j=1}^d (M^TM)_j (y_j)^2 \varphi\left(y\right)dy \\ = & \sum_{j=1}^d (M^TM)_j \int_{\mathbb{R}^d} (y^j)^2 \varphi\left(y\right)dy \\ = & \frac{1}{d} C_{\varphi 2} Tr(M^TM) = \frac{1}{d} C_{\varphi 2} \|M\|^2 \quad . \end{aligned} \tag{3.1.32}$$

Therefore, we get

$$QJ \geq c_\Theta^0 \left\|(BA_R+\delta A)^{-1}\right\|^2 \left(\lambda^2 \frac{C_{\varphi 2}}{C_\varphi d}\|M\|^2 + |\mu|^2\right) - O(\lambda^{-m})\|\mathcal{M}\|_\lambda^2 > C\|\mathcal{M}\|_\lambda^2 \,. \tag{3.1.33}$$

Since all other contributions of $\partial_{\delta\mathcal{A}^2}\tilde{h}_\lambda(\mathcal{M})$ are $O(\lambda^{-1})\|\mathcal{M}\|_\lambda^2$ or smaller we get a lower bound for the second derivative $\partial_{\mathcal{A}}^2 h_\lambda$

$$\begin{aligned}\partial_{\delta\mathcal{A}^2}\tilde{h}_\lambda(\mathcal{M},\mathcal{M}) \geq & c_\Theta^0 \left\|(BA_R+\delta A)^{-1}\right\|^2 \left(\lambda^2 \frac{C_{\varphi 2}}{C_\varphi d}\|M\|^2 + |\mu|^2\right) \\ & - O(\lambda^{-1}\|\mathcal{M}\|_\lambda^2 \quad .\end{aligned} \tag{3.1.34}$$

We apply Lemma B.1.1 in the appendix combined with the estimates (3.1.19) satisfying condition (B.1.2) and the estimate (3.1.34) satisfying condition (B.1.1). The there exists a unique local minimizer that fulfills

$$\|\delta\mathcal{A}\|_\lambda \leq O(\lambda^{-1}) \quad . \tag{3.1.35}$$

Hence, δA is maximal $O(\lambda^{-2})$ and $\delta\tau$ is maximal $O(\lambda^{-1})$ for the minimizer. Therefore, the argument of W is not only smaller than Θ_W but actually $O(\lambda^{-1})$

Step 2: Improving the estimates Instead of estimating $\nabla W(\delta A(x_i - x) + \delta\tau)$ in (3.1.27) with the local convexity one can also estimate it with a Taylor-expansion

$$\nabla^2 W(\delta A(x_i - x) + \delta\tau) = \nabla^2 W(0) + \frac{1}{2}\nabla^4 W(0) O(\lambda^{-2}) \quad . \tag{3.1.36}$$

If we go through the calculation above with the modified estimate, we get similarly to (3.1.34)

$$\begin{aligned}\partial_{\delta\mathcal{A}}^2\tilde{h}_\lambda[\mathcal{M}] = & \left\|(BA_R+\delta A)^{-1}\right\|^2 \left(\lambda^2 \frac{C_{\varphi 2}}{C_\varphi d} Tr(M^T\nabla^2 W(0)M) + \mu\nabla^2 W(0)\mu\right) \\ & + O(\lambda^{-2}\|\mathcal{M}\|_\lambda^2 \quad .\end{aligned} \tag{3.1.37}$$

Because $|A_R^{-1}B^{-1}| < C_A$ we can bound the change of $\|(BA_R+\delta A)^{-1}\|^2$ by the change of δA (see Lemma B.2.3), and gets

$$\begin{aligned}\partial_{\delta\mathcal{A}}^2\tilde{h}_\lambda[\mathcal{M}] = & \left\|(BA_R)^{-1}\right\|^2 \left(\lambda^2 \frac{C_{\varphi 2}}{C_\varphi d} Tr(M^T\nabla^2 W(0)M)^2 + \mu\nabla^2 W(0)\mu\right) \\ & + O(\lambda^{-2}\|\mathcal{M}\|_\lambda^2) \quad .\end{aligned} \tag{3.1.38}$$

Again, we can bound $\partial_{\delta\mathcal{A}}^2\tilde{h}_\lambda[\mathcal{M}]$ from below and above by

$$\langle M, C_+ M\rangle < \partial_{\delta\mathcal{A}}^2\tilde{h}_\lambda[\mathcal{M}] < \langle M, C_+ M\rangle \quad , \tag{3.1.39}$$

where

$$C_\pm = \left(\lambda^2 \left\|(BA_R)^{-1}\right\|^2 \frac{C_{\varphi 2}}{C_\varphi d}\left(\nabla^2 W(0)\otimes Id_{\mathbb{R}^d} \pm O(\lambda^{-2})\right) \oplus \left(\nabla^2 W(0)\right) \pm O(\lambda^{-2})\right) . \tag{3.1.40}$$

The inverse of $C_\pm$ is

$$C_\pm^{-1} = \left\|(BA_R)^{-1}\right\|^{-2} \lambda^{-2} \frac{C_\varphi d}{C_{\varphi 2}} \left(\left(\nabla^2 W(0)\right)^{-1} \otimes Id_{\mathbb{R}^d} \pm O(\lambda^{-2}) \right) \oplus \left\|(BA_R)^{-1}\right\|^{-2} \left(\nabla^2 W(0)\right)^{-1} \pm O(\lambda^{-2}) \quad . \tag{3.1.41}$$

If we apply Lemma B.1.2 together with equation (3.1.19), we get Hence, we get from the estimates (B.1.18) and (B.1.19)

$$\tilde{h}_\lambda \left(\delta \mathcal{A}_{min}, \chi_{\mathcal{A}_R}\right) = F\left(BA_R\right) + \vartheta \det(BA_R) - \vartheta \rho_\lambda - \frac{1}{2\lambda^2 \left\|A_R^{-1} B^{-1}\right\|^2} \frac{C_\varphi d}{C_{\varphi 2}} Tr\left(M_0^T (\nabla^2 W(0))^{-1} M_0\right) + O\left(\lambda^{-4}\right) \quad . \tag{3.1.42}$$

With Lemma (2.1.2) we can estimate $\vartheta\rho_\lambda = \det BA_R + O(\lambda^{-4})$ and get the estimate (3.1.14). And the estimate (B.1.19) gives

$$\left\|(BA_R)^{-1}\right\|^2 \left(\lambda^2 \frac{C_{\varphi 2}}{C_\varphi d} Tr\left(\alpha^T \nabla^2 W(0) \alpha\right) + \mu \nabla^2 W(0) \mu \right) \le M_0 O(\lambda^{-4}) M_0 \quad . \tag{3.1.43}$$

where

$$\alpha := \delta A_{min} + \frac{1}{\lambda^2 \left\|A_R^{-1} B^{-1}\right\|^2} \frac{C_\varphi d}{C_{\varphi 2}} \left(\nabla^2 W(0)\right)^{-1} M_0 \quad . \tag{3.1.44}$$

This implies the first part of (3.1.13). Next we use Lemma B.1.2 from the appendix one more time, This time withwe use $(\delta A_{min}, 0)$ as a starting point, and we just minimize with respect to $\delta\tau$

$$\partial_{\delta\tau} \tilde{h}_\lambda(\delta A_{min}, 0, \chi_{\mathcal{A}_R}, x) = \frac{\|(BA_R + \delta A_{\min})^{-1}\|^2}{C_\varphi \lambda^d} \sum_i \nabla W\left(\delta A_{min}\left(x_i - x\right) + \delta\tau\right) \varphi \ . \tag{3.1.45}$$

Again can pass from the discrete estimate to the continuum estimate using Lemma 2.1.2. We define

$$\widetilde{\delta A} := \lambda \delta A \quad ,$$
$$\psi(X) := \nabla W \left(\widetilde{\delta A}\left(x_i - x\right) + \delta\tau \right) \varphi(X) \quad , \tag{3.1.46}$$

We get

$$\partial_{\delta\tau} \tilde{h}_\lambda = \frac{\|(BA_R + \delta A)^{-1}\|^2}{C_\varphi \lambda^d} \int \nabla W\left(\delta A y\right) \varphi\left(y\right) dy + O(\lambda^{-m}) \|\nabla^m \psi\|_\infty \quad . \tag{3.1.47}$$

Then $\int \nabla W\left(\delta A y\right) \varphi\left(y\right) dy$ is the integral of an odd function over an even domain. Therefore, it is zero. Since $|\delta A| = O(\lambda^{-2})$, we have $\nabla^m \psi = O(1)$. We already obtained that $\partial^2_{\delta\tau}\tilde{h}_\lambda$ is strictly positive and $O(1)$. Hence, the application of Lemma B.1.2 leads to

$$\delta\tau = O(\lambda^{-m}) \quad . \tag{3.1.48}$$

Step 3: Differentiability of the minimizers: We calculate

$$\begin{aligned}
&\partial_{\mathcal{A}_R}\partial_{\delta\mathcal{A}}\tilde{h}_\lambda(\mathcal{M}_1,\mathcal{M}_2)\\
=&\partial_{\mathcal{A}_R}\left(\frac{\|(BA_R+\delta A)^{-1}\|^2}{C_\varphi\lambda^d}\sum_i\langle\nabla W, M\,(x_i-x)+\mu\rangle\,\varphi\right)[\mathcal{M}_2]\\
&+\partial_{\mathcal{A}_R}\frac{\partial_{\delta\mathcal{A}}\|(BA_R+\delta A)^{-1}\|^2\,[M]}{C_\varphi\lambda^d}\sum_i W\left(\delta A\,(x_i-x)+\delta\tau\right)\varphi[\mathcal{M}_2]\\
&+\left(\partial^2_A F\right)(BA_R+\delta A)\,(M_1,BM_2)+\vartheta\left(\partial^2_A\det\right)(BA_R+\delta A)\,[M_1,BM_2] \quad .
\end{aligned} \tag{3.1.49}$$

We see that F and $\vartheta\det A$ give contributions of order $O(\lambda^{-2}\|\mathcal{M}_1\|_\lambda\|\mathcal{M}_2\|_\lambda)$. Furthermore, $\nabla W\left(\delta A\,(x_i-x)+\delta\tau\right)$ is $O(\lambda^{-1})$ and $W\left(\delta A\,(x_i-x)+\delta\tau\right)$ is $O(\lambda^{-1})$. Therefore, the term where the derivative $\partial_{\mathcal{A}_R}$ is applied on the $\|(BA_R+\delta A)^{-1}\|^2$ are $O(\lambda^{-2}\|\mathcal{M}_1\|_\lambda\|\mathcal{M}_2\|_\lambda)$. If the derivative is applied on the atom positions $x_i = A_R^{-1}(z_i-\tau_R)$, we get a factor $(z_i-\tau_R)$ for the A_R derivative. If we apply the derivative on the argument of W, we also get an inner derivative $\delta A=\lambda^{-2}$. If we apply this on the atom position in φ, we get λ^{-1}. We have

$$\partial_{\mathcal{A}_R}\partial_{\delta\mathcal{A}}\tilde{h}_\lambda(\mathcal{M}_1,\mathcal{M}_2) = O(\lambda^{-2}\|\mathcal{M}_1\|_\lambda\|\mathcal{M}_2\|_\lambda) \quad . \tag{3.1.50}$$

Therefore, we can apply the second part of Lemma B.1.1 □

We encountered the first technical difficulty of the model δA is not zero for most lattice. This means even in the 'best possible' case that is when the atom configuration is exactly a Bravais lattice the fitted lattice will not exactly coincide with it. We also notice that $|\delta\tau|$ is much smaller than $|\delta A|$. Hence, the model fits τ much better than A when the configuration is a Bravais lattice.

We studied the local minimizers of the pre-energy density h_λ for the case that the configuration is a Bravais lattice in Lemma 3.1.4 Now we will proof that one of these minimizers is in fact the global minimizer, if the energy density is low enough. In particular in a neighborhood of the ground state E this will always be true. This means on the one hand that the effective elastic potential is given by one of the minima described in lemma 3.1.4. On the other hand we can use this information when we perturb the lattice as described in Section 3.2.

Theorem 3.1.5. *For all $C_A\in\mathbb{R}$ and $n\in\mathbb{N}$ there exists $\hat{\lambda}\in\mathbb{R}$ and $\hat{\epsilon}>0$ such that for all $\lambda\geq\hat{\lambda}$, all $A_R\in Gl_d(\mathbb{R})$ and all $\tau_R\in R^d$ such that $F(A_R)\leq\hat{\epsilon}$ the* *following holds. There exists $B \in Gl_d(\mathbb{Z})$ and $t \in \mathbb{Z}^d$ such that*

$$\begin{aligned}\hat{h}_\lambda(\chi_{\mathcal{A}_R}, x) =&h_\lambda\left(BA_R + \delta\hat{A}, B\tau_R + BA_R x + t + \delta\hat{\tau}, \chi_{\mathcal{A}_R}, x\right) \quad ,\\ =&F\left(BA_R\right) + \vartheta\det(BA_R) - \vartheta\rho_\lambda\\ &- \frac{1}{2\lambda^2\left\|A_R^{-1}B^{-1}\right\|^2}\frac{C_\varphi d}{C_{\varphi 2}}Tr\left(M_0^T(\nabla^2 W(0))^{-1}M_0\right) \pm O\left(\lambda^{-4}\right) \quad ,\end{aligned} \tag{3.1.51}$$

where

$$\begin{aligned}\delta\hat{A} =& -\frac{1}{\lambda^2\left\|A_R^{-1}B^{-1}\right\|^2}\frac{C_\varphi d}{C_{\varphi 2}}(c_\Theta^0)^{-1}M_0 + O(\lambda^{-3}) \quad ,\\ |\delta\hat{\tau}| \le& O(\lambda^{-n}) \quad .\end{aligned} \tag{3.1.52}$$

Proof. Because of the translation invariance 2.1.3 we can assume w.o.l.o.g $x = 0$. We estimate

$$\hat{h}_\lambda\left(\chi_{\mathcal{A}_R}, 0\right) = \inf_{\mathcal{A}}\left\{h_\lambda\left(\mathcal{A}, \chi_{\mathcal{A}_R}, 0\right)\right\} \le h_\lambda\left(BA_R, B\tau_R - t, \chi_{\mathcal{A}_R}, 0\right) = F(BA_R) \quad . \tag{3.1.53}$$

Hence, for $F(A_R)$ small enough and λ large enough we can use Theorem 2.4.3 and get that 0 is regular with $\mathcal{A}$

$$\begin{aligned}C_A =&2\sqrt{d}\left(2\left|E\right|\right)^{d-1}\det E^{-1} \quad ,\\ \epsilon_\rho =&2\det E^{-1}\max\left\{\left(\mu_1 - \vartheta\right)^{-1}, \vartheta^{-1}\right\}F(BA_R) + \frac{\mu_1^2}{4C_\phi^W\left(\mu_1 - \vartheta\right)\lambda^2} \quad ,\\ \epsilon_J =&4\frac{\mu_1}{\mu_1 - \vartheta}\det E^{-1}F(BA_R) + \frac{\vartheta\mu_1^2}{2\left(\mu_1 - \vartheta\right)C_\phi^W\lambda^2} \quad .\end{aligned} \tag{3.1.54}$$

Furthermore, according to Lemma 2.1.2 $|\det A_R - \rho_\lambda(\chi_{\mathcal{A}_R})| \le O(\lambda^{-m})$. By Lemma 2.2.1 we have

$$\epsilon_J\rho \ge \frac{C_0^W}{C_\varphi\lambda^d}\sum_{x_i\in\chi}\mathrm{dist}^2(x_i, \chi_{\mathcal{A}})\varphi\left(\lambda^{-1}\left|x_i\right|\right) \quad . \tag{3.1.55}$$

The conditions of Lemma 2.3.4 are fulfilled for small enough $F(A_R)$ and large enough λ. Therefore, there has to exists $B \in Gl_d(\mathbb{Z})$ and $t \in Z^d$ with

$$\begin{aligned}\left\|1 - A^{-1}BA_R\right\| <& \left(\frac{C_0^W C_{\varphi 2}}{dC_\varphi}\det A_R - 8C_0^W(\det A_R - \rho)\right)^{-\frac{1}{2}}\frac{\sqrt{J_\lambda}}{\lambda} \quad ,\\ \left\|B\tau_R - \tau + t\right\| <&\left\|A\right\|\left(C_0^W(2\rho - \det A_R)\right)^{-\frac{1}{2}}\sqrt{J_\lambda} \quad .\end{aligned} \tag{3.1.56}$$

For small enough $F(A_R)$ it holds

$$\begin{aligned}\|\delta A\| =&\|A - BA_R\| \leq \|A\|\|1 - A^{-1}BA_R \\ \leq&\| \leq s_o^{-1}\left(\frac{C_0^W C_{\varphi 2}}{dC_\varphi}\det A_R - 8C_0^W(\det A_R - \rho)\right)^{-\frac{1}{2}}\frac{\sqrt{J_\lambda}}{\lambda} \\ \leq&\frac{\Theta_W}{3\lambda} \quad ,\end{aligned} \tag{3.1.57}$$

and for $\delta\tau$

$$\begin{aligned}|\delta\tau| =& |\tau - B\tau_R - t| \\ \leq& s_0^{-1}\left(C_0^W(2\rho - \det A_R)\right)^{-\frac{1}{2}}\sqrt{\epsilon_J \rho} \\ \leq&\frac{\Theta_W}{3} \quad .\end{aligned} \tag{3.1.58}$$

The minimizer fulfills the conditions of Lemma 3.1.4 and one of the local minimizers described in this corollary has to be the global minimizer. □

Remark: This theorem implies that there exists $B \in Gl_d(\mathbb{Z})$ such that

$$F_\lambda(G,z) \leq F\left(BG^{-1}\right) - \frac{1}{2\lambda^2\left\|GB^{-1}\right\|^2}\frac{C_\varphi d}{C_{\varphi 2}}Tr\left(M_0^T(\nabla^2 W(0))^{-1}M_0\right) \pm O\left(\lambda^{-4}\right) \quad , \tag{3.1.59}$$

where

$$M_0 := (\partial_A F)\left(BG^{-1}\right) + \vartheta(\partial_A \det)(BG^{-1}) \quad . \tag{3.1.60}$$

This estimate is independent of z. Hence, the same estimate holds for $F_\lambda(G)$. In particular for the effective elastic potential holds

$$F_\lambda(G) = \min\left\{F(BG^{-1})|B \in Gl_d(\mathbb{Z})\right\} + O(\lambda^{-2}) \quad . \tag{3.1.61}$$

Corollary 3.1.6. *If the atom configuration is an Bravais lattice $\chi_{\mathcal{A}_R}$, all conditions of Lemma 3.1.4 are fulfilled and additionally W is locally quadratic, then the local minimizers defined in Lemma 3.1.4 fulfills*

$$\delta\hat{\tau}_B = \delta\hat{A}\left(x - \bar{x}\right) \quad , \tag{3.1.62}$$

where $\bar{x}$ is the center of mass of the atom distribution weighted with $\varphi\left(\frac{|x_i - x|}{\lambda}\right)$.

$$\bar{x} = \frac{1}{C_\varphi \lambda^d}\sum_i x_i \varphi\left(\frac{|x_i - x|}{\lambda}\right) \quad . \tag{3.1.63}$$

Proof. We consider a local minimizing $\delta\tau$. Since, $\delta\tau$ is local minimizing the derivative in $\delta\tau$ direction is zero and since J_λ is the only term where $\delta\tau$ appears. Hence, we get

$$\begin{aligned}0 =&\partial_{\delta\tau} J_\lambda\left(x, \delta\mathcal{A}, \chi_{\mathcal{A}_R}\right)\\ =&\frac{\left\|(BA_R + \delta A)^{-1}\right\|^2}{C_\varphi \lambda^d} \sum_i \nabla W(\delta A\left(x_i - x\right) + \delta\tau)\varphi\left(\frac{|x_i - x|}{\lambda}\right) \quad , \qquad (3.1.64)\end{aligned}$$

which simplifies to

$$0 = \sum_i \nabla W(\delta A\left(x_i - x\right) + \delta\tau)\varphi\left(\frac{|x_i - x|}{\lambda}\right) \quad . \qquad (3.1.65)$$

Since, we consider W to be locally quadratic around $\mathbb{Z}^d$, we have

$$\begin{aligned}0 &= \sum_i \nabla^2 W(0)(\delta A\left(x_i - x\right) + \delta\tau)\varphi\left(\frac{|x_i - x|}{\lambda}\right) \quad ,\\ 0 &= \sum_i (\delta A\left(x_i - x\right) + \delta\tau)\varphi\left(\frac{|x_i - x|}{\lambda}\right) \quad . \qquad (3.1.66)\end{aligned}$$

Solving this with respect to $\delta\tau$ we obtain

$$\delta\tau = -\delta A \frac{\sum_i \left(x_i - x\right)\varphi\left(\frac{|x_i - x|}{\lambda}\right)}{\sum_i \varphi\left(\frac{|x_i - x|}{\lambda}\right)} \quad . \qquad (3.1.67)$$

□

Remark 3.1.7. We note that all our estimates are independent of x. However the pre-energy density itself depends on x. Furthermore, we have estimate 3.1.13 that shows that δA will scale with λ^{-2}, but only an estimate that $\delta\tau$ has to scale less than λ^{-m}. This means that it still could be zero. This would be very nice because it would make further calculations much easier. Unfortunately this is generally not the case. We will address this question in the following .

Why consider $\delta\tau \neq 0$? We will explain why it is a rare event that $\delta\tau = 0$. Since we have not introduced any probability measure, rare event is meant purely heuristically, in the sense only for special positions or special parameter values. We have calculated in Lemma 3.1.6 that $\delta\tau = 0$ is connected to the distance between the center of mass and x. It is a rare event that the center of mass of the atom configuration equals x. This can be best seen, if we consider a configuration where the x is no special symmetry point. Then, there exists an atom that has a distance to x that no other atoms has. If we change φ of this special distance we move the center of mass only very little but we move it. Therefore, only at one special weight the center of mass can equal x. Hence, for generic φ and x we can not expect this to happen automatically. Additionally, we see that $\delta\tau$ generally will depends on x. Of course, this proofs nothing for W not quadratic. But, we can not expect that higher orders will solve the problem automatically.

Why consider the x-dependence of h_λ for one local minimizer In Lemma 3.1.4 we have calculated the existence of local minimizers. Furthermore we have proven that the local minimizers are differentially functions of x. For this we will get

$$\frac{d}{dx}h_\lambda(\delta\mathcal{A}_{min}(x),\chi_{\mathcal{A}_R},x)=\partial_x h_\lambda(\delta\mathcal{A}_{min}(x),\chi_{\mathcal{A}_R},x)+\partial_{\delta\mathcal{A}}h_\lambda(\delta\mathcal{A}_{min}(x),\chi_{\mathcal{A}_R},x)\frac{d\delta\mathcal{A}}{dx}. \tag{3.1.68}$$

Since for local minimizers holds $\partial_{\delta\mathcal{A}}h_\lambda(\delta\mathcal{A}_{min}(x),\chi_{\mathcal{A}_R},x))=0$, we have

$$\begin{aligned}&\frac{d}{dx}h_\lambda(\delta\mathcal{A}_{min}(x),\chi_{\mathcal{A}_R},x)\\ =&\partial_x h_\lambda(\delta\mathcal{A}_{min}(x),\chi_{\mathcal{A}_R},x)\\ =&\frac{\|(BA_R+\delta A)^{-1}\|^2}{C_\varphi\lambda^d}\sum_i \nabla W\left(\delta A\left(x_i-x\right)+\delta\tau\right)\delta A\varphi\left(\frac{|x_i-x|}{\lambda}\right)\\ &+\frac{1}{C_\varphi\lambda^d}\sum_i\left(\left\|(BA_R+\delta A)^{-1}\right\|^2 W\left(\delta A\left(x_i-x\right)+\delta\tau\right)-\vartheta\frac{1}{\lambda}\nabla\tilde{\varphi}\left(\frac{x_i-x}{\lambda}\right)\right)\quad .\end{aligned} \tag{3.1.69}$$

The minimizer fulfills

$$\begin{aligned}0=&\partial_{\delta\tau}h_\lambda(\delta\mathcal{A}_{min}(x),\chi_{\mathcal{A}_R},x)\\ =&\frac{\|(BA_R+\delta A)^{-1}\|^2}{C_\varphi\lambda^d}\sum_i \nabla W\left(\delta A\left(x_i-x\right)+\delta\tau\right)\varphi\left(\frac{|x_i-x|}{\lambda}\right)\quad .\end{aligned} \tag{3.1.70}$$

Hence, equation (3.1.69) implies

$$\frac{d}{dx}h_\lambda\frac{1}{C_\varphi\lambda^d}\sum_i\left(\left\|(BA_R+\delta A)^{-1}\right\|^2 W\left(\delta A\left(x_i-x\right)+\delta\tau\right)-\vartheta\right)\frac{1}{\lambda}\nabla\tilde{\varphi}\left(\frac{x_i-x}{\lambda}\right)\quad . \tag{3.1.71}$$

Again for some generic x find an atom, that has a distance to x that no other atom has to. If we deform φ in a way that change $\varphi'(y)$ but not the φ' of any other atom we automatically change $\frac{d}{dx}h_\lambda(\delta\mathcal{A}_{min}(x),\chi_{\mathcal{A}_R},x)$. Hence, the local minimizer can not be expected to be constant. One might hope that $\delta\mathcal{A}_{min}$ could change accordingly to keep the local minimum constant. But $\delta\mathcal{A}_{min}$ is uniquely defined by

$$
\begin{aligned}
0 =&\partial_{\delta\mathcal{A}} h_\lambda(\delta\mathcal{A}_{min}(x), \chi_{\mathcal{A}_R}, x)\mathcal{M} \\
=&\frac{\left\|(BA_R+\delta A)^{-1}\right\|^2}{C_\varphi \lambda^d} \sum_i \nabla W\left(\delta A\left(x_i-x\right)+\delta\tau\right)\left(M\left(x_i-x\right)+\mu\right)\varphi \\
&+\frac{\partial_{\delta\mathcal{A}}\left\|(BA_R+\delta A)^{-1}\right\|^2}{C_\varphi \lambda^d} \sum_i W\left(\delta A\left(x_i-x\right)+\delta\tau\right)\varphi \\
&+\left(\partial_A F\right)\left(BA_R+\delta A\right) M+\vartheta\left(\partial_A \det\right)\left(BA_R+\delta A\right) M \quad .
\end{aligned} \tag{3.1.72}
$$

In this equation only φ enters but not φ'. Since we can deform φ in a way that $\varphi'(y)$ changes but not $\varphi(y)$, the change of $\delta\mathcal{A}$ can not compensate the change of $\varphi'(y)$. These small fluctuations tend to make calculations complicated, since they are existing already in the most regular configurations. They causes an error depending on λ. For sufficiently large system size L. The integral over this small errors can still lead to a big error in the energy.

Since we have found out that in case that the configuration is a Bravais lattice the energy density and the minimizer $\hat{\mathcal{A}}$ are still dependent on x. We study the symmetries of this the minimizers and minima of $h_\lambda(\cdot, \chi, x)$. The minimizing $\hat{A}$ and $\hat{\tau}$ have the periodicity of the lattice. Additionally $\hat{A}$ is symmetric to each lattice point. And τ is antisymmetric to each lattice point.

Lemma 3.1.8. *Let $A_R \in Gl_d(\mathbb{R})$ and $\tau_R \in \mathbb{R}^d$ If the configuration is the Bravais lattice, then it holds*

$$\chi_{\mathcal{A}_R} = A_R\left(\mathbb{Z}^d - \tau_R\right) \tag{3.1.73}$$

Then it holds

1) Periodicity: For all positions $x \in \mathbb{R}^d$ and all $\mathbf{j} \in Z^d$, it holds

$$
\begin{aligned}
\min_{\mathcal{A}\in Gl_d(\mathbb{R})\times\mathbb{R}^d} h_\lambda(\mathcal{A}, \chi_{\mathcal{A}_R}, x) &= \min_{\mathcal{A}\in (Gl_d(\mathbb{R}),\mathbb{R}^d)} h_\lambda(\mathcal{A}, \chi_{\mathcal{A}_R}, x + A_R^{-1}\mathbf{j}) \\
\arg\min_{\mathcal{A}\in Gl_d(\mathbb{R})\times\mathbb{R}^d} h_\lambda(\mathcal{A}, \chi_{\mathcal{A}_R}, x) &= \arg\min_{\mathcal{A}\in Gl_d(\mathbb{R})\times\mathbb{R}^d} h_\lambda(\mathcal{A}, \chi_{\mathcal{A}_R}, x + A_R^{-1}\mathbf{j})
\end{aligned} \tag{3.1.74}
$$

2) Point Symmetry for any lattice point: For all positions $x \in \mathbb{R}^d$ and all lattice points $x_j \in \chi_{\mathcal{A}_R}$ it holds

$$\min_{\mathcal{A}\in Gl_d(\mathbb{R})\times\mathbb{R}^d} h_\lambda(\mathcal{A}, \chi_{\mathcal{A}_R}, x_j + x) = \min_{\mathcal{A}\in Gl_d(\mathbb{R})\times\mathbb{R}^d} h_\lambda(\mathcal{A}, \chi_{\mathcal{A}_R}, x_j - x) \tag{3.1.75}$$

Furthermore the minimizer satisfies

$$
\begin{aligned}
&\left(\hat{A}, \hat{\tau}\right) \in \arg\min_{\mathcal{A}\in Gl_d(\mathbb{R})\times\mathbb{R}^d} h_\lambda(\mathcal{A}, \chi_{\mathcal{A}_R}, x_j + x) \\
\Leftrightarrow &\left(\hat{A}, -\hat{\tau}\right) \in \arg\min_{\mathcal{A}\in Gl_d(\mathbb{R})\times\mathbb{R}^d} h_\lambda(\mathcal{A}, \chi_{\mathcal{A}_R}, x_j - x) \quad .
\end{aligned} \tag{3.1.76}
$$

3) For positions $x \in \chi_{\mathcal{A}_R}$ and all $z \in Z^d$ the unique local minimizer with $|\tau - z| \leq \frac{\Theta_W}{3}$ fulfills $\tau = z$

Proof. Because of the frame indifference of the model (see Lemma 2.1.3) we can set $\tau_R = 0$ without lose of generality

1) Periodicity: For all $\mathbf{j} \in \mathbb{Z}^d$ we calculate

$$\begin{aligned}
&c_\varphi \lambda^d \left\|A^{-1}\right\|^{-2} J_\lambda \left(\mathcal{A}, \chi_{\mathcal{A}_R}, x\right) \\
=&\sum_{\mathbf{i} \in \mathbb{Z}^d} W\left(A\left(A_R^{-1}\mathbf{i} - x\right) - \tau\right) \varphi\left(\lambda^{-1}\left|-A_R^{-1}\mathbf{i} + x\right|\right) \\
=&\sum_{\mathbf{i} \in \mathbb{Z}^d} W\left(A\left(A_R^{-1}\left(\mathbf{i}+\mathbf{j}\right) - x - A_R^{-1}\mathbf{j}\right)\right) - \tau\right) \varphi\left(\lambda^{-1}\left|A_R^{-1}\left(\mathbf{i}+\mathbf{j}\right) - x - A_R^{-1}\mathbf{j}\right|\right) \\
=&\sum_{\mathbf{k} \in \mathbb{Z}^d} W\left(A\left(A_R^{-1}\mathbf{k} - (x + A_R^{-1}\mathbf{j})\right) - \tau\right) \varphi\left(\lambda^{-1}\left|A_R^{-1}\left(\mathbf{k} - (x - G\mathbf{j})\right)\right|\right) \\
=&c_\varphi \lambda^d \left|A^{-1}\right|^{-2} J_\lambda \left(\mathcal{A}, A_R^{-1}\mathbb{Z}^d, x + A_R^{-1}\mathbf{j}\right) \quad . \qquad (3.1.77)
\end{aligned}$$

We have the same J_λ for both points with the same $\mathcal{A}$. ρ_λ can be treated the same way and $F(A)$ and $\det A$ are not changed. Therefore, we get

$$h_\lambda \left(\mathcal{A}, \chi_{\mathcal{A}_R}, x\right) = h_\lambda \left(\mathcal{A}, \chi_{\mathcal{A}_R}, x + G\mathbf{j}\right) \quad . \qquad (3.1.78)$$

Since this holds for every A and τ, we can also get the minimizer at one position from the minimizer at the other and they give the same energy.

2) Point symmetry: For all $A \in Gl_d(\mathbb{R}), \tau \in \mathbb{R}^d$ we have

$$c_\varphi \lambda^d J_\lambda \left(\mathcal{A}, \chi_{\mathcal{A}_R}, x\right) = \left\|A^{-1}\right\|^2 \sum_{\mathbf{i}} W(A\left(x_{\mathbf{i}} - x\right) + \tau) \varphi\left(\lambda^{-1}\left|x_{\mathbf{i}}\right|\right) \quad . \qquad (3.1.79)$$

We use the symmetry $W(-X) = W(X)$

$$\begin{aligned}
&c_\varphi \lambda^d J_\lambda \left(\mathcal{A}, \chi_{\mathcal{A}_R}, x\right) \\
=&\left\|A^{-1}\right\|^2 \sum_{\mathbf{i} \in \mathbb{Z}^d} W\left(-A\left(A_R^{-1}\mathbf{i} - x\right) - \tau\right) \varphi\left(\lambda^{-1}\left|-A_R^{-1}\mathbf{i} + x\right|\right) \\
=&\left\|A^{-1}\right\|^2 \sum_{\mathbf{i} \in \mathbb{Z}^d} W\left(A\left(-A_R^{-1}\mathbf{i} - (-x)\right) - \tau\right) \varphi\left(\lambda^{-1}\left|A_R^{-1}\mathbf{i} - (-x)\right|\right) \\
=&\left\|A^{-1}\right\|^2 \sum_{-\mathbf{k} \in \mathbb{Z}^d} W\left(A\left(A_R^{-1}\mathbf{k} - (-x)\right) - \tau\right) \varphi\left(\lambda^{-1}\left|A_R^{-1}\left(\mathbf{k} - (-x)\right)\right|\right) \\
=&c_\varphi \lambda^d J_\lambda \left(A, -\tau, A_R^{-1}\mathbb{Z}^d, -x\right) \quad . \qquad (3.1.80)
\end{aligned}$$

Since the change of τ only influences J_λ we can conclude

$$h_\lambda \left(\mathcal{A}, G\mathbb{Z}^d, x\right) = h_\lambda \left(\mathcal{A}, A_R^{-1}\mathbb{Z}^d, -x\right) \quad . \qquad (3.1.81)$$

Now we apply the periodicity case to get

$$h_\lambda\left(\mathcal{A}, A_R^{-1}\mathbb{Z}^d, x + A_R^{-1}\mathbf{j}\right) = h_\lambda\left(\mathcal{A}, A_R^{-1}\mathbb{Z}^d, -x + A_R^{-1}\mathbf{j}\right) \quad . \tag{3.1.82}$$

3) Lemma 3.1.4) says that there is an unique local minimizer around zero . The point symmetry say that $+\tau$ and $-\tau$ has the same energy. Which implies for the unique local minimizer $\tau = -\tau$ and therefore $\tau = 0$. Hence, if one is the minimizer the other has to be the minimizer too. Therefore, it holds $\tau = 0$. If we combine this with the periodicity of the local minimizers, we get the conclusion

□

In the next lemma we will summarize the symmetries of the effective elastic potentials. These are mostly direct consequences of the general symmetries of the model described in Lemma 2.1.3 and the symmetries of the minimizers described in Lemma 3.1.8.

Lemma 3.1.9. *The effective elastic energy density has the following symmetries:*

1) The effective elastic potential is invariant under reparametrisation: For all $G \in Gl_d(\mathbb{R})$, $z \in \mathbb{R}^d$, $B \in Gl_d(\mathbb{Z})$ and $t \in \mathbb{Z}^d$ it holds

$$\begin{aligned} F_\lambda(G,z) =& F_\lambda(GB, B^{-1}z + t) \quad , \\ F_\lambda(G) =& F_\lambda(GB) \quad . \end{aligned} \tag{3.1.83}$$

2) The effective elastic potential is frame indifferent: For all $G \in Gl_d(\mathbb{R})$, $z \in \mathbb{R}^d$ and $R \in SO_d(\mathbb{R})$ it holds

$$\begin{aligned} F_\lambda(G,z) =& F_\lambda(RG, z) \quad , \\ F_\lambda(G) =& F_\lambda(RG) \quad . \end{aligned} \tag{3.1.84}$$

3) The local effective elastic potential is point symmetric to 0: For all $G \in Gl_d(\mathbb{R})$ and$z \in \mathbb{R}^d$ we have

$$F_\lambda(G,z) = F_\lambda\left(G, -z\right) \quad . \tag{3.1.85}$$

4) The effective elastic energy function has the full symmetry group of $\chi_{G^{-1}}e,g$ for all $G \in Gl_d(\mathbb{R})$ and$z \in \mathbb{R}^d$ it holds, if $R \in SO_d(\mathbb{R})$ and $B \in \mathrm{GL_d}(\mathbb{Z})$ satisfy $\tilde{R}G = GB$, then we have

$$F_\lambda(G,z) = F_\lambda(G, B^{-1}z) \quad . \tag{3.1.86}$$

Proof. 1) Invariance under reparametrisation:

$$\begin{aligned}F_\lambda(G,z) =&\hat{h}_\lambda\left(G\left(\mathbb{Z}^d - z\right),0\right)\\ =&\hat{h}_\lambda\left(G\left(B\left(\mathbb{Z}^d - t\right) - BB^{-1}z\right),0\right)\\ =&\hat{h}_\lambda\left((GB)\left(\mathbb{Z}^d - \left(B^{-1}z+t\right)\right),0\right)\\ =&F_\lambda(GB, B^{-1}z+t) \quad .\end{aligned} \tag{3.1.87}$$

Furthermore by a coordinate change $z = By$ we get

$$\begin{aligned}F_\lambda(G) =& \int_{[0,1]^d} F_\lambda(G,z)dz\\ =& \int_{[0,1]^d} F_\lambda(GB, B^{-1}z)dz\\ =& \int_{B[0,1]^d} F_\lambda(GB,y)\det B dy \quad .\end{aligned} \tag{3.1.88}$$

Since the determinant of B is one, we consider $F_\lambda(GB,y) = F_\lambda(GB,y+t)$ for $t \in \mathbb{Z}^d$. For every $y \in B[0,1]^d$ there exists a $\tilde{z} \in [0,1]^d$ and a $t \in \mathbb{Z}^d$ such that $y + t = \tilde{z}$. Furthermore, if there are two $y_1, y_2 \in B[0,1]^d$ with $t_1, t_2 \in \mathbb{Z}^d$ and $y_1 + t_1 = x = y_2 + t_2$, then we have

$$B^{-1}\left(y_1 - y_2\right) = B^{-1}\left(t_1 - t_2\right) \in \mathbb{Z}^d \quad . \tag{3.1.89}$$

Therefore, this can happen only on the boundary of $B^{-1}[0,1]^d$. Since the volume of $B[0,1]^d$ is given by $\det B = 1$ we have

$$F_\lambda(G) = \int_{B[0,1]^d} F_\lambda(GB,y)dy = \int_{[0,1]^d} F_\lambda(GB,y)dy = F_\lambda(G) \quad . \tag{3.1.90}$$

2) The point symmetry is the direct consequence of the point symmetry of the local minimizers (see 3.1.8)

3) The frame indifference follows from the frame indifference of the model (see 2.1.3) and the calculation:

$$\begin{aligned}F_\lambda(G,z) =&\hat{h}_\lambda\left(G\left(\mathbb{Z}^d - z\right),0\right)\\ =&\hat{h}_\lambda\left(RG\left(\mathbb{Z}^d - z\right),R0\right)\\ =&F_\lambda(RG,z) \quad .\end{aligned} \tag{3.1.91}$$

If this linear equation holds for every z, it holds also for the average over one unit cell. Therefore, we have the corresponding equation for the average effective elastic potential.

4) Rotation group: For every $A \in Gl_d(\mathbb{R}), \tau \in \mathbb{R}^d$ we have

$$
\begin{aligned}
& c_\varphi \lambda^d J_\lambda\left(A, \tau, G\left(\mathbb{Z}^d - z\right), 0\right) \\
=& \left\|A^{-1}\right\|^2 \sum_{\mathbf{i} \in \mathbb{Z}^d} W(AG(\mathbf{i} - z) + \tau) \varphi\left(\lambda^{-1}\left|G(\mathbf{i} - z)\right|\right) \\
=& \left\|A^{-1}\right\|^2 \sum_{i \in \mathbb{Z}^d} W(AGBB^{-1}(\mathbf{i} - z) + \tau) \varphi\left(\lambda^{-1}\left|GBB^{-1}(\mathbf{i} - z)\right|\right) \\
=& \left\|A^{-1}\right\|^2 \sum_{i \in \mathbb{Z}^d} W(ARG\left(B^{-1}\mathbf{i} - B^{-1}z\right) + \tau) \varphi\left(\lambda^{-1}\left|RG\left(B^{-1}\mathbf{i} - B^{-1}z\right)\right|\right) \\
=& \left\|A^{-1}R^{-1}\right\|^2 \sum_{j \in \mathbb{Z}^d} W(ARG\left(\mathbf{j} - B^{-1}z\right) + \tau) \varphi\left(\lambda^{-1}\left|RG\left(\mathbf{J} - B^{-1}z\right)\right|\right) \\
=& c_\varphi \lambda^d J_\lambda\left(AR, \tau, G\left(\mathbb{Z}^d - B^{-1}z\right), 0\right) \quad .
\end{aligned} \tag{3.1.92}
$$

We can apply the same calculation to ρ. Furthermore $\det A = \det(AR)$ and $F(AR) = F(A)$ Hence, we get

$$
\begin{aligned}
F_\lambda(G, z) =& \inf_{A,\tau} h_\lambda(A, \tau, G\left(\mathbb{Z}^d - z\right), x) \\
=& \inf_{A,\tau} h_\lambda(A\tilde{R}^{-1}, \tau, \tilde{R}^{-1}\mathbb{Z}, \tilde{R}x) = F_\lambda(G, B^{-1}z) \quad .
\end{aligned} \tag{3.1.93}
$$

□

Finally, we remember the effective particle potential defined in 2.2.8. Since we have found out so much about the minimizing $\hat{\mathcal{A}}$ we can use this knowledge to calculate the effective particle potential in this specific case. If we use the symmetries of the minimizers we can proof that $\hat{\mathcal{A}}$ can be chosen such that the minima of the effective particle potential are exactly the lattice position. Furthermore the the effective particle potential is locally quadratic in the neighborhood of these minima.

Lemma 3.1.10. *There exists $\hat{\lambda} \in \mathbb{R}$ and $\hat{\epsilon} > 0$ such that for all $\lambda \geq \hat{\lambda}$, $A_R \in Gl_d(\mathbb{R})$ such that $F(A_R) \leq \hat{\epsilon}$ and all $\tau_R \in R^d$ it holds: For the configuration $\chi_{\mathcal{A}_R} = A_R^{-1}\left(\mathbb{Z}^d - z\right)$ there is a effective particle potential as defined in 2.2.8 such that for $\tilde{y} = A_R^{-1}(\mathbf{j} - z) + \delta y$ with $|\delta y| \leq |A_R|^{-1}\Theta_W$ we have*

$$
\frac{1}{2} C_\Theta^0 |\delta y|^2 \leq V_{\mathcal{A}}(\tilde{y}) \leq \frac{9}{8}|C_A|^2|E|^2|\delta y|^2 \quad . \tag{3.1.94}
$$

Proof.

$$
\begin{aligned}
\nabla V_{\mathcal{A}}(y) =& \int_{B_{2\lambda}(\Omega)} \frac{\left\|A^{-1}(x)\right\|^2}{C_\varphi \lambda^d} \nabla W(A(x)(y - x) + \tau(x)) A(x) \varphi\left(\lambda^{-1}|y - x|\right) \\
&+ \int_{B_{2\lambda}(\Omega)} \frac{\left\|A^{-1}(x)\right\|^2}{C_\varphi \lambda^d} W(A(x)(y - x) + \tau(x)) A(x) \nabla\tilde{\varphi}\left(\lambda^{-1}(y - x)\right) \lambda^{-1}.
\end{aligned} \tag{3.1.95}
$$

We know from Lemma 3.1.8 that $A(x)$ can be chosen symmetric to $y = A_R^{-1}(\mathbf{j} - \tau_R)$ and $\tau(x)$ can be chosen antisymmetric to $y = A_R^{-1}\mathbf{j}$. Since W and φ are symmetric, ∇W and $\nabla\tilde{\varphi}$ are antisymmetric. Hence, $\nabla V_{\mathcal{A}}(A_R^{-1}\mathbf{j})$ is an odd function integrated over an even domain and is exactly zero as a result. The second derivative of the effective particle potential tested with $\mu \in \mathbb{R}^d$ satisfies

$$\begin{aligned}\nabla^2 V_{\mathcal{A}}(y)[\mu] =& \int_{B_{2\lambda}(\Omega)} \frac{\|A^{-1}(x)\|^2}{C_\varphi \lambda^d} \nabla^2 W[A(x)\mu]\varphi \\ &+ 2\int_{B_{2\lambda}(\Omega)} \frac{\|A^{-1}(x)\|^2}{\lambda C_\varphi \lambda^d} \langle \nabla W, A(x)\mu\rangle \langle \nabla\tilde{\varphi}, \mu\rangle \\ &+ \int_{B_{2\lambda}(\Omega)} \frac{\|A^{-1}(x)\|^2}{\lambda^2 C_\varphi \lambda^d} W\nabla^2\tilde{\varphi}[\mu]. \end{aligned} \tag{3.1.96}$$

The second line of (3.1.96) is $O(\lambda^{-1})$ and the third line is $O(\lambda^{-2})$. Hence, the dominating contribution comes from the first line.Furthermore with Lemma 3.1.8 we can calculate

$$\begin{aligned}A(x)\,(y-x) + \tau(x) =& \left(BA_R + \delta A(x)\right)(y-x) + B\tau_R + BA_R x + t + \delta\tau(x) \\ =& \delta A(x)\,(y-x) + \delta\tau(x) + B\tau_R + BA_R y + t \quad . \end{aligned} \tag{3.1.97}$$

Using $\tilde{y} = A_R^{-1}(\mathbf{j} - \tau_R) + \delta y$, the periodicity of W, $\delta A = O(\lambda^{-2})$ and $|\delta\tau| \leq O(\lambda^{-2})$ we get

$$\nabla^2 W(A(x)\,(\tilde{y}-x) + \tau(x)) = \nabla^2 W(BA_R\delta y + O(\lambda^{-1})) \quad . \tag{3.1.98}$$

For $|\delta y| \leq |A_R|^{-1}\Theta_W$ the argument is in the local convex part of W. Hence, we get an upper bound

$$\begin{aligned}\nabla^2 V_{\mathcal{A}}(y)[\mu] \leq& \int_{B_{2\lambda}(\Omega)} \frac{\|A^{-1}(x)\|^2}{C_\varphi \lambda^d} C_\Theta^1 |A(x)|^2 \varphi\left(\lambda^{-1}|y-x|\right) \\ \leq& \frac{9}{4}|C_A|^2|E|^2|\mu|^2 + O(\lambda^{-1}) \quad , \end{aligned} \tag{3.1.99}$$

and a lower bound

$$\begin{aligned}\mu\nabla^2 V_{\mathcal{A}}(y)\mu \geq& \int_{B_{2\lambda}(\Omega)} \frac{\|A^{-1}(x)\|^2}{C_\varphi \lambda^d} C_\Theta^0 |A^{-1}(x)|^{-2} \varphi\left(\lambda^{-1}|y-x|\right) \\ \geq& C_\Theta^0|\mu|^2 \quad . \end{aligned} \tag{3.1.100}$$

Hence, the stationary points at the lattice positions are minima and the potential is quadratic in a neighborhood around them. □

3.2 Perturbation of a lattice

In this section we will derive a method to calculate upper bounds for the energy costs of a deformation of a lattice in our model. The aim is to get an upper bound that is precise that we can calculate an upper bound for the energy density of a pair of dislocations in an arbitrary large crystal. Hence, the estimate needs to be very precise in all areas that are far away from the dislocations. Otherwise small errors there integrated over the volume of the crystal will give an error larger than the energy barrier itself. Since we do not know the energy of the lattice itself exact prevent this. We need to estimate the energy of the configuration by comparing it with the energy of the lattice. We assume that our configuration has the for $\psi(\mathbb{Z}^d)$. We will estimate the energy density of the configuration in the point $\psi(z)$ with the local effective elastic potential $F_\lambda(\nabla\psi(z), z)$. This is a the energy of a Bravais lattice. Hence, the first step is to calculate how the energy density changes if we deform a Bravais lattice $\chi_{\mathcal{A}_R}$ add a perturbation to the lattice around this one point(Lemma 3.2.1). Up to some error terms we obtain

$$\begin{aligned}&h_\lambda(\mathcal{A}, A_R^{-1}(\mathbb{Z}), x)\\ \leq &h_\lambda(\mathcal{A}, A_R^{-1}(\mathbb{Z}), x)\\ &+ 2|c_\Theta^1|\lambda^4 \left\|A_R^{-1}B^{-1}\right\|^2 \|BA_R\|^2 |A_R|^4 \det A_R \times \max_{y\in B_{2\lambda}(x)} \{\|\nabla^2 u(A_R y)\|\}^2 \end{aligned} \quad (3.2.1)$$

If we adapt the estimate 3.2.1 to every point of $\psi(z)$ and integrate, we get up to some error terms

$$\begin{aligned}\int_{\psi(\tilde\Omega)} \hat h(\chi, x)dx \leq &\int_{\tilde\Omega} F_\lambda\left(\nabla\psi(z), z\right) \det\nabla\psi(z)dz\\ &+ C_Q|(\nabla\psi(z))^{-1}|^4\lambda^4 \int_{\tilde\Omega} \|\nabla^2\psi(\psi^{-1}(z))\|^2 \det\nabla\psi(z)dz \quad .\end{aligned} \quad (3.2.2)$$

In Lemma 3.2.2 we calculate an estimate for the change of the effective elastic potential. Namely we show that

$$\begin{aligned}F_\lambda(G_1, z)\det(G_1) \leq &F_\lambda(G_0, z)\det(G_0) + (\nabla F)_{loc}\left(G_0, z\right)[G_1 - G_0]\\ &+ \frac{1}{2}(\nabla^2 F)_{loc}\left(G_0, z\right)[G_1 - G_0] + O\left((G_1 - G_0)^3\right) \quad .\end{aligned} \quad (3.2.3)$$

Then we can use this estimate to convert the integral of the local effective elastic potential in an integral of the global effective elastic potential at the cost of some boundary error X_S, more precisely

$$\begin{aligned}\int h_\lambda(\psi(\mathbb{Z}^d), \psi(z))dz \leq &\int F_\lambda(\nabla\psi(z))\det\nabla\psi(z)\\ &+ C_Q|(\nabla\psi(z))^{-1}|^4\lambda^4\|\nabla^2\psi(z)\|^2 dz + X_S v \quad .\end{aligned} \quad (3.2.4)$$

Finally, in Theorem 3.2.3 we estimate the energy difference between a lattice $A_R^{-1}\mathbb{Z}^d$ and a deformed lattice $\psi(\mathbb{Z}^d)$ that have equal atom positions at the boundary, and conclude that

$$\begin{aligned}&\int h_\lambda(\psi(\mathbb{Z}^d),\psi(z))dz-\int h_\lambda(A_R^{-1}\mathbb{Z}^d,A_R^{-1}z)dz\\ \leq&\int(\nabla F)_{av}\left(A_R^{-1}\right)\left[\nabla\psi-A_R^{-1}\right]dz+\int\frac{1}{2}(\nabla^2F)_{av}\left(A_R^{-1}\right)\left[\nabla\psi-A_R^{-1}\right]dz\\ &+C_Q|(\nabla\psi(z))^{-1}|^4\lambda^4\|\nabla^2\psi(z)\|^2dz\quad.\end{aligned}\tag{3.2.5}$$

We also derive an upper bound for a particular configuration, in dimension two consisting of two dislocations, and construct a continuous path that leads from the elastically deformed Bravais lattice to a plastically deformed configuration of lower energy. The energy barrier of this path scales at most like λ^2.

In the first lemma we proof that if we deform a lattice in a neighborhood of the point x with some deformation $|u(z_i)|\leq C(x_i-x)^2$, then the energy will increase by a term that scales like λ^4C^2 up to lower order terms. If u is three times differentiable, some cancellation takes place

Lemma 3.2.1. *For all $C_A>0$ and all $m\in N$ there exists $\hat\lambda\in\mathbb{R}$ such that for all $\lambda>\hat\lambda$ and for all $A_R,\in Gl_d(\mathbb{R})$,$\tau_R\in\mathbb{R}^d$, $B\in Gl_d(\mathbb{R})$ and $t\in\mathbb{Z}^d$ satisfying $\left|BA_R^{-1}\right|<C_A$ and $x\in\Omega$ we have Let $\mathcal{A}\in Gl_d(\mathbb{R})\times\mathbb{R}^d$ be*

$$\mathcal{A}:=\arg\min\left\{h_\lambda(\tilde{\mathcal{A}},A_R^{-1}(\mathbb{Z}),x)\,\middle|\,\tilde{\mathcal{A}}\in Gl_d(\mathbb{R})\times\mathbb{R}^d,\lambda\|\delta A\|\leq\frac{\Theta_W}{3},|\delta\tau|\leq\frac{\Theta_W}{3}\right\}.\tag{3.2.6}$$

where

$$\delta\mathcal{A}=(\delta A,\delta\tau)=(\tilde{A}-BA_R,B\tau_R+BA_Rx+\tilde{t}-\tau)\quad.\tag{3.2.7}$$

Moreover we consider an atom configuration $\chi=\{x_i|i=1...N\}$ defined by

$$x_i:=A_R^{-1}z_i+u(z_i)\quad,\tag{3.2.8}$$

where u has the following properties

1) u is at least 3 times differentiable,

2) $\nabla u(A_Rx)=0$,

3) $\lambda^2|\nabla^2u(A_Rx)|\leq\frac{1}{4}\theta c_6^{-1}(\det A_R)|A_R|^{-2}$,

4) $\lambda^3|\nabla^3u(A_Ry)|\leq\frac{3}{8}\theta c_6^{-1}(\det A_R)|A_R|^{-3}$ for all $y\in B_{2\lambda}(x)$, *where c_6 is as in Lemma 2.2.7, then*

$$\begin{aligned} h_\lambda(\mathcal{A},\chi,x) \leq & h_\lambda(\mathcal{A},A_R^{-1}(\mathbb{Z}),x) \\ & + 2c_\Theta^1\lambda^4 \left\|A_R^{-1}B^{-1}\right\|^2 \|BA_R\|^2|A_R|^4 \max_{B_{2\lambda}(x)}\{\|\nabla^2 u(A_R y)\|\}^2 \det A_R \\ & + 0(\lambda^{-n})\nabla^2 u(A_R x) + O(\lambda^2\nabla^3 u) \quad . \end{aligned} \tag{3.2.9}$$

Proof. We consider the Taylor expansion

$$\begin{aligned} h_\lambda(\mathcal{A},\chi,x) = & h_\lambda(\mathcal{A},A_R^{-1}\mathbb{Z},x) + \frac{d}{ds}h_\lambda(A(s),\tau(s),\chi(s),x)|_{t=0} \\ & + \int_0^1\int_0^s \frac{d}{ds}^2 h_\lambda(\mathcal{A}(v),\chi(v),x)dvds \quad . \end{aligned} \tag{3.2.10}$$

We calculate the first order contribution

$$\begin{aligned} & \frac{d}{ds}h_\lambda(\mathcal{A},\chi(s),x)|_{s=0} \\ = & \sum_i \frac{\partial}{\partial x_i}h_\lambda(\mathcal{A},\chi(s),x)|_{t=0}\frac{dx_i}{ds} \\ = & \frac{\|A^{-1}\|^2}{C_\varphi\lambda^d}\sum_i \langle\nabla W(A\left(x_i(0)-x\right)+\tau), Au(A_R x_i(0))\rangle\,\varphi\left(\lambda^{-1}\left|x_i(0)-x\right|\right) \\ & + \frac{\|A^{-1}\|^2}{C_\varphi\lambda^d}\sum_i \left(W(A\left(x_i(0)-x\right)+\tau)-\vartheta\right)\left\langle\partial_{x_i}\varphi\left(\lambda^{-1}\left|x_i(0)-x\right|\right), u(A_R x_i(0))\right\rangle . \end{aligned} \tag{3.2.11}$$

$\chi(0)$ is a Bravais lattice and $\mathcal{A}_0$ a corresponding local minimizer. Furthermore $\chi(0) = A_R\mathbb{Z}^d = A_R^{-1}B^{-1}\mathbb{Z}^d$ Hence, we relabel $\mathbb{Z}^d$ as follows

$$x_i = A_R^{-1}z_i = A_R^{-1}B^{-1}(Bz_i) = (A_R^{-1}B^{-1})z_j \quad . \tag{3.2.12}$$

With this we can apply Lemma 3.1.3 and get

$$\begin{aligned} W(A\left(x_j(0)-x\right)+\tau) = & W(\delta A\left(x_j(0)-x\right)+\delta\tau) \quad , \\ \nabla W(A\left(x_j(0)-x\right)+\tau) = & \nabla W(\delta A\left(x_j(0)-x\right)+\delta\tau) \quad . \end{aligned} \tag{3.2.13}$$

According to Lemma 3.1.4 $\delta A = O(\lambda^{-2})$ and $\delta\tau(0) \leq O(\lambda^{-m})$ Therefore, it holds

$$\begin{aligned} W(\delta A\left(x_i(0)-x\right)+\delta\tau) = & O(\lambda^{-2}) \quad , \\ \nabla W(\delta A\left(x_i(0)-x\right)+\delta\tau) = & O(\lambda^{-1}) \quad . \end{aligned} \tag{3.2.14}$$

We rewrite equation (3.2.11) as

$$\begin{aligned} \frac{d}{ds}h_\lambda(0) = & \frac{\|A^{-1}\|^2}{C_\varphi\lambda^d}\sum_i \langle\nabla W(\delta A\left(x_i(0)-x\right)+\delta\tau), Au(A_R x_i(0))\rangle\,\varphi \\ & + \frac{\|A^{-1}\|^2}{C_\varphi\lambda^d}\sum_i \left(W\left(\delta A\left(x_i(0)-x\right)+\delta\tau\right)-\vartheta\right)\langle\partial_{x_i}\varphi, u(A_R x_i(0))\rangle \quad . \end{aligned} \tag{3.2.15}$$

A Taylor expansion of $u(x_i)$ gives

$$u(A_R x_i(0)) = \nabla^2 u(A_R x)[A_R x_i(0) - x] + O(\nabla^3 u \lambda^3) \quad . \tag{3.2.16}$$

Hence, there is one contribution with $\nabla^2 u(A_R x)$ and one of higher order. The derivative on φ is $O(\lambda^{-1})$, furthermore $W = O(\lambda^{-2})$ and $\nabla W = O(\lambda^{-1})$. Hence, the higher order contribution in the estimate (3.2.15) is $O(\lambda^2 \nabla^3 u)$. The second order contribution can be bounded form above by $O(\lambda \nabla^2 u)$ with the same argument. However, this estimate can be improved further. We apply Lemma 2.1.2 to estimate the sum with an integral

$$\begin{aligned} \tilde{\delta A} :=& \lambda \delta A \quad , \\ \psi_1(X) :=& \left\langle \nabla W(\lambda \delta A X + \delta\tau), A\nabla^2 u[A_R X] \right\rangle \varphi\left(X\right) \quad , \\ \psi_2(X) :=& \left(W(\delta A y + \delta\tau) - \vartheta\right) \left\langle \nabla\tilde{\varphi}\left(X\right), \nabla^2 u[A_R X] \right\rangle \quad . \end{aligned} \tag{3.2.17}$$

We get

$$\begin{aligned} &\frac{d}{ds} h_\lambda(\mathcal{A}, \chi(s), x)|_{t=0} \\ =&\frac{\left\|A^{-1}(0)\right\|^2 \lambda^2}{C_\varphi} \int_{\mathbb{R}^d} \left\langle \nabla W(\delta A y + \delta\tau), A\nabla^2 u(A_R x)[A_R y] \right\rangle \varphi\left(|y|\right) dy \det A_R \\ &+ \frac{\left\|A^{-1}(0)\right\|^2 \lambda}{C_\varphi} \int_{\mathbb{R}^d} \left(W(\delta A y + \delta\tau) - \vartheta\right) \left\langle \nabla\tilde{\varphi}\left(y\right), \nabla^2 u(A_R x)[A_R y] \right\rangle dy \det A_R \\ &+ O(\lambda^2 \nabla^3 u) + O(\lambda^{-m-1} \nabla^2 u) \quad . \end{aligned} \tag{3.2.18}$$

The contribution of the ϑ-term in equation (3.2.18) is zero because it is the integral of an odd function over an even domain. If $\delta\tau$ would be zero, the same would hold true for the two other integrals in equation (3.2.18). However, thought $\delta\tau$ does not have to be zero, we have $\delta\tau \leq O(\lambda^{-m})$ by Lemma 3.1.4. Next we expand W in orders of $\delta\tau$ [3]

$$\begin{aligned} W(\delta A y + \delta\tau) =& W(\delta A y) + \nabla W(\delta A y) O(\lambda^{-m}) \quad , \\ \nabla W(\delta A y + \delta\tau) =& \nabla W(\delta A y) + \nabla^2 W(\delta A y) O(\lambda^{-m}) \quad . \end{aligned} \tag{3.2.19}$$

Since the integral of an odd function over a even domain is zero, we get

$$\begin{aligned} 0 =& \int_{\mathbb{R}^d} \left\langle \nabla W(\delta A y + \delta\tau), A\nabla^2 u(A_R x)[A_R y] \right\rangle \varphi\left(|y|\right) dy \quad , \\ 0 =& \int_{\mathbb{R}^d} W(\delta A y) \left\langle \nabla\tilde{\varphi}\left(y\right), \nabla^2 u(A_R x)[A_R y] \right\rangle \quad . \end{aligned} \tag{3.2.20}$$

[3]Because of symmetry the third derivative of W is $O(\lambda^{-1})$ near the minimum of W

Hence, we get

$$\begin{aligned}
&\frac{d}{ds}h_\lambda(\mathcal{A},\chi(s),x)|_{t=0}\\
=&\frac{\lambda\left\|A^{-1}\right\|^2}{C_\varphi}\int_{\mathbb{R}^d}\left\langle O(\lambda^{-m}),\nabla^2W(\delta Ay)A\nabla^2u(A_Rx)[A_Ry]\right\rangle dy\varphi\left(\lambda^{-1}\left|y\right|\right)\det A_R\\
&+\frac{\left\|A^{-1}\right\|^2\lambda}{C_\varphi}\int_{\mathbb{R}^d}\left\langle\nabla W(\delta Ay),O(\lambda^{-m}\right\rangle\left\langle\nabla\tilde{\varphi}\left(\lambda^{-1}\left|y\right|\right),\nabla^2u(A_Rx)[A_Ry]\right\rangle dy\det A_R\\
&+O(\lambda^2\nabla^3u)+O(\lambda^{-m-1})\nabla^2u(A_Rx)\\
=&O(\lambda^2\nabla^3u)+O(\lambda^{2-m})\nabla^2u(A_Rx)\quad.
\end{aligned}\tag{3.2.21}$$

The contribution of the second order is

$$\frac{d^2}{ds^2}h_\lambda(\mathcal{A},\chi(s),x)=\sum_i\sum_j\left\langle\frac{dx_i}{ds},\frac{\partial^2}{\partial x_i\partial x_j}h_\lambda\frac{dx_j}{ds}\right)>\quad.\tag{3.2.22}$$

We first calculate $\frac{\partial^2}{\partial x_i\partial x_j}h_\lambda$ omitting the argument of W and φ.

$$\begin{aligned}
C_\varphi\lambda^d\frac{\partial^2}{\partial x_i\partial x_j}h_\lambda=&\frac{\partial}{\partial x_i\partial x_j}J_\lambda-\vartheta\frac{\partial}{\partial x_i\partial x_j}\rho_\lambda\\
=&\left\|A^{-1}\right\|^2A^T\nabla^2WA\varphi\delta_{ij}+\left\|A^{-1}\right\|^2(\nabla WA)\otimes\partial_{x_i}\varphi\delta_{ij}\\
&+\left\|A^{-1}\right\|^2\partial_{x_i}\varphi\otimes(\nabla WA)\delta_{ij}+\left\|A^{-1}\right\|^2(W-\vartheta)\,\partial_{x_i}\partial_{x_j}\varphi\delta_{ij}\quad.
\end{aligned}\tag{3.2.23}$$

Each derivative on φ produces a factor λ^{-1}.

$$C_\varphi\lambda^d\frac{\partial}{\partial x_i\partial x_j}h_\lambda=\left\|A^{-1}\right\|^2A^T\nabla^2WA\varphi\delta_{ij}+O(\lambda^{-1})\quad.\tag{3.2.24}$$

Hence, we get that

$$\frac{d^2}{ds^2}h_\lambda(\mathcal{A},\chi(s),x)=\frac{\left\|A^{-1}\right\|^2}{C_\varphi\lambda^d}\sum_i\nabla^2W(A(x_i(s)-x)+\tau)[Au(A_Rx_i)]\varphi+O(\lambda^{-1}|u|^2)\quad.\tag{3.2.25}$$

Furthermore we have $\left\|A^{-1}\right\|^2=\|A_R^{-1}B^{-1}\|^2+O(\lambda^{-1})$ due to Lemma 3.1.4. Hence, we get

$$\frac{d^2}{ds^2}h_\lambda=\frac{\left\|A_R^{-1}B^{-1}\right\|^2}{C_\varphi\lambda^d}\sum_i\nabla^2W[BA_Ru(A_Rx_i)]\varphi(\lambda^{-1}(x_i(s)-x))+O(\lambda^{-1}|u|^2)\quad.\tag{3.2.26}$$

The changes in the $x_i(s)$ are only $O(1)$. The derivative $\partial_{x_i}\varphi$ is $O(\lambda^{-1})$. Hence, we get

$$\frac{d^2}{ds^2}h_\lambda = \frac{\left\|A_R^{-1}B^{-1}\right\|^2}{C_\varphi \lambda^d}\sum_i \nabla^2 W[BA_R u(A_R x_i(0))]\varphi(\lambda^{-1}(x_i(0)-x))O(\lambda^{-1})O(u^2) \quad . \tag{3.2.27}$$

Performing a Taylor expansion of $u(x)$ and by means of the assumptions we impose on the derivatives of u, we optain

$$\begin{aligned} u(A_R y) =& \frac{1}{2}\nabla^2 u(A_R x)\,[A_R(y-x)] \\ &+ \int_0^1\int_0^w\int_0^v \nabla^3 u\,(A_R x + sA_R(y-x))\,[(A_R(y-x))]\,dsdvdw \\ |BA_R u(A_R x_i(0))| \le& \frac{1}{2}|BA_R||A_R|^2|x_i(0)-x|^2\|\nabla^2 u(A_R x)\| \\ &+ 1/6|BA_R||A_R|^3|x_i(0)-x|^3|\nabla^3 u| \\ \le& \theta \quad . \end{aligned} \tag{3.2.28}$$

Hence, for sufficiently large λ it holds

$$\operatorname{dist}(A(s)(x_i(s)-x)+\tau(s),\mathbb{Z}^d) \le \theta \quad . \tag{3.2.29}$$

Therefore, the argument of W is always in the convex region and we get

$$\begin{aligned} \frac{d^2}{ds^2}h_\lambda \le& \frac{\left\|A_R^{-1}B^{-1}\right\|^2}{C_\varphi\lambda^d}\sum_i c_\Theta^1|BA_R u(A_R x_i)|^2\varphi(\lambda^{-1}(x_i(0)-x)) \\ &+ O(\lambda^{-1}|u|^2) \quad . \end{aligned} \tag{3.2.30}$$

Since $u(A_R x)=0$ and $\nabla u(A_R x)=0$ We have

$$|u(A_R x_i(0))| \le \frac{1}{2}\max_{B_{2\lambda}(x)}\{\|\nabla^2 u(A_R y)\|\}\,(2|A_R|\lambda)^2 \quad . \tag{3.2.31}$$

Hence, we get

$$\frac{d^2}{ds^2}h_\lambda \le 4\lambda^4\frac{\left\|A_R^{-1}B^{-1}\right\|^2}{C_\varphi\lambda^d}\sum_i \max_{B_{2\lambda}(x)}\{\|\nabla^2 u(A_R y)\|\}^2 c_\Theta^1|BA_R|^2|A_R|^4\varphi \quad . \tag{3.2.32}$$

With Lemma 2.1.2 we get

$$\frac{d^2}{ds^2}h_\lambda \le 4c_\Theta^1\lambda^4\left\|A_R^{-1}B^{-1}\right\|^2|BA_R|^2|A_R|^4\max_{B_{2\lambda}(x)}\{\|\nabla^2 u(A_R y)\|\}^2\det A_R \quad . \tag{3.2.33}$$

□

Now we study how the effective elastic potential depends on its argument. We consider the local minimizers of the pre-energy density $h_\lambda(\cdot, (G\mathbb{Z}^d - z, 0)$. the branches of local minimizer and the local minima are differentiable functions of G. However the global minimizer may jump in an uncontrolled fashion between the branches. Furthermore the global minima will be continuous but do not have to be differentiable or locally convex. Therefore, the effective elastic potential does not have to be differentiable as a function of G. However, the Taylor expansion containing the branch that is the global minimizer for G_0 still gives an upper for the effective elastic potential for G close to G_0 of the form

$$\begin{aligned} F_\lambda(G_1)\det(G_1) \leq & F_\lambda(G_0)\det(G_0) + (\nabla F)_{av}(G_0, z)[G_1 - G_0] \\ & + \frac{1}{2}(\nabla^2 F)_{av}(G_0)[G_1 - G_0] + O(|G_1 - G_0|^3) \quad . \end{aligned} \tag{3.2.34}$$

Lemma 3.2.2. *There exists $\hat{\lambda} \in \mathbb{R}$ and $\hat{\epsilon} > 0$ such that for all $\lambda \geq \hat{\lambda}$ it holds For all $G_0 \in Gl_d(\mathbb{R})$ that satisfies $F(G_0) \leq \hat{\epsilon}$ there exist $B(G_, z) \in Gl_d(\mathbb{Z})$ and $r \geq 0$ such that for all $G_1 \in Gl_d(\mathbb{R})$ that satisfies $|G_1 - G_0| \leq r$ it holds*

$$\begin{aligned} F_\lambda(G_1, z)\det(G_1) \leq & F_\lambda(G_0, z)\det(G_0) + (\nabla F)_{loc}(G_0, z)[G_1 - G_0] \\ & + \frac{1}{2}(\nabla^2 F)_{loc}(G_0, z)[G_1 - G_0] + O(|G_1 - G_0|^3) \quad , \end{aligned} \tag{3.2.35}$$

where $(\nabla F)_{loc}$ is a linear form defined for any $M \in \mathbb{R}^{d\times d}$

$$\begin{aligned} (\nabla F)_{loc}(G_0, z)[M] = & \partial_A F(BG_0^{-1})\left[BG_0^{-1}MG_0^{-1}\right] \\ & + F(BG_0^{-1})Tr(G_0^{-1}M)\det G_0 + O(\lambda^{-2})M \quad , \end{aligned} \tag{3.2.36}$$

and $(\nabla^2 F)_{loc}$ is a quadratic form fulfilling

$$\begin{aligned} & (\nabla^2 F)_{loc}(G_0, z)[M] \\ = & \partial_A^2 F(BG_0^{-1})\left[BG_0^{-1}MG_0^{-1}\right]\det G_0 \\ & + 2\partial_A F\left(BG_0^{-1}\right)\left[Tr\left(G_0^{-1}M\right)BG_0^{-1}MG_0^{-1} - G_0^{-1}MG_0^{-1}MG_0^{-1}\right]\det G_0 \\ & - F\left(BG_0^{-1}\right)\left(Tr\left(G_0^{-1}M\right)^2 - Tr\left(G_0^{-1}MG_0^{-1}M\right)\right)\det G_0 + O\left(\lambda^{-2}M^2\right) \quad . \end{aligned} \tag{3.2.37}$$

This implies for the effective elastic potential

$$\begin{aligned} F_\lambda(G_1)\det(G_1) \leq & F_\lambda(G_0)\det(G_0) + (\nabla F)_{av}(G_0, z)[G_1 - G_0] \\ & + \frac{1}{2}(\nabla^2 F)_{av}(G_0)[G_1 - G_0] \quad , \end{aligned} \tag{3.2.38}$$

where

$$\begin{aligned} (\nabla F)_{av}(G_0)X &= \int_{[0,1]^d}(\nabla F)_{loc}(G_0, z)X dz \quad , \\ (\nabla^2 F)_{av}(G_0)(X, X) &= \int_{[0,1]^d}(\nabla^2 F)_{loc}(G_0)(X, X) dz \quad . \end{aligned} \tag{3.2.39}$$

Proof. We define $G(s) = sG_1 + (1-s)G_0$, and consider

$$\begin{aligned} F_\lambda(G(s), z) \det G(s) =& \hat{h}_\lambda(0, G(s)(\mathbb{Z}^d - z)) \det G(s) \\ =& \inf_{\mathcal{A}} h_\lambda(\mathcal{A}, 0, G(s)(\mathbb{Z}^d - z)) \det G(s) \quad . \end{aligned} \tag{3.2.40}$$

According to Lemma 3.1.5, for λ large enough and $F(G^{-1}) < \hat{\epsilon}$ small enough, there is a $B \in Gl_d(\mathbb{Z})$ such that the global minimizer $\hat{\mathcal{A}} \in Gl_d(\mathbb{R})$ satisfies

$$\begin{aligned} \left| BG - \hat{A} \right| =& O(\lambda^{-2}) \quad , \\ |\tau - Bz - t| \leq& O(\lambda^{-m}) \quad . \end{aligned} \tag{3.2.41}$$

The global minimizer is also a local minimizer as described in Lemma 3.1.4. According to Lemma 3.1.4 the local minimizer is a differentiable function of the lattice parameter $G(s)$. Since for all s the configuration $G(s)\left(\mathbb{Z}^d - z\right)$ is a lattice we can as in Lemma 3.1.3 and conclude that

$$\begin{aligned} &\tilde{h}\left(\delta\mathcal{A}(s), G(s), z)\right) := h_\lambda(\mathcal{A}(s), G(s)(\mathbb{Z}^d - z), 0) \det G(s) \\ =& C_\varphi^{-1} \lambda^{-d} \left\| \left(BG^{-1}(s) + \delta A(s) \right)^{-1} \right\|^2 \det G(s) \\ &\times \sum_{\mathbf{i} \in \mathbb{Z}^d} W(\delta A(s) G(s) B^{-1} (\mathbf{i} - z) + \delta\tau(s)) \varphi\left(\lambda^{-1} |x_i - x| \right) \\ &+ F(\delta A(s) + BG^{-1}(s)) \det G(s) + \vartheta \det\left(\delta A(s) + BG^{-1}(s) \right) \det G(s) \\ &- \frac{\vartheta}{C_\varphi \lambda^d} \sum_{\mathbf{i} \in \mathbb{Z}^d} \varphi\left(\lambda^{-1} \left| G(s) B^{-1} (\mathbf{i} - z) \right| \right) \det G(s) \quad . \end{aligned} \tag{3.2.42}$$

Moreover we have

$$\begin{aligned} \tilde{h}_\lambda(\delta\mathcal{A}(1), G(1), z) =& \tilde{h}_\lambda(\delta\mathcal{A}(0), G_0, z) + \frac{d}{ds} \tilde{h}_\lambda(\delta\mathcal{A}(0), G_0, z) \\ &+ \int_0^1 \int_0^v \frac{d^2}{ds^2} h_\lambda(\delta\mathcal{A}(s), G(s), z) ds dv \quad . \end{aligned} \tag{3.2.43}$$

Since we have selected $\delta\mathcal{A}(0)$ to be the global minimizer, by construction we have $\tilde{h}_\lambda(\delta\mathcal{A}(0), G_0, z) = F(G_1, z)$. Furthermore the global minimum for $t = 1$ has to be smaller or equal $\tilde{h}_\lambda(\delta\mathcal{A}(1), G(1), z)$. Hence, it holds

$$\begin{aligned} F_\lambda(G_1, z) \det G_1(s) \leq& F_\lambda(G_0, z) \det G_0 + \frac{d}{ds} \tilde{h}_\lambda(\delta\mathcal{A}(0), G(0), z) \\ &+ \int_0^1 \int_0^t \frac{d^2}{ds^2} \tilde{h}_\lambda(\delta\mathcal{A}(s), G(s), z) ds ds \quad . \end{aligned} \tag{3.2.44}$$

By Lemma B.1.3 and the chain rule we get

$$\frac{d}{ds} \tilde{h}_\lambda(\mathcal{A}(0), G_0, z) = \frac{\partial}{\partial G} \left(\tilde{h}_\lambda(\mathcal{A}(0), G_0, z) \right) [G_1 - G_0] \quad . \tag{3.2.45}$$

For the ease of exposition we will omit the argument of W and φ in the following calculation. For all test matrices $M \in \mathbb{R}^{d\times d}$ we have

$$\begin{aligned}
&\frac{\partial}{\partial G}\tilde{h}_\lambda(\mathcal{A}(G_0), x, G_0(\mathbb{Z}^d - z))[M] \\
=&\partial_G \left(F(BG_0^{-1} + \delta A(0)) \det G_0\right)[M] + \vartheta \partial_A \det\left(B + \delta A(0) G_0\right)[\delta A(0) M] \\
&- \vartheta \partial_G \left(\rho_\lambda \det G_0\right)[M] \\
&+ \frac{\partial_G \left\| \left(BG_0^{-1} + \delta A(0)\right)^{-1}\right\|^2 [M]}{C_\varphi \lambda^d} \sum_{\mathbf{i}\in\mathbb{Z}^d} W \varphi \det G_0 \\
&+ \frac{\left\| \left(BG_0^{-1} + \delta A(0)\right)^{-1}\right\|^2}{C_\varphi \lambda^d} \sum_{\mathbf{i}\in\mathbb{Z}^d} \left\langle \nabla W, \delta A(0) M B^{-1}(\mathbf{i} - z)\right\rangle \varphi \det G_0 \\
&+ \frac{\left\| \left(BG_0^{-1} + \delta A(0)\right)^{-1}\right\|^2}{C_\varphi \lambda^d} \sum_{\mathbf{i}\in\mathbb{Z}^d} W \left\langle \nabla \tilde{\varphi}, M B^{-1}(\mathbf{i} - z)\right\rangle \det G_0 \\
&+ J_\lambda\left(BG_0^{-1} + \delta A(0), \delta\tau(0) + Bz + t, G^{-1}\left(\mathbb{Z}^d - z\right), 0\right) \partial_A \det G_0[M] \quad .
\end{aligned} \tag{3.2.46}$$

Since we know that $\delta A = O(\lambda^{-2})$ and $\delta\tau \leq O(\lambda^{-k})$. We get that W is $O(\lambda^{-2})$ and ∇W is $O(\lambda^{-1})$. So J_λ itself is $O(\lambda^{-2})$, and all contributions of J_λ in equation (3.2.46) are of order $O(\lambda^{-2}|M|)$. Furthermore, because $\delta A = O(\lambda^{-2})$, also the contribution of $\vartheta \det A$ is $O(\lambda^{-2})$. In contrast, the contribution of F is $O(1)$. We see this using Lemma B.2.3. In fact

$$\begin{aligned}
&\partial_G \left(F(BG_0^{-1} + \delta A(0)) \det G_0\right)[M] \\
=&\left(\partial_A F[BG_0^{-1} + \delta A)\left[BG_0^{-1} M G_0^{-1}\right] + F(BG_0^{-1} + \delta A(0)) Tr(G_0^{-1} M)\right) \det G_0 \\
=&\left(\partial_A F(BG_0^{-1})\left(BG_0^{-1} M G_0^{-1}\right) + F(BG_0^{-1}) Tr(G_0^{-1} M)\right) \det G_0 + O(\lambda^{-2} M) \quad .
\end{aligned} \tag{3.2.47}$$

We focus on the term from $\partial_G\left(\rho_\lambda \det G\right)$. We use Lemma 2.1.2 with the functions ψ defined by

$$\psi(X) := \frac{1}{C_\varphi} \nabla\tilde{\varphi}(X)\left(G_1 - G_0\right) G_0^{-1} X \quad . \tag{3.2.48}$$

Since φ is C_C^∞ so are ψ and we get

$$\partial_G \rho_\lambda[M] == \quad \frac{1}{C_\varphi} \int_{\mathbb{R}^d} \left\langle \nabla\tilde{\varphi}(y), M G_0^{-1} y\right\rangle dy \det\left(BG_0^{-1}\right) + O(\lambda^{-k} M) \quad . \tag{3.2.49}$$

Partial integration leads to

$$\begin{aligned}\partial_G\rho_\lambda[M] =& -\frac{1}{C_\varphi}\int_{\mathbb{R}^d}\tilde{\varphi}\,(y)\left\langle\nabla, MG^{-1}y\right\rangle dy\det G^{-1}+O(\lambda^{-k})M\\ =& -\frac{1}{C_\varphi}\int_{\mathbb{R}^d}\tilde{\varphi}\,(y)\,Tr\left(MG^{-1}\right)dy\det G^{-1}+O(\lambda^{-k}|M|)\\ =& -Tr\left(MG^{-1}\right)\det G^{-1}+O(\lambda^{-k}M)\quad .\end{aligned}\tag{3.2.50}$$

Due to Lemma B.2.3 we can conclude that

$$\begin{aligned}\partial_G\left(\rho_\lambda\det G\right)[M] =&\partial_G\left(\rho_\lambda\right)[M]\det G+\rho_\lambda\partial_G\det G[M]\\ &-Tr\left(MG^{-1}\right)+O(\lambda^{-k}M)+Tr\left(MG^{-1}\right)\\ =&O(\lambda^{-k})\quad .\end{aligned}\tag{3.2.51}$$

We summarize

$$\begin{aligned}\frac{d}{ds}h_\lambda(\mathcal{A}(G_0),G_0,z) =&\partial_A F(BG_0^{-1})\left(BG_0^{-1}\left(G_1-G_0\right)G_0^{-1}\right)\\ &+F(BG_0^{-1})Tr(G_0^{-1}(G_0-G_1))\det G_0+O(\lambda^{-2})\left(G_1-G_0\right).\end{aligned}\tag{3.2.52}$$

For the second order term we get as in Lemma B.1.3

$$\begin{aligned}\frac{d^2}{ds^2}\tilde{h}_\lambda(\delta\mathcal{A}(s),G(s),z) =&\frac{\partial^2\tilde{h}_\lambda}{\partial G^2}(\delta\mathcal{A}(s),G(s),z)\left[\frac{dG}{ds}\right]\\ &-\left(\frac{\partial^2\tilde{h}_\lambda}{\partial\delta\mathcal{A}^2}\right)^{-1}\left[\frac{\partial}{\partial\delta\mathcal{A}}\left(\frac{\partial\tilde{h}_\lambda}{\partial_G}\left[\frac{dG}{ds}\right]\right)\right].\end{aligned}\tag{3.2.53}$$

As already seen in Lemma 3.1.4 $0\leq\frac{\partial^2\tilde{h}_\lambda}{\partial\delta\mathcal{A}^2}$, and therefore $0\leq\left(\frac{\partial^2\tilde{h}_\lambda}{\partial\delta\mathcal{A}}\right)^{-1}$. The second term in (3.2.53) is always negative and for an upper bound we only need to estimate the first term. We explicitly calculate $\frac{\partial^2\tilde{h}_\lambda}{\partial G^2}(\delta\mathcal{A}(s),G(s),z)\,[M]$, again for the ease of exposition we omit the arguments of W and φ, and we also write G for $G(s)$ and δA for $\delta A(s)$. we have

$$\begin{aligned}&\frac{\partial^2\tilde{h}_\lambda}{\partial G^2}(\delta\mathcal{A},G,z)\,[M]\\ =&\partial_G^2\left(F(BG^{-1}+\delta A)\det G\right)[M]\det G-\vartheta\partial_G\left(\rho_\lambda\det G\right)[M]\\ &\vartheta\partial_A^2\det\left(B+\delta AG\right)[\delta AM]+2\partial_G^2J_\lambda[M]\det G\\ &+2\partial_G J_\lambda[M]\partial_G\det G[M]+J_\lambda\partial_G^2\partial_G^2\det G[M]\quad .\end{aligned}\tag{3.2.54}$$

The second derivative of J_λ is

$$\begin{aligned}
&C_\varphi \lambda^d \partial_G^2 J_\lambda[M]\\
=&\partial_G^2 \left\| \left(BG^{-1}+\delta A\right)^{-1} \right\|^2 [M] \sum_{\mathbf{i}\in\mathbb{Z}^d} W\varphi\\
&+\left\| \left(BG^{-1}+\delta A\right)^{-1} \right\|^2 \sum_{\mathbf{i}\in\mathbb{Z}^d} \nabla^2 W \left[\delta A \left(G_1-G_0\right) B^{-1} \left(\mathbf{i}-z\right)\right] \varphi\\
&+\left\| \left(BG^{-1}+\delta A\right)^{-1} \right\|^2 \sum_{\mathbf{i}\in\mathbb{Z}^d} W \nabla^2 \tilde{\varphi} \left[\left(\left(G_1-G_0\right) B^{-1} \left(\mathbf{i}-z\right)\right)\right]\\
&+2\partial_G \left\| \left(BG^{-1}+\delta A\right)^{-1} \right\|^2 [M] \sum_{\mathbf{i}\in\mathbb{Z}^d} \left\langle \nabla W, \delta A M B^{-1} \left(\mathbf{i}-z\right)\right\rangle \varphi\\
&+2\partial_G \left\| \left(BG^{-1}+\delta A\right)^{-1} \right\|^2 [M] \sum_{\mathbf{i}\in\mathbb{Z}^d} \left\langle W\nabla\tilde{\varphi}, \left(MB^{-1}\left(\mathbf{i}-z\right)\right)\right\rangle\\
&+2\left\| \left(BG^{-1}+\delta A\right)^{-1} \right\|^2 \sum_{\mathbf{i}\in\mathbb{Z}^d} \left\langle \nabla W\left(\delta A M B^{-1}\left(\mathbf{i}-z\right)\right), \nabla\tilde{\varphi}\left(MB^{-1}\left(\mathbf{i}-z\right)\right)\right\rangle .
\end{aligned} \tag{3.2.55}$$

Again we use that $\delta A = O(\lambda^{-2})$ and $\delta\tau \leq O(\lambda^{-2})$ and therefore W is $O(\lambda^{-2})$ and ∇W is $O(\lambda^{-1})$. As calculated above J_λ and $\partial_G J$ are both $O(\lambda^{-2})$. So all terms coming from J_λ are $O(\lambda^{-2})$. Because $\delta A = O(\lambda^{-2})$ the contribution of ($\vartheta \det A \det G$ is $O(\lambda^{-4})$). In contrast $\partial_G^2 \left(F \det G\right)$ is $O\left(1\right)$. in fact

$$\begin{aligned}
&\partial_G^2 \left(F\left(BG^{-1}+\delta A\right) \det G\right)[M]\\
=&\partial_A^2 F\left[\partial_G A[M]\right] \det G + \partial_A F\left[\partial_G^2 A[M]\right] \det G\\
&+2\partial_A F\left(\partial_G A[M]\right) \partial G \det G[M] + F\partial_G^2 \det G[M] \quad .
\end{aligned} \tag{3.2.56}$$

The argument of F equals BG^{-1} up to $O(\lambda^{-2})$. We use Lemma B.2.3 for the derivatives of $\det G$ and G^{-1}. We get

$$\begin{aligned}
&\partial_G^2 \left(F\left(BG^{-1}+\delta A\right) \det G\right)[M]\\
=&\partial_A^2 F(BG^{-1})\left[BG^{-1}MG^{-1}\right] \det G - 2\partial_A F\left(BG^{-1}\right)\left[G^{-1}MG^{-1}MG^{-1}\right] \det G\\
&+2\partial_A F\left(BG^{-1}\right)\left[BG^{-1}MG^{-1}\right] Tr\left(G^{-1}M\right) \det G\\
&-F\left(BG^{-1}\right) Tr\left(G^{-1}MG^{-1}M\right) \det G\\
&F\left(BG^{-1}\right) Tr\left(G^{-1}(G_1-G_0)\right)^2 \det G + O(\lambda^{-2}(G_1-G_0)^2) \quad .
\end{aligned} \tag{3.2.57}$$

For the contribution of the density $(\rho_\lambda \det G)$ we can apply the same calculation as we did for the first order contribution and receive

$$\partial_G^2 \left(\rho_\lambda \det G\right)[M] - O(\lambda^{-k}) \quad . \tag{3.2.58}$$

Hence, $\partial_G^2 (\rho_\lambda \det G)(G_1 - G_0, G_1 - G_0)$ gives no contribution of leading order. The only remaining part of leading order comes from F. We finally remember that $G = G(s) = G_0 + O(G_1 - G_0)$. If we apply this on the estimate (3.2.57) and put this into the estimate (3.2.53) we get the second order contribution for the estimate (3.2.44) together with equation (3.2.52) we get the conclusion. □

Next we study a configuration satisfying $\chi = \psi(\mathbb{Z}^d)$ in some area $\psi(\tilde{\Omega})$. We now combine Lemma 3.2.1 and Lemma 3.2.2 to bound the integral of the energy density over the $\psi(\tilde{\Omega})$ from above by the integral over the local effective elastic energy plus the integral over some term that scales like $\lambda^4\|\nabla^2\psi\|^2$ plus many lower order terms. If additionally χ is a perturbation of a lattice e.g $\chi = A_R^{-1}\mathbb{Z}^d + u(z_i)$ such that $u = 0$ at the boundary of $\psi(\tilde{\Omega})$, we can bound the energy of the configuration from above by the energy of the lattice lattice plus a linear term in ∇u and a quadratic term in ∇u coming from the expansion of the average effective elastic potential plus the $\lambda^4\|\nabla^2 u\|^2$ term and many lower order terms.

Theorem 3.2.3. *There exists $\hat{\lambda} \in \mathbb{R}$ and $\hat{\epsilon} > 0$ such that for all $\lambda \geq \hat{\lambda}$, holds: If there is a set $\tilde{\Omega} \subset \mathbb{R}^n$ and a map $\psi \in C^3\left(\mathbb{R}^d, \mathbb{R}^d\right)$ such that $\psi(\tilde{\Omega}) \subset \Omega$ all points $x \in B_{2\lambda}\left(\psi\left(\tilde{\Omega}\right)\right)$ satisfies*

1) $\chi \cap B_{2\lambda}\left(\psi\left(\tilde{\Omega}\right)\right) = \psi(\mathbb{Z}) \cap B_{2\lambda}\left(\psi\left(\tilde{\Omega}\right)\right)$,

2) $F\left(\nabla\psi(z) \leq \hat{\epsilon}\right.$ for $z \in \tilde{\Omega}$,

3) $\lambda^2|\nabla^2\psi(\psi^{-1}(x))| \leq \frac{1}{4}\theta c_6^{-1}|\nabla\psi^{-1}(x)|^{-2}$ for $x \in B_{2\lambda}(\psi(\tilde{\Omega}))$,

4) $\lambda^3|\nabla^3\psi(\psi^{-1}(x))| \leq \frac{3}{8}\theta c_6^{-1}|\nabla\psi^{-1}(x)|^{-3}$ for $x \in B_{2\lambda}(\psi(\tilde{\Omega}))$,

then the energy fulfills

$$\begin{aligned}\int_{\psi(\tilde{\Omega})} \hat{h}(\chi, x)dx = &\int_{\tilde{\Omega}} F_\lambda\left(\nabla\psi(z), z\right)\det\nabla\psi(z)dz \\ &+ C_Q|(\nabla\psi(z))^{-1}|^4\lambda^4\int_{\tilde{\Omega}} \max_{B_{2\lambda}(\psi(z))}\{\|\nabla^2\psi(\psi^{-1}(y))\|\}^2\det\nabla\psi(z)dz \\ &+ \int_{\psi^{-1}(\tilde{\Omega})}\int 0(\lambda^{2-k})\nabla^2\psi(z) + O(\lambda^2|\nabla^3\psi(y)|)\det\nabla\psi(z) \quad ,\end{aligned} \tag{3.2.59}$$

where $C_Q := 2dc_4^2c_6^2$ and c_4 and c_6 are as in Lemma 2.2.6. If additionally it holds

$$\psi(z) = A_R^{-1}z + u(z) \quad , \tag{3.2.60}$$

then we get for the difference of the energy

$$\begin{aligned}
&\int_{\psi(\tilde\Omega)} \hat h(\chi,x)dx - \int_{A_R^{-1}\tilde\Omega} \hat h(A_R^{-1}\mathbb{Z},x)dx + O(|\nabla u|^3) \\
&\leq \int_{\tilde\Omega} (\nabla F)_{av}\left(A_R^{-1}\right)[\nabla u(z)] + \frac{1}{2}(\nabla^2 F)_{av}\left(A_R^{-1}\right)[\nabla u(z)]\,dz \\
&\quad + C_Q\lambda^4|(\nabla\psi(z))^{-1}|^4 \int_{\tilde\Omega} \max_{B_{2\lambda}(\psi(z))}\{\|\nabla^2\psi(\psi^{-1}(y))\|\}^2 dz \\
&\quad + \int_{\tilde\Omega}\int_{[-\frac12,\frac12]^d} (\nabla F)_{loc}\,(\nabla\psi(z-w),z)\,[\nabla^2\psi(z)w] + O(\nabla^3\psi) + O(\left|\nabla^2 u\right|^2)dwdz \\
&\quad + \int_{\tilde\Omega} 0(\lambda^{2-m})\nabla^2\psi(z) + O(\lambda^2)\max_{B_{2\lambda}(\psi(z))}\|\nabla^3\psi\|\left(\psi^{-1}(y)\right)dz + |X_S - X_S^G|,
\end{aligned} \tag{3.2.61}$$

with a boundary term

$$\begin{aligned}
|X_S - X_S^G| = &\int_{[-\frac12,\frac12]^d}\int_{\left(w+\tilde\Omega\right)/\tilde\Omega} \left|(\nabla F)_{loc}\left(A_R^{-1},\tilde z\right)\right| |\nabla u(\tilde z)| + O(u^2)d\tilde z)dw \\
&\int_{[-\frac12,\frac12]^d}\int_{\tilde\Omega/\left(\tilde\Omega+w\right)} \left|(\nabla F)_{loc}\left(A_R^{-1}+\nabla u(\tilde z-w),\tilde z\right)\right| |\nabla u(\tilde z)|\,d\tilde z dw \\
&\int_{[-\frac12,\frac12]^d}\int_{\left(\left(w+\tilde\Omega\right)/\tilde\Omega\right)\cup\left(\tilde\Omega/\left(\tilde\Omega+w\right)\right)} O((\nabla u)^2) + O(\lambda^{-2}\nabla u)d\tilde z dw \quad .
\end{aligned} \tag{3.2.62}$$

Proof. **Step 1: Rewriting the energy with local elastic potential**

We consider near the point $x=\psi(z)$ the lattice $\tilde\chi(x)$ with

$$\begin{aligned}
\tilde x_i :=&\psi(z) + \nabla\psi(z)\,(z_i - z) \quad , \\
\tilde x_i - x =&\nabla\psi(z)\,(z_i - z) \quad .
\end{aligned} \tag{3.2.63}$$

This implies

$$\begin{aligned}
\hat h_\lambda\,(\tilde\chi(x),x) =&\hat h_\lambda(\nabla\psi(z)\left(\mathbb{Z}^d - z\right),0) \\
=&F_\lambda\,(\nabla\psi(z),z) \quad .
\end{aligned} \tag{3.2.64}$$

Because of $F(\nabla\psi(z)) \leq \hat\epsilon$ and $\lambda \geq \hat\lambda$ the conditions of Lemma 3.1.5 are fullfilled. Hence, we have a global minimizer for $h_\lambda(\cdot,\tilde\chi,x)$ that is close to $B\nabla\psi(z), Bz+t$ for some $B\in Gl_d(\mathbb{Z})$ and $t\in Z^d$. We call this global minimizer $\mathcal{A}_0\,(x)$ and get

$$\hat h_\lambda\,(\tilde\chi(x),x) = h_\lambda(\mathcal{A}_0(x)\,(x)\,,\tilde\chi(x),x) \quad . \tag{3.2.65}$$

On the other hand $\tilde\chi(x)$ is a lattice. If we define

$$\begin{aligned}
u(z_i) :=&x_i - \tilde x_i \\
=&\psi(z_i) - \psi(z) - \nabla\psi(z)\,(z_i - z) \quad .
\end{aligned} \tag{3.2.66}$$

we have $u(z) = 0$, $\nabla u(z) = 0$ and $\nabla^k u(z) = \nabla^k \psi(z)$ for $k \geq 2$. Since the assumptions of Lemma 3.2.1 are fulfilled, we get

$$\begin{aligned} &h_\lambda(\mathcal{A}_0(x), \chi, x) + 0(1)\nabla^2\psi(z) + O(\lambda^2\nabla^3\psi) \\ \leq &h_\lambda(\mathcal{A}_0(x), \tilde{\chi}, x) \\ &+ 2\lambda^4 c_\Theta^1 |(\nabla\psi)^{-1}|^4 \left\|\nabla\psi^{-1}B^{-1}\right\|^2 \|B\nabla\psi\|^2 |(\nabla\psi)^{-1}|^4 \\ &\max_{B_{2\lambda}(x)} \{\|\nabla^2\psi(\psi^{-1}(y))\|\}^2 \det(\nabla\psi)^{-1} \quad . \end{aligned} \tag{3.2.67}$$

We have chosen $\mathcal{A}$ to be the global minimizer for $\tilde{\chi}$ furthermore $h_\lambda(\mathcal{A}_0, \chi, x)$ has to be larger than the infimum over all $\mathcal{A}$ According to Lemma 3.1.5 $B\nabla\psi$ is $O(\lambda^{-2})$ away from the global minimizer A_0. And according to Lemma 2.2.7 the global minimizers fulfill $|A_0^{-1}| \leq c_4$ and $|A_0| \leq c_3$ Hence, we get the upper bound

$$\begin{aligned} \hat{h}(\chi, x) \leq &F_\lambda\left(\nabla\psi(z), z\right) \\ = &+ C_Q \lambda^4 |(\nabla\psi(z))^{-1}|^4 \max_{B_{2\lambda}(\psi(z))} \{\|\nabla^2\psi(\psi^{-1}(y))\|\}^2 \det(\nabla\psi)^{-1} \\ &+ 0(1)\nabla^2\psi(z) + O(\lambda^2\nabla^3\psi(y)) \quad . \end{aligned} \tag{3.2.68}$$

Integrating this, we get

$$\begin{aligned} \int_{\psi(\tilde{\Omega})} \hat{h}(\chi, x) dx = &\int_{\tilde{\Omega}} \hat{h}(\chi, \psi(z)) \det\left(\nabla\psi(z)\right) dz \\ = &\int_{\tilde{\Omega}} F_\lambda\left(\nabla\psi(z), z\right) \det\left(\nabla\psi(z)\right) dz \\ &+ C_Q \lambda^4 |(\nabla\psi(z))^{-1}|^4 \int_{\tilde{\Omega}} \max_{B_{2\lambda}(\psi(z))} \{\|\nabla^2\psi(\psi^{-1}(y))\|\}^2 dz \\ &+ \int_{\tilde{\Omega}} 0(1)\nabla^2\psi(z) + O(\lambda^2) \max_{B_{2\lambda}(\psi(z))} \|\nabla^3\psi\| \left(\psi^{-1}(y)\right) dz \quad . \end{aligned} \tag{3.2.69}$$

Step 2: Changing from the local to the average elastic potential We now compare the integral of the average effective elastic potential, with the integral over the local elastic potential. We use the abbreviation

$$\tilde{F}_\lambda\left(G, z\right) = F_\lambda\left(G, z\right) \det G \quad . \tag{3.2.70}$$

We use the periodicity $F_\lambda\left(G, w\right) = F_\lambda\left(G, w + t\right)$ for $t \in \mathbb{Z}^d$. If we integrate over one periodicity cell the integral is not changing if we move this cell. Hence, we get

$$\begin{aligned} \int_{\tilde{\Omega}} F_\lambda\left(\nabla\psi(z)\right) \det\left(\nabla\psi(z)\right) dz = &\int_\Omega \tilde{F}_\lambda\left(\psi(z), z\right) dz \\ = &\int_{\tilde{\Omega}} \int_{[0,1]^d} \tilde{F}_\lambda\left(\nabla\psi(z), w\right) dw dz \\ = &\int_{\tilde{\Omega}} \int_{[-\frac{1}{2}, \frac{1}{2}]^d} \tilde{F}_\lambda\left(\nabla\psi(z), w + z\right) dw dz \quad . \end{aligned} \tag{3.2.71}$$

Next we substitute$\tilde{z} = z - w$.

$$\begin{aligned}\int_{\tilde{\Omega}} F_\lambda\left(\nabla\psi(z)\right)\det\left(\nabla\psi(z)\right)dz &= \int_{[-\frac{1}{2},\frac{1}{2}]^d}\int_{\tilde{\Omega}+w}\tilde{F}_\lambda\left(\nabla\psi(\tilde{z}-w),\tilde{z}\right)d\tilde{z}dw \\ &= \int_{\tilde{\Omega}}\int_{[-\frac{1}{2},\frac{1}{2}]^d}\tilde{F}_\lambda\left(\nabla\psi(\tilde{z}-w),\tilde{z}\right)dwd\tilde{z} + X_S \quad .\end{aligned} \tag{3.2.72}$$

X_S is a surface term given by

$$\begin{aligned}X_S = &\int_{[-\frac{1}{2},\frac{1}{2}]^d}\int_{\left(w+\tilde{\Omega}\right)/\tilde{\Omega}}\tilde{F}_\lambda\left(\nabla\psi(\tilde{z}-w),\tilde{z}\right)d\tilde{z}dw \\ &-\int_{[-\frac{1}{2},\frac{1}{2}]^d}\int_{\tilde{\Omega}/\left(\tilde{\Omega}+w\right)}\tilde{F}_\lambda\left(\nabla\psi(\tilde{z}-w),\tilde{z}\right)d\tilde{z}dw \quad .\end{aligned} \tag{3.2.73}$$

We get for the integral over the effective elastic potential

$$\begin{aligned}&\int_{\tilde{\Omega}} F_\lambda\left(\nabla\psi(z),z\right)\det\left(\nabla\psi(z)\right)dz \\ =&\int_{\tilde{\Omega}}\tilde{F}_\lambda\left(\nabla\psi(z),z\right)dz = \int_{\tilde{\Omega}}\int_{[-\frac{1}{2},\frac{1}{2}]^d}\tilde{F}_\lambda\left(\nabla\psi(z),z\right)dwdz \\ =&\int_{\tilde{\Omega}} F_\lambda\left(\nabla\psi(z)\right)\det\left(\nabla\psi(z)\right)dt - X_S \\ &+\int_{\tilde{\Omega}}\int_{[-\frac{1}{2},\frac{1}{2}]^d}\tilde{F}_\lambda\left(\nabla\psi(z),z\right) - \tilde{F}_\lambda\left(\nabla\psi(z-w),z\right)dwdx.\end{aligned} \tag{3.2.74}$$

We use the first part of Lemma 3.2.2 and get

$$\begin{aligned}&\int_{\tilde{\Omega}} F_\lambda\left(\nabla\psi(z),z\right)\det\left(\nabla\psi(z)\right)dz \\ =&\int_{\tilde{\Omega}} F_\lambda\left(\nabla\psi(z)\right)\det\left(\nabla\psi(z)\right)dz \\ &+\int_{\tilde{\Omega}}\int_{[-\frac{1}{2},\frac{1}{2}]^d}(\nabla F)_{loc}\left(\nabla\psi(z-w),z\right)\left[\nabla\psi(z)-\nabla\psi(z-w)\right] \\ &+\frac{1}{2}(\nabla^2 F)_{loc}\left(\nabla\psi(z-w),z\right)\left[\nabla\psi(z)-\nabla\psi(z-w)\right]dwdx - X_S \\ =&\int_{\tilde{\Omega}} F_\lambda\left(\nabla\psi(z)\right)\det\left(\nabla\psi(z)\right)dz \\ &+\int_{\tilde{\Omega}}\int_{[-\frac{1}{2},\frac{1}{2}]^d}(\nabla F)_{loc}\left(\nabla\psi(z-w),z\right)\left[\nabla^2\psi(z)w\right]dwdz \\ &+\int_{\tilde{\Omega}} O(\nabla^3\psi) + O(\left|\nabla^2 u\right|^2)dwdz + X_S \quad .\end{aligned} \tag{3.2.75}$$

Step 3: Comparison with the lattice: If we apply the calculation above to $\psi(\tilde{\mathbb{Z}}^d) = A_R^{-1}\mathbb{Z}^d$ here $\nabla\psi = A_R^{-1}$ is constant and equation (3.2.74) turns into

$$\int_{\tilde{\Omega}} F_\lambda\left(A_R^{-1}, z\right)\det\left(A_R^{-1}\right)dz = \int_{\tilde{\Omega}} F_\lambda\left(A_R^{-1}\right)\det\left(A_R^{-1}\right)dz + X_S^G \quad . \tag{3.2.76}$$

with the boundary term

$$\begin{aligned} X_S^G = &\int_{[-\frac{1}{2},\frac{1}{2}]^d}\int_{\left(w+\tilde{\Omega}\right)/\tilde{\Omega}} \tilde{F}_\lambda\left(A_R^{-1}, \tilde{z}\right)d\tilde{z}dw \\ &- \int_{[-\frac{1}{2},\frac{1}{2}]^d}\int_{\tilde{\Omega}/\left(\tilde{\Omega}+w\right)} \tilde{F}_\lambda\left(A_R^{-1}, \tilde{z}\right)d\tilde{z}dw \quad . \end{aligned} \tag{3.2.77}$$

If we calculate the difference between the two boundary terms, we get

$$\begin{aligned} X_S - X_S^G = &\int_{[-\frac{1}{2},\frac{1}{2}]^d}\int_{\left(w+\tilde{\Omega}\right)/\tilde{\Omega}} \tilde{F}_\lambda\left(A_R^{-1} + \nabla u(\tilde{z}), \tilde{z}\right) - \tilde{F}_\lambda\left(A_R^{-1}, \tilde{z}\right)d\tilde{z}dw \\ &- \int_{[-\frac{1}{2},\frac{1}{2}]^d}\int_{\tilde{\Omega}/\left(\tilde{\Omega}+w\right)} \tilde{F}_\lambda\left(A_R^{-1} + \nabla u(\tilde{z}-w), \tilde{z}\right) - \tilde{F}_\lambda\left(A_R^{-1}, \tilde{z}\right)d\tilde{z}dw \quad . \end{aligned} \tag{3.2.78}$$

With the help of Lemma 3.2.2 this term can be estimate from above by

$$\begin{aligned} |X_S - X_S^G| \leq &\int_{[-\frac{1}{2},\frac{1}{2}]^d}\int_{\left(w+\tilde{\Omega}\right)/\tilde{\Omega}} \left|(\nabla F)_{loc}\left(A_R^{-1}, \tilde{z}\right)\right| |\nabla u(\tilde{z})| + O\left((\nabla u)^2\right)d\tilde{z}) \\ &+ O(\lambda^{-2}\nabla u) + O\left((\nabla u)^2\right)dw \\ &\int_{[-\frac{1}{2},\frac{1}{2}]^d}\int_{\tilde{\Omega}/\left(\tilde{\Omega}+w\right)} \left|(\nabla F)_{loc}\left(A_R^{-1} + \nabla u(\tilde{z}-w), \tilde{z}\right)\right| |\nabla u(\tilde{z})| \\ &+ O(\lambda^{-2}\nabla u) + O(\nabla u^2)d\tilde{z}dw \quad . \end{aligned} \tag{3.2.79}$$

Furthermore we expand $F_\lambda\left(\nabla\psi(z)\right)\det\left(\nabla\psi(z)\right)$ using the second part of Lemma 3.2.2 and get

$$\begin{aligned} F_\lambda\left(\nabla\psi(z)\right)\det\left(\nabla\psi(z)\right) \geq &F_\lambda\left(A_R^{-1}\right)\det\left(A_R^{-1}\right) + (\nabla F)_{av}\left(A_R^{-1}\right)[\nabla u(z)] \\ &+ \frac{1}{2}(\nabla^2 F)_{av}\left(A_R^{-1}\right)[\nabla u(z)] \quad . \end{aligned} \tag{3.2.80}$$

Finally, we get

$$\begin{aligned} &\int_{\tilde{\Omega}} F_\lambda\left(A_R^{-1} + \nabla u(z), z\right)\det\left(A_R^{-1} + \nabla u(z)\right)dz - \int_{\tilde{\Omega}} F_\lambda\left(A_R, z\right)\det\left(\nabla\psi(z)\right)dz \\ \leq &\int_{\tilde{\Omega}} (\nabla F)_{av}\left(A_R^{-1}\right)[\nabla u(z)] + \frac{1}{2}(\nabla^2 F)_{av}\left(A_R^{-1}\right)[\nabla u(z)]\,dz \\ &+ \int_{\tilde{\Omega}}\int_{[-\frac{1}{2},\frac{1}{2}]^d} (\nabla F)_{loc}\left(\nabla\psi(z-w), z\right)\nabla^2\psi(z)w + O(\nabla^3\psi) + \\ &O(\left|\nabla^2 u\right|^2)dwdz + |X_S - X_S^G|. \end{aligned}$$

If we use this for the estimate (3.2.69). We get the estimate (3.2.75) ☐

Remark 3.2.4. We consider the term

$$\int_{\tilde{\Omega}} \int_{[-\frac{1}{2},\frac{1}{2}]^d} (\nabla F)_{loc} (\nabla \psi(z-w), z) \nabla^2 \psi(z) w dw dz \quad . \tag{3.2.81}$$

Since the integral of an odd function over an even domain is zero, we have

$$\int_{\tilde{\Omega}} \int_{[-\frac{1}{2},\frac{1}{2}]^d} (\nabla F)_{loc} (\nabla \psi(z), z) \nabla^2 \psi(z) w dw dz = 0 \quad . \tag{3.2.82}$$

Therefore, this terms apears only due to fluctuations in $(\nabla F)_{loc} (\nabla \psi(z-w), z)$. If the global minimizer $\mathcal{A}$ is not jumping between different parametrisations, then this is actually a $O(\nabla \psi^2)$ term. If it is jumping then its size depend on the size of the jump in $(\nabla F)_{loc}$.

3.3 Upper bound for the energy barrier

In this section we calculate an upper bound for the energy barrier of plastic relaxation in dimension two. For this we construct an explicit continuous path of configurations, that starts with a sheared Bravais lattice and ends with a plastically deformed configuration of lower energy. To construct this path we consider the example configuration consisting of two dislocations, whose cores have distance a. In Lemma 3.3.1 we calculate an upper bound for the energy of this configuration using Theorem 3.2.3. With this estimate it is easy to show that in a proper regime of parameter the energy of a pair of dislocations get smaller than the energy of a sheared Bravais lattice for sufficiently large a and that the energy barrier scales at most like λ^2.

First we will define the example configuration χ_a. The configuration χ_a is based on an undeformed lattice $A_R^{-1}\mathbb{Z}^2$. We consider two dislocations. The centers of this dislocations have the distance $2a \geq O(\lambda)$ and the distance vector is be parallel to b. We introduce coordinates such that the first dislocation has the Burgers vector $b_1 = 2\pi b = 2\pi(1,0)$ and center $(-a, 0)$. The second has the Burgers vector $b_2 = -2\pi b$ and center $(a, 0)$. With ϕ_i we denote the angle between the distance vector of the centers of the dislocations and the distance vector between the center of the i dislocation and the point z. We assume $A_R^{-1} B_L(0) \subset \Omega$ with $L \geq O(a\lambda)$. For $z \in B_L(0)$ we define

$$\begin{aligned} \chi_a :=& \psi_a(\mathbb{Z}^2) \quad , \\ \psi(z) :=& A^{-1} z + u(z) \quad , \\ u(z) :=& u_1(z) + u_2(z) + u_L \quad , \\ u_i(z) :=& \frac{b_i}{2\pi} \phi_i \quad , \\ u_L(z) :=& -by\frac{a}{L^2} \quad . \end{aligned} \tag{3.3.1}$$

For $z \in B_{4\lambda}(\Omega)/B_L(0)$ u is discontinuous. However, since the atoms are moved parallel to the discontinuity, there are no collisions of atoms along the discontinuity line. Hence the hard core potential condition may be violated only directly at the center of the dislocation. There the atoms are moved to fulfill the hard core condition.

In some way this is a really bad example for a configuration with two dislocations since we just guessed the structure. However, we will calculate that the leading order part of the energy will come from $\lambda^4\|\nabla^2 u\|^2$ at the core of the dislocation. Therefore, there are lots of possible improvements, but they will not really make a difference as long as the core energy is so big and its estimate is not better. More Information about dislocations can be found in [6].

Now, we proof that the difference between the energy of the example configuration and the energy of the undeformed lattice, can be bounded from above by one term for the core energy that scales like λ^2 and on term for the elastic relaxation scaling like $a(\nabla F_{av})(b^\perp \times b)$ and many lower order contributions. The logarithmic part of the elastic energy is a lower order contribution in our model.

Lemma 3.3.1. *There exists $\hat{\lambda} \in \mathbb{R}$ and $\hat{\epsilon} > 0$ such that for all $\lambda > \hat{\lambda}$ and all $A_R \in Gl_d(\mathbb{R})$ with $F(A_R) \le \hat{\epsilon}$ the configuration χ_a of two dislocations, as defined above in* (3.3.1)*, has energy*

$$\begin{aligned} H_\lambda(\chi_a) - H_\lambda\left(A_R^{-1}\mathbb{Z}^d\right) =& 2\pi \det A_R^{-1}\hat{r}^2\delta h_{max} + \frac{8\pi C_Q|A_R^4|b^2\lambda^4}{(\hat{r}-3A_R\lambda)^2} \\ &+ 4\pi(\nabla F)_{av}\left(A_R^{-1}\right)\left[b^\perp \otimes e_1\right] \\ &+ 2\|(\nabla^2 F)_{av}\left(A_R^{-1}\right)\|\pi b^2 \ln(\frac{2a}{\hat{r}}) + O\left(\ln\left(\frac{a}{\hat{r}}\right)\right) \\ &+ O(\lambda) + O(a^6L^{-5}\lambda) + O(a^2\lambda^3L^{-3}) \\ &+ O(a^3L^{-2}) + O(a\lambda L^{-1}) \quad , \end{aligned} \tag{3.3.2}$$

where

$$\begin{aligned} \delta h_{max} =& \left(\vartheta(\det E - \det A_R) - F(A_R) + \left\|E^{-1}\right\|^2 \int_{[0,1]^d} W(\tau)d\tau \det A_R\right) \quad , \\ \hat{r} =& 3|A_R|\lambda\left(1 + \max\left\{\left(\frac{|b|c_6}{\Theta_W}\det A_R\right)^{\frac{1}{2}}, \left(3\frac{|b|c_6}{\Theta_W}\det|A_R|\right)^{1/3}\right\}\right) \quad . \end{aligned} \tag{3.3.3}$$

and c_6 is as in Lemma 2.2.7.

Proof. The gradient in polar coordinates is

$$\nabla\psi(r,\phi) = e_r\partial_r\psi(r,\phi) + \frac{1}{r}e_\phi\partial_\phi\psi(r,\phi) \quad . \tag{3.3.4}$$

We get

$$\begin{aligned}\nabla u_i =& b_i \otimes r^{-1} e_{\phi i} \quad , \\ \nabla^2 u_i =& - b_i r_i^{-2} \otimes (e_{ri} \otimes e_{\phi i} + e_{\phi i} \otimes e_{ri}) \quad , \\ \nabla^3 u_i =& 2 b_i r_i^3 \otimes (e_{ri} \otimes e_{\phi i} \otimes e_{\phi i} + e_{\phi i} \otimes e_{ri} \otimes e_{\phi i} + e_{\phi i} \otimes e_{\phi i} \otimes e_{ri} - e_{\phi i} \otimes e_{\phi i} \otimes e_{\phi i}) \, .\end{aligned} \tag{3.3.5}$$

In particular $|\nabla u_i| \leq |b| r_i^{-1}$ and $|\nabla^2 u_i| \leq 2|b| r_i^{-2}$ and $|\nabla^2 u_i| \leq 8|b| r_i^{-3}$. We consider the set of regular positions

$$\begin{aligned}\tilde{\Omega} :=& B_{\tilde{L}}(0) \, / \, (B_{\hat{r}}(a,0) \cup B_{\hat{r}}(-a,0)) \quad , \\ \tilde{L} :=& L - 2|A_R|\lambda \quad , \\ \hat{r} :=& 3|A_R|\lambda \left(1 + \max \left\{ \left(\frac{|b| c_6}{\Theta_W} \det A_R \right)^{\frac{1}{2}} , \left(3 \frac{|b| c_6}{\Theta_W} \det A_R \right)^{1/3} \right\} \right) \quad .\end{aligned} \tag{3.3.6}$$

There is a circles of radius $\hat{r}$ around the centers of the dislocations, because the derivative of u is not bounded there. Furthermore, the regular area does not cover the whole ball $B_L(0)$, because u is not differentiable at the boundary. However, we can use this estimate for point z close tho the x-axis even for $x \in (-a, a)$, since we can describe the atoms in a $B_{2\lambda}$ with a continuous expansion of $\tilde{u}$ with $\nabla \tilde{u}(\tilde{z}) = \nabla u(\tilde{z})$. BDue to $|\nabla u_i| \leq |b| r_i^{-1}$ we know that $\nabla \psi(z) = A_R^{-1} + O(\lambda^{-1})$. Hence, for large enough λ for every $\tilde{z}$ with $|\psi(\tilde{z}) - \psi(z)| \leq 2\lambda$, we have

$$\begin{aligned}\lambda^2 |\nabla^2 u(\tilde{z})| \leq& |\nabla^2 u_1| + |\nabla^2 u_1| + O(L^{-1}) \leq 2|b| \left(r_1^{-2} + r_1^{-2} \right) O(L^{-1}) \quad , \\ \leq& 4|b| \hat{r}_0^{-2} + O(L^{-1}) \leq 1/4 \Theta_W c_6^{-1} | \left(\nabla \psi(z) \right)^{-1} |^{-2} \quad , \\ \lambda^3 |\nabla^3 u(\tilde{z})| \leq& |\nabla^3 u_1| + |\nabla^3 u_1| \leq 2|b| \left(r_1^{-3} + r_1^{-3} \right) \leq 8|b| \hat{r}_0 \\ \leq& 3/8 \Theta_W c_6^{-1} | \left(\nabla \psi(z) \right)^{-1} |^{-2} \quad .\end{aligned} \tag{3.3.7}$$

The regular area $\tilde{U}$ satisfy Theorem 3.2.3.

$$\begin{aligned}E_{reg} =& \int_{\psi(\tilde{\Omega})} \hat{h}(\chi, x) dx - \int_{A_R^{-1} \tilde{\Omega}} \hat{h}(A_R^{-1} \mathbb{Z}, x) dx \\ =& \int_{\tilde{\Omega}} (\nabla F)_{av} \left(A_R^{-1} \right) [\nabla u(z)] + \frac{1}{2} (\nabla^2 F)_{av} \left(A_R^{-1} \right) [\nabla u(z)] \, dz \\ &+ \int_{\tilde{\Omega}} \int_{[-\frac{1}{2}, \frac{1}{2}]^d} (\nabla F)_{loc} \left(\nabla \psi(z - w), z \right) [\nabla^2 \psi(z) w] + O(\nabla^3 \psi) + O(\nabla^2 \psi^2) dw dz \\ &+ \int_{\tilde{\Omega}} C_Q \lambda^4 |(\nabla \psi(z))^{-1}|^4 \int_{\tilde{\Omega}} \max_{B_{2\lambda}(\psi(z))} \{ \| \nabla^2 \psi(\psi^{-1}(y)) \| \}^2 dz + |X_S - X_S^G| \\ &+ \int_{\tilde{\Omega}} 0(1) \nabla^2 \psi(z) + O(\lambda^2) \max_{B_{2\lambda}(\psi(z))} \| \nabla^3 \psi \| \left(\psi^{-1}(y) \right) dz \quad .\end{aligned} \tag{3.3.8}$$

We note that $\psi(\tilde{\Omega})$, $A_R^{-1}\tilde{\Omega}$ and $B_{2\lambda}(\Omega)$ are in fact three different sets. However, in $B_{2\lambda}(\Omega)/\psi(B_L(0))$ the lattice and the example configuration are equal. In $B_{2\lambda}(\Omega)/B_{2\lambda}(\psi(B_L(0)))$ the energy density of the deformed configuration and the lattice are equal. Between $\psi(\tilde{\Omega})$ and $B_{2\lambda}(\Omega)/B_{2\lambda}(\psi(B_L(0)))$ there is an area of measure $O(\lambda L)$ We call the contribution of this area the boundary energy E_{Bound} Additionally, there is an area of size λ^2 in the center of each dislocation, that is not covered by $\psi(\tilde{\Omega})$. We call the contribution of this energy the core energy E_{Core}. Last, $\psi(\tilde{\Omega})$ and $A_R^{-1}\tilde{\Omega}$ are nearly the same set but not exactly. We call this energy of the misfit E_{mis} and obtain

$$H_\lambda(\chi) - H_\lambda(A_R^{-1}\mathbb{Z}^d) \leq E_{Core} + E_{Bound} + E_{mis} + E_{reg} \quad . \tag{3.3.9}$$

The core energy E_{Core} First, the center of the dislocations are not covered by $\psi(\tilde{\Omega})$. We use the general upper bound for the energy density from Lemma 2.2.3

$$\hat{h}_\lambda(x,\chi) \leq \vartheta \det E - \vartheta\rho_\lambda + \left\|E^{-1}\right\|^2 \int_{[0,1]^d} W(\tau) d\tau \rho_\lambda \quad . \tag{3.3.10}$$

The area not included in $\psi(\tilde{\Omega})$ is the image of two circles of radius $\hat{r}^2$ has the area $2\pi\hat{r}^2 \det A_R^{-1} + O(\lambda^{-1})$

$$\delta E_{core} = 2\pi \det A_R^{-1} \hat{r}^2 \vartheta \left(\det E - \det A_R\right) - F(A_R) + \left\|E^{-1}\right\|^2 \int_{[0,1]^d} W(\tau) d\tau \det A_R. \tag{3.3.11}$$

The energy of the boundary We calculate the deformation $u(z)$ at the boundary of $\tilde{\Omega}$. If we move the whole line connecting the point z with the center of a dislocation parallel to the x-axis, the angle do not change. If ϕ is the angle between the x-axis and the position vector z, $B_L(0)$ we get for the points at the boundary

$$\begin{aligned}
u(z) =& u_1(z) + u_2(z) + u_L \\
=& b\left(\phi_1(z) - \phi_2(z)\right) - 2by\frac{a}{L^2} \\
=& b\left(\phi(z+a) - \phi(z-a)\right) - 2by\frac{a}{L^2} \\
=& 2b\nabla\phi(z)(a,0) + 1/3b\nabla^3\phi(\tilde{z})((a,0)^3) - 2by\frac{a}{L^2} \\
=& b_i \otimes r^{-2}(y,-x)\cdot(a,0) - 2by\frac{a}{L^2} + O(a^3L^{-3}) \\
=& O(a^3L^{-3}) \quad .
\end{aligned} \tag{3.3.12}$$

Since the boundary zone is an domain of width $O(\lambda)$, the derivative of u is relevant at the boundary too. In the same way for z at a $O(\lambda)$ distance to the boundary of $\tilde{\Omega}$ we get

$$\begin{aligned}\nabla u(z) =& b\left(\nabla\phi(z+a) - \nabla\phi(z-a)\right) - 2b\frac{a}{L^2}X \\ =& 2b\nabla^2\phi(\tilde{z})((a,0),X) - 2b\frac{a}{L^2}X \\ =& O(\frac{a}{L^2})X \quad .\end{aligned} \tag{3.3.13}$$

In a 4λ neighborhood of the boundary we get

$$|u(z)| \leq O(a^3L^{-3}) + O(a\lambda L^{-2}) \quad . \tag{3.3.14}$$

Lemma 2.2.9 says that we can estimate the energy difference between our configuration and that of a lattice from above with the effective particle potential and the local effective elastic potential. According to Lemma 3.1.10 the minima of the effective particle potential of the lattice are exactly at the lattice positions. And the potential is quadratic around them. The increase of the energy density δh_B at the boundary is

$$\delta h_B = O(\delta u^2) = O(a^6L^{-6}) + O(a^2\lambda^2L^{-4}) \quad . \tag{3.3.15}$$

The energy contribution of the boundary is given by δH_B. Hence, we get

$$E_{Bound} = O(a^6L^{-5}\lambda) + O(a^2\lambda^3L^{-3}) \quad . \tag{3.3.16}$$

Now, we estimate the different terms of (3.3.8). We do not need to treat the boundary between $\tilde{\Omega}_U$ and $\tilde{\Omega}_O$, because in a 2λ neighborhood of this boundary the atom configuration is equal to $A_R^{-1}z_i + \tilde{u}(z_i)$ with a continuous $\tilde{u}_i$ and $\nabla u = \nabla\tilde{u}$

The misfit energy E_{mis} The sets $\psi\left(\tilde{\Omega}\right)$ and $A_R^{-1}\tilde{\Omega}$ are different because of the $u(z)$ at the boundary of $\tilde{\Omega}$. We know that at the boundary of $B_{\tilde{L}}$ the deformation u is $O(a^3L^{-3}) + O(a\lambda L^{-2})$ The energy is $O(1)$. Hence we get

$$E_{mis} = O(a^3L^{-2}) + O(a\lambda L^{-1}) \quad . \tag{3.3.17}$$

Since the Burgers Vector is parallel to the the x-axis, there is no misfit between $\psi\tilde{\Omega}_U$ and $\tilde{\Omega}_O$ Otherwise, we would get an $O(a)$ term here.

Estimate for the part linear in ∇u The same term appears in the linear elasticity theory for dislocations. Hence, it was treated extensively (see for example [3]) For the linear map $(\nabla F)_{av}\left(A_R^{-1}\right)$ there exists a matrix such that the application of the map on a matrix A equals the scalar product of A with the map. We call this matrix $(\nabla F)^{av}$.

$$\sum_{i,j}(\nabla F)^{av}_{i,j}A_{i,j} = \langle(\nabla F)_{av}, A\rangle =: (\nabla F)_{av}\left(A_R^{-1}\right)[A] \quad . \tag{3.3.18}$$

With this matrix we can write

$$\int_{\tilde{\Omega}_1} (\nabla F)^{av} \left(A_R^{-1}\right) [\nabla u(z)]\, dz = \int_{\tilde{\Omega}_1} \langle (\nabla F)_{av}, \nabla u(z)\rangle\, dz$$
$$= \int_{\tilde{\Omega}_1} \operatorname{div} \left(u_(z)(\nabla F)_{av}\right) dz \quad . \tag{3.3.19}$$

By Gauss theorem we have

$$\int_{\tilde{\Omega}_1} (\nabla F)_{av} \left(A_R^{-1}\right) [\nabla u(z)]\, dz = \int_{\partial\tilde{\Omega}_1} \left\langle \left((\nabla F)_{av} u_(z)\right), dn\right\rangle$$
$$=(\nabla F)_{av} \left(A_R^{-1}\right) \left(\int_{\tilde{\Omega}_1} u(z) \otimes dS\right) \quad . \tag{3.3.20}$$

The boundary of $\tilde{\Omega}$ consists of the boundary of $\partial B_{\tilde{L}}(0)$ and S_a the section of the $x - axis$ between the dislocations. We denote S_a with S_a^-, if its is approached coming from negative y and S_a^-, if it is approached coming from positive y.

$$S_a :=\{(x,0), |x \in (-a+\hat{r}, a-\hat{r})\} \quad ,$$
$$\partial\tilde{\Omega} =S_a^+ \cup S_a^- \cup \partial B_{\hat{r}}(-a,0) \cup \partial B_{\hat{r}}(-a,0) \cup \partial B_{\tilde{L}}(0) \quad . \tag{3.3.21}$$

The important contribution comes from S_a the boundary between the dislocations on the x-axis. At this boundary the normal vector changes sign depending on the side we approaching it. On the other side u is discontinuous there too. If we come from above, it holds $\lim_{y\to 0+} \phi_1 = 0$ and $\lim_{y\to 0+} \phi_2 = \pi$. In contrast, if we approach from below, it holds $\lim_{y\to 0-} \phi_1 = 2\pi$ and $\lim_{y\to 0-} \phi_2 = \pi$. Therefore, we have

$$(\nabla F)_{av} \left(A_R^{-1}\right) \int_{S_a^+ \cup S_a^-} [u(z) \otimes dS]$$
$$= \int_{-a+\hat{r}}^{a+\hat{r}} (\nabla F)_{av} \left(A_R^{-1}\right) \left[\lim_{y\to 0+} u(x,y) \otimes (-e_1) + \lim_{y\to 0-} u(x,y) \otimes (e_1) dx\right] dx \tag{3.3.22}$$
$$=a(\nabla F)_{av} \left(A_R^{-1}\right) [b \otimes e_1] \left(\lim_{y\to 0+} (\phi_2 - \phi_1) + \lim_{y\to 0-} (\phi_1 - \phi_2)\right)$$
$$= (2a - \hat{r})\, (\nabla F)_{av} \left(A_R^{-1}\right) [b_1 \otimes e_1] \quad . \tag{3.3.23}$$

We have already calculated that on the boundary of $B_{\tilde{L}}(0)$ Hence, it holds

$$|u(z)| \leq O(a^3 L^{-3}) + O(a\lambda L^{-2}) \quad . \tag{3.3.24}$$

We get

$$(\nabla F)_{av} \left(A_R^{-1}\right) \left[\int_{\partial B_{\tilde{L}}(0)} u(z) \otimes dS\right] = O(a^3 L^{-2}) + O(a\lambda L^{-1}) \quad . \tag{3.3.25}$$

Finally, on the circles around the dislocations we have

$$\begin{aligned}
&(\nabla F)_{av}\left(A_R^{-1}\right)\left[\int_{\partial B_{\hat{r}}(-a,0)} u(z)\otimes dS\right] \\
=&(\nabla F)_{av}\left(A_R^{-1}\right)\left[\int_{\partial B_{\hat{r}}(-a,0)} (u_1(z)+u_2(z)+u_L)\otimes dS\right] \\
=&\hat{r}\int_0^{2\pi}(\nabla F)_{av}\left(A_R^{-1}\right)[b\otimes e_{r1}]\left(\phi_1-\phi_2-y\frac{a}{L^2}\right)d\phi_1 \\
&+O((\nabla F)_{av}\hat{R})+O((\nabla F)_{av}\lambda) \quad .
\end{aligned} \tag{3.3.26}$$

In summary, we get

$$\begin{aligned}
\int_{\tilde{\Omega}_1}(\nabla F)_{av}\left(A_R^{-1}\right)[\nabla u(z)]\,dz =&2a(\nabla F)_{av}\left(A_R^{-1}\right)[b_1\otimes e_1] \\
&+O(a^3L^{-3})+O(a\lambda L^{-2})+O((\nabla F)_{av}\lambda) \quad .
\end{aligned} \tag{3.3.27}$$

Estimate for the part quadratic in ∇u Also this term appears in the linear elasticity theory for dislocations (see for example [3]). We present a calculation for completeness. We estimate

$$\int \tilde{\Omega}\frac{1}{2}(\nabla^2 F)_{av}\left(A_R^{-1}\right)[\nabla u(z)]\,dz \le \frac{1}{2}|^2(\nabla^2 F)_{av}\left(A_R^{-1}\right)\| \int \tilde{\Omega}\|\nabla u(z)\|^2 dz \quad . \tag{3.3.28}$$

We need an estimate for $\int_{\tilde{\Omega}}\|\nabla u\|^2 dz$. We realize that

$$\Delta u_i = b\,\mathrm{div}\,(e_{\phi i}) = b\left(e_r\partial_r+\frac{1}{r}e_\phi\partial_\phi\right)e_\phi = 0 \quad . \tag{3.3.29}$$

Additionally, it holds $\Delta u_L = 0$, because it is a linear function. Therefore, due to the linearity of the Laplace-operator, u is a solution of the laplace equation. Using Gauss theorem we obtain

$$\begin{aligned}
\int_{\tilde{\Omega}}\|\nabla u\|dz =& \int_{\tilde{\Omega}}\partial_i u_k\partial_i u_k dz \\
=& \int_{\tilde{\Omega}}\partial_i\left(u_k\partial_i u_k\right)-u_k\partial_i\partial_i u dz \\
=& \int_{\partial\Omega}u_k\partial_i u_k dF_i \quad .
\end{aligned} \tag{3.3.30}$$

The section of the x-axis $S_a = \{(x,0),|x\in(-a+\hat{r},a-\hat{r})\}$ can be treated as in the case of the linear contribution

$$\begin{aligned}\int_{S_a^+\cup S_a^-} u_k\partial_i u_k dF_i =& \int_{-a+\hat{r}}^{a-\hat{r}} \partial_1 u_k \left(\lim_{y\to 0-} u_k(x,y) - \lim_{y\to 0+} u_k(x,y)\right) dx \\ =&2\pi b^2 \int_{-a+\hat{r}}^{a-\hat{r}} \left(r_1^{-1} + r_2^{-1} - \frac{a}{L^2}\right) \\ =&4\pi b^2 \ln\left(\frac{2a-\hat{r}}{\hat{r}}\right) - 2\pi b^2 \frac{a^2}{L^2} \quad . \end{aligned} \tag{3.3.31}$$

For the outer boundary $\partial B_{\tilde{L}}(0)$ we get

$$\begin{aligned}\int_{\partial B_{\tilde{L}}} u_k\partial_i u_k dF_i =&O(L)\left(O(a^3L^{-3}) + O(a\lambda L^{-2})\right)O(a\lambda L^{-2}) \\ =&O(a^4L^{-4}) + O(a^2\lambda L^{-3} \quad . \end{aligned} \tag{3.3.32}$$

On the boundary around the dislocation we notice that $\nabla u = r_i^{-1} b \otimes e_{\phi i}$ is orthogonal to e_{ri} the normal vector to the surface and we get

$$\begin{aligned}\int_{\partial B_{\tilde{L}}} u_k\partial_i u_k dF_i =&\hat{r}\int_0^2 \pi u(\nabla u_1 + \nabla u_2 + \nabla u_L) e_{\phi 1} d\phi_1 \\ &+ \hat{r}O(1\hat{r})(O(a^{-1}) + O(aL^{-2})) = (O(a^{-1}) + O(aL^{-2})) \quad . \end{aligned} \tag{3.3.33}$$

Therefore, we obtain

$$\begin{aligned}&\int_{\tilde{\Omega}} \frac{1}{2}(\nabla^2 F)_{av}\left(A_R^{-1}\right)[\nabla u(z)]\, dz \\ \leq& 2\pi|^2(\nabla^2 F)_{av}\left(A_R^{-1}\right)\|b^2\left(\ln\left(\frac{2a-\hat{r}}{\hat{r}}\right)\right) \\ &+ O(a^2L^{-2}) + (O(a^{-1}) + O(aL^{-2})) + O(a^4L^{-4}) + O(a^2\lambda L^{-3}) \quad . \end{aligned} \tag{3.3.34}$$

The contribution of the term quadratic in $\nabla^2 u$ We search for an upper bound for

$$E_{22} = \int_{\tilde{\Omega}} C_Q\lambda^4 \int_{\tilde{\Omega}} |(\nabla\psi(z))^{-1}|^4 \max_{B_{2\lambda}(\psi(z))}\{\|\nabla^2\psi(\psi^{-1}(y))\|\}^2 dz \quad . \tag{3.3.35}$$

For $y \in \psi^{-1}\left(B_{2\lambda}\psi\tilde{\Omega}\right)$ we have $|(\nabla\psi(z))^{-1}|^4 \leq |A_R|^4 + O(\lambda^{-1})$. Furthermore, it holds $\nabla^2 u_L = 0$ and wee can estimate

$$\begin{aligned}\|\nabla^2 u(z)\|^2 =&\|\nabla^2 u_1 + \nabla^2 u_2\|^2 = 2\|\nabla^2 u_1\|^2 + 2|\nabla u_2\|^2 \\ =&4b^2\left(r_1^{-4} + r_2^{-4}\right) \quad . \end{aligned} \tag{3.3.36}$$

We need to estimate $\max_{B_{2\lambda}(\psi(z))}\{\|\nabla^2\psi(\psi^{-1}(y))\|\}^2$ and not just $\nabla^2\psi(z)$ With $\nabla\psi(y) = A_R^{-1} + 0(\lambda^{-1})$ and $y\psi^{-1} \in B_{2\lambda}(\psi(z))$ we know that

$$|r_i(z) - r_i(y)| \leq |z - y| \leq |A_R|3\lambda = \delta r \quad . \tag{3.3.37}$$

Our estimates (3.3.36) turns into

$$\max_{B_{2\lambda}(\psi(z))}\{\|\nabla^2\psi(\psi^{-1}(y))\|\}^2 dz \leq 4b^2\left((r_1-\delta r)^{-4} + (r_2 - \delta r)^{-4}\right) \quad . \tag{3.3.38}$$

We can integrate this estimate and get

$$\begin{aligned}\int_\Omega \frac{1}{(r_1-\delta r)^4} + \frac{1}{(r_2-\delta r)^4} dz \leq& 2\left(2\pi\int_{\hat r}^\infty \frac{1}{(r-\delta r)^4} r dr\right)\\ =&4\pi\left(\int_{\hat r - \delta r}^{2a-\delta r}\frac{\tilde r + \delta r}{\tilde r^4} d\tilde r\right)\\ =&\frac{2\pi}{(\hat r - \delta r)^2} \quad .\end{aligned} \tag{3.3.39}$$

Furthermore, we have

$$\begin{aligned}E_{22} =& \int_{\tilde\Omega} C_Q|A_R|^4\lambda^4\int_{\tilde\Omega}\max_{B_{2\lambda}(\psi(z))}\{\|\nabla^2\psi(\psi^{-1}(y))\|\}^2 dz\\ \leq&\frac{8\pi C_Q|A_R|^4b^2\lambda^4}{(\hat r-\delta r)^2} \quad .\end{aligned} \tag{3.3.40}$$

Since $\hat r$ and δr are $O(\lambda)$, this contribution is $O(\lambda^2)$.

Estimate for the Error terms in E_{reg} The formula (3.3.8) for E_{ref} the energy of the regular area includes the volume error terms

$$\begin{aligned}E_{reg1} =& \int_{\tilde\Omega}\int_{[-\frac12,\frac12]^d}(\nabla F)_{loc}\left(\nabla\psi(z-w), z\right)[\nabla^2\psi(z)w]dwdz \quad ,\\ E_{reg2} =& \int_{\tilde\Omega} 0(1)\nabla^2\psi(z)dz \quad ,\\ E_{reg3} =& \int_{\tilde\Omega}\int_{[-\frac12,\frac12]^d} O(\nabla^3\psi) + O(\left|\nabla^2 u\right|^2)dwdz \quad ,\\ E_{reg4} =& O(\lambda^2)\max_{B_{2\lambda}(\psi(z))}\|\nabla^3\psi\|\left(\psi^{-1}(y)\right)dz \quad .\end{aligned} \tag{3.3.41}$$

Furthermore, we have the surface error term $|X_S - X_S^G|$. We consider E_{reg1} first. If $F(G,z)$ is differentiable in a neighborhood of A_R^{-1}, then E_1 is actually $\int O(|\nabla^2 u|^2)dz$. Otherwise we can estimate

$$\int_{\tilde\Omega}\int_{[-\frac12,\frac12]^d}(\nabla F)_{loc}\left(\nabla\psi(z-w), z\right)[\nabla^2\psi(z)w]dwdz \leq \int_{\tilde\Omega} O(\nabla^2 u(z))dz \quad . \tag{3.3.42}$$

$\nabla^2 u = O(r^{-2})$ near the dislocations and $O(ar^{-3})$ for $r >> a$. We get

$$\begin{aligned}E_{reg1}z \leq & CO\left(\nabla F_{\text{loc}}\left(A_R^{-1}\right)\int_{\hat{r}}^{a} O(r^{-2})rdr + \int_{a}^{L} O(ar^{-3})rdr\right) \\ = & O\left(\left|\nabla F_{\text{loc}}\left(A_R^{-1}\right)\right|\ln\left(\frac{a}{\hat{r}}\right)\right) + O\left(a^{-2}\right) \quad .\end{aligned} \tag{3.3.43}$$

In the same way we can estimate E_{reg2} to be

$$E_{reg2}z = O\left(\ln\left(\frac{a}{\hat{r}}\right)\right) + O\left(a^{-2}\right) \quad . \tag{3.3.44}$$

Next, we consider E_{reg3}. We calculated an upper bound for $\|\nabla^2 u\|^2$ already. Only this term does not have the factor λ^4. Hence, this term is $O(\lambda^{-2})$. The third order term $\nabla^3 u$ is $O(r^{-3})$

$$\begin{aligned}E_{reg3}z \leq & \int_{\hat{r}}^{a} O(r^{-3})rdr + \int_{\hat{r}}^{L} O(r^{-3})rdr + O(\lambda^{-2}) \\ = & O(\frac{1}{\hat{r}}) + O(\lambda^{-2}) = O(\lambda^{-1}) \quad .\end{aligned} \tag{3.3.45}$$

Analogous to our calculation for $\max_{B_{2\lambda}(\psi(z))} \|\nabla^2 u\|^2 \left(\psi^{-1}(y)\right)$ we get for E_{reg4}

$$E_{reg4} = \lambda^2 \int_{\hat{r}-\delta r}^{\infty} O(r^{-3})rdr = O(\lambda) \quad . \tag{3.3.46}$$

Finally, the boundary term $|X_S - X_S^G|$. According to Theorem 3.2.3)

$$\begin{aligned}|X_S - X_S^G| \leq & \int_{[-\frac{1}{2},\frac{1}{2}]^d} \int_{\left(w+\tilde{\Omega}\right)/\tilde{\Omega}} \left|(\nabla F)_{loc}\left(A_R^{-1}\right)\right| |\nabla u(\tilde{z})| + O(\nabla u^2) d\tilde{z}) dw \\ & + \int_{[-\frac{1}{2},\frac{1}{2}]^d} \int_{\tilde{\Omega}/\left(\tilde{\Omega}+w\right)} |(\nabla F)_{loc}\left(A_R^{-1} + u(\tilde{z}-w)\right)| |u(\tilde{z})| dw \\ & + \int_{[-\frac{1}{2},\frac{1}{2}]^d} \int_{\left(\left(w+\tilde{\Omega}\right)/\tilde{\Omega}\right)\cup\left(\tilde{\Omega}/\left(\tilde{\Omega}+w\right)\right)} O(\lambda^{-2}\nabla u) + O\left(((\nabla u)^2\right) d\tilde{z} dw \quad .\end{aligned} \tag{3.3.47}$$

We remember that at the boundary of our regular area $\tilde{\Omega}$ the gradient of u fulfills $\nabla u = O(aL^{-2})$. The sets $\left(w+\tilde{\Omega}\right)/\tilde{\Omega}$ and $\tilde{\Omega}/\left(\tilde{\Omega}+w\right)$, that are located at the boundary of $B_{\tilde{L}(0)}$, have a maximal broadness of $|w|$ and a length of L. The area of these sets scales like $O(L)$. $O(\lambda^{-2}\nabla u)$ and $O\left(((\nabla u)^2\right)$ are much smaller. Therefore, the contribution of the outer boundary scales like $O(aL^{-1})$ Additional, we have the boundary between $\tilde{\Omega}_L$ and $\tilde{\Omega}$. There the ∇u is $O(r^{-1})$ for $r < a$ and $O(ar^{-2})$ for $r \geq a$. We get

$$X_S - X_S^G \leq O\left(|\nabla F_{loc}\left(A_R^{-1}\right)| \ln\left(\frac{a}{\lambda}\right) + O(1)|\nabla F_{loc}\left(A_R^{-1}\right)\right) \quad . \tag{3.3.48}$$

□

Next, we use the result of Lemma 3.3.1 to construct a path for plastic relaxation with an energy barrier $O(\lambda^2)$. If there is a lattice vector $b \in A_R^{-1}\mathbb{Z}$ such that $\nabla F_a v(b \times b) < 0$ and the domain Ω is large enough, then there exists a continuous path of configurations, that starts at the undeformed Bravais lattice $A_R^{-1}\mathbb{Z}^d$, leads to a configuration of lower energy and has a energy barrier scaling like $O(\lambda^2)$. The path consists of a pair of dislocations with the burgers vectors b and $-b$ nucleated in one point and then moved apart.

Theorem 3.3.2. *There exits $\hat{\lambda} \in \mathbb{R}$ and $\hat{\epsilon} > 0$ such that for all $\lambda > \hat{\lambda}$, $A_R \in Gl_2(\mathbb{R})$, $b \in A_R^{-1}\mathbb{Z}^2$, $x_0 \in \Omega$ and $L > \hat{a}^{3/2}$ satisfying the assumptions*

1) $F(A_R) \leq \hat{\epsilon}$,

2) $(\nabla F)_{av}\left(A_R^{-1}\right)\left[b \otimes b^{\perp}\right] \leq 0$,

3) $B_{|A_R^{-1}|L}(x_0) \subset \Omega$,

there exists a path continuous $\chi(s) : [0,1] \to (\mathbb{R}^2)^N$ with the properties

1) $\chi(0) = A_R^{-1}\mathbb{Z}^2 \cap B_{4\lambda}(\Omega)$

2) $\chi \cap B_{4\lambda}(\Omega)/\Omega = A_R^{-1}\mathbb{Z}^d(\Omega)/\Omega$

3) $H(\chi(1)) < H(A_R^{-1}\mathbb{Z}^2 \cap B_{4\lambda}(\Omega))$

4) $\max_{s\in[0,1]} H(\chi(s)) \leq H(0) + C_{max}\lambda^2$

Here C_{max} and $\hat{a}$ are defined as

$$\begin{aligned} C_{max} :=& 2\pi\lambda^{-2}\hat{r}^2\left(\vartheta\left(\det EA_R^{-1} - 1\right) - F(A_R)\det A_R^{-1} + \left\|E^{-1}\right\|^2\int_{[0,1]^d} W(\tau)d\tau\right) \\ &+ \frac{9\pi C_Q|A_R|^4 b^2\lambda^2}{(\hat{r} - 3A_R\lambda)^2} \quad , \\ \hat{a} =& \frac{C_{max}\lambda^2}{|2\pi(\nabla F)_{av}\left(A_R^{-1}\right)[b \otimes (0,1)]\,|} \quad . \end{aligned} \tag{3.3.49}$$

Proof. We introduce our coordinate system with origin x_0 and x- Axis parallel to the vector b. We define the path

$$\chi(s) = \chi_{\hat{a}t} \quad , \tag{3.3.50}$$

where $\chi_{\hat{a}t}$ is the example configuration defined in Section 3.3.1. For $a = 0$ th dislocations chancel. The starting value $\chi(0) = A_R^{-1}\mathbb{Z}^d \cap B_{4\lambda}(\Omega)$ is assumed. Due to $\chi(s)/\psi\tilde{\Omega} = A_R^{-1}\mathbb{Z}^d/\psi\tilde{\Omega}$ and $\psi\tilde{\Omega} \subset B_{|A_R^{-1}|}(0)$ the boundary condition $\chi(s)/\psi\tilde{\Omega} \subset A_R^{-1}\mathbb{Z}^d/\psi\tilde{\Omega}$ is fulfilled. The positions of the dislocations change continuously with t. The angels ϕ_i are continuous functions of the vector between a position in space and the position of the centers of the dislocations everywhere but in the centers of the dislocation. Therefore, the atom positions are continuous functions of $\chi(s)$ and defines a continuous path. [4] According to Lemma 3.3.1 the energy of $\chi(s)$ is

$$\begin{aligned} H_\lambda(\chi(s)) - H_\lambda\left(A_R^{-1}\mathbb{Z}^d\right) \leq & C_{max}\lambda^2 + 4\pi(\nabla F)_{av}\left(A_R^{-1}\right)[b\otimes(0,t\hat{a})] \\ & + \frac{1}{2}\|(\nabla^2 F)_{av}\left(A_R^{-1}\right)\|\pi b^2\left(\ln\left(\frac{2\hat{a}t}{\lambda}\right)\right) + O\left(\ln\left(\frac{\hat{a}t}{\hat{r}}\right)\right) \\ & + O(\lambda) + O(\hat{a}^6 t^6 L^{-5}\lambda) + O(\hat{a}^2 t^2 \lambda^3 L^{-3}) \\ & + O(\hat{a}^3 t^3 L^{-2}) + O(a\lambda L^{-1}) \quad . \end{aligned} \tag{3.3.51}$$

If it holds $L > \hat{a}^{3/2}$, then we have for all $t \in [0,1]$

$$\begin{aligned} O\left(\ln\left(\frac{\hat{a}t}{\hat{r}}\right)\right) \leq & O(\lambda) \quad , \\ O(\hat{a}^6 t^6 L^{-5}\lambda) \leq & O(\lambda^{-2}) \quad , \\ O(\hat{a}^2 t^2 \lambda^3 L^{-3}) \leq & O(\lambda^{-2}) \quad , \\ O(\hat{a}^3 t^3 L^{-2}) \leq & O(1) \quad , \\ O(a\lambda L^{-1}) \leq & O(\lambda^{-1}) \quad . \end{aligned} \tag{3.3.52}$$

All these terms are smaller $O(\lambda)$ and does not change the scaling of the upper bound. Since $4\pi(\nabla F)_{av}\left(A_R^{-1}\right)[b\otimes(0,t\hat{a})]$ is negative, we have for all $t \in [0,1]$

$$\chi(s) - H_\lambda \leq C_{max}\lambda^2 \quad . \tag{3.3.53}$$

Finally, by construction we have

$$H_\lambda(\chi(1)) - H_\lambda(A_R^{-1}\mathbb{Z}^d \cap B_{4\lambda}(\Omega)) \leq -C_{max}\lambda^2 + O(\lambda) \quad . \tag{3.3.54}$$

Hence, the path leads to an decrease of energy. □

Perspective 3.3.3. Dislocations with empty core If one wants to get a better upper bound for the energy barrier, one should consider the possibility, that in the core of the dislocations the effective elastic particle potential (see definition 2.2.8) is very high. Hence, we know that we can reduce the energy removing atoms from the cores of the dislocations and move them near to occupied lattice position somewhere far from the dislocations. This will reduce the leading order of the energy.

Further plastic relaxation:

[4] If one of the dislocations moves directly through on atom. The atom can have to be moved separately continuously, since this happens in the core region it does not change our estimates.

1) Finally, the dislocations will get close two the the boundary of the domain. Since we fixed the atoms of the boundary, the atoms can not adapt to the dislocation that leads to an increase of energy. In $O(\delta x)$ distance to a dislocation ∇u is $O(\delta x)$. If we want to reduce this over a $O(\delta x)$ distance to zero and have to pay $\lambda^4|\nabla^2 u|^2$ over the density, the cost scales like $O(\lambda^4 \delta x^{-3})$. The elastic gain from moving the dislocation further scales like $O(x + \delta x)$. If we minimize this cost, we get that we expect the dislocation to stop in distance $\delta x = O(\lambda^2)$ from the boundary.

2) After both dislocations have stopped further plastic relaxation needs the creation of a new pair of dislocations. Since the first two dislocation line, that has moved through the crystal, has reduced the elastic energy a little bit, ∇F is a little bit lower now. Hence, it will take a little bit longer to overcome the energy barrier. However the crystal is really big and we moved just one single dislocation. Therefore, the effect on the lattice is

$$A_2 - A - 1 = \frac{b}{L} < O(\lambda^{-3}) \quad . \tag{3.3.55}$$

We need to move $O(L)$ dislocations this way before we significantly change the lattice structure. And before the energy barrier changes significantly.

The situation in $3d$

We can do a similar calculation for $3D$. We use a dislocation line in shape of a closed loop of length $2\pi R$, given by a map $x_b[0,1] \to \mathbb{R}^3$. The dislocation line means that we prescribe on our local strain $G(z)$ the condition

$$\operatorname{rot} G(z) = \int_0^1 \delta(z - x_b(s)) \frac{dx_b(s)}{ds} \left| \frac{dx_b(s)}{ds} \right|^{-1} ds \quad . \tag{3.3.56}$$

We get an area of irregular points around the dislocation line with a radius scaling like $\hat{r} = O(\lambda)$. If the curvature of x_b is significantly smaller than $\hat{r}^{-1}$, the volume of the irregular area will be approximately $2\pi^2 R \hat{r}^2$. Hence, we have a core energy of

$$E^1_{core} = \pi \delta h_{max} \hat{r}^2 R = O(\lambda^2 R) \quad . \tag{3.3.57}$$

Furthermore, since $x_b[0,1]$ describes a dislocation line. For points with distance r to the dislocation, with a r bigger than $\hat{r}$ but smaller than the curvature of the dislocation line, we expect have $\nabla^2 u^2 = O(r^{-2})$. This leads to an energy density proportional to $b^2 \lambda^4 \|\nabla^2 u\|^2$. Integrated over the regular area close to the dislocation line this gives another contribution of order $E^2_{core} = O(\lambda^2 R)$. Therefore, in summary we expect a core energy of the form

$$E_{Core} \approx C_1 \lambda^2 R \quad . \tag{3.3.58}$$

The contribution of the elastic energy is

$$\int \tilde{F}(G(z))dz = \int \tilde{F}(A_R^{-1})dz + \int \nabla F_{av}\left(A_R^{-1}\right)\left(G(z) - A_R^{-1}\right)dz$$
$$+ \frac{1}{2}\int \nabla F_{av}\left(A_R^{-1}\right)\left(G(z) - A_R^{-1}, G(z) - A_R^{-1}\right)dz \quad . \qquad (3.3.59)$$

We expect the quadratic contribution to be dominated by the core energy or by the elastic energy gain for every radius r. A calculation for this energy contribution can be found in [2]. The first contribution is equal to the energy of the undeformed lattice. For the second contribution we use the condition prescribed by the dislocation. If we choose any surface S_b, that has the dislocation line as its boundary, it holds $x_b = \partial S_b$. The rest of the domain is simple connected and the rotation of $G(z)$ is zero there. Hence, $G(z)$ is the gradient of some $u(z)$ and we can use gauss theorem to integrate $u(z)$ over the boundary instead of $G(z)$ over the domain. The surface S_b appears two times as the boundary one time from below one time from above.

$$\int \left(G(z) - A_R^{-1}\right)dz = \int_{\partial\tilde{\Omega}} u(z)dS \quad . \qquad (3.3.60)$$

Since the normal vectors are flipped depending from which side of the boundary we are looking at it, the contribution of S_b is proportional to the discontinuity of $u(z)$.

$$\int_{S_b^+ \cup S_b^-} u(z)dS = \int_{S_b} u^+(z) - u^-(z) \otimes dS \quad . \qquad (3.3.61)$$

Since the gradient of $u(z)$ is $G(z)$, we can take for $z \in S_b$ any curve $x_z(0,1) \to \mathbb{R}^d$ connecting the two sides of the surface in z through the regular area. We calculate the discontinuity of u as the integral over G.

$$u^+(z) - u^-(z) = \int_0^1 \nabla u(x_z(\tilde{s}))d\tilde{z}$$
$$= \int_0^1 \nabla G(x_z(d\tilde{s}))d\tilde{s} \quad . \qquad (3.3.62)$$

On the other hand this is the integral over a closed loop of the differentiable vector field G. Therefore, according to stokes theorem this equals the integral of the rotation of G over any surface S_z with boundary x_z. But the rotation of G

is given by the dislocation and we get

$$\begin{aligned}\int_{S_b^+ \cup S_b^-} u(z) dS &= \int_{S_b} \int_0^1 \nabla G(x_z(\tilde{s})) d\tilde{s} \otimes dS \\ &= \int_{S_b} \int_{S_z} \operatorname{rot} G dS_z \otimes dS_b \\ &= \int_{S_b} b \otimes dS \quad .\end{aligned} \tag{3.3.63}$$

As in our calculation for $d = 2$ we expect the contributions of the other parts of the boundary to be small.

$$\int \nabla F_{av} \left(A_R^{-1}\right) \left(G(z) - A_R^{-1}\right) dz \quad . \tag{3.3.64}$$

For a circle of radius R we get

$$E_{el} \approx -C_2 R^2 |\nabla F_{av} \left(A_R^{-1}\right) (b \otimes n)| \quad . \tag{3.3.65}$$

Putting the core energy and the elastic energy together we get

$$\delta E(R) = C_1 R \lambda^2 - C_2 R^2 |\nabla F_{av} \left(A_R^{-1}\right) (b \otimes n)| \quad . \tag{3.3.66}$$

The R of maximal energy is then

$$R_{max} \approx \frac{C_1 \lambda^2}{2 C_2 \nabla F_{av} \left(A_R^{-1}\right) (b \otimes n)} \quad . \tag{3.3.67}$$

And the energy barrier is

$$E_{Bar} = \frac{C_1^2 \lambda^4}{2 C_2 \nabla F_{av} \left(A_R^{-1}\right) (b \otimes n)} \quad . \tag{3.3.68}$$

Nucleation Instead of creating a dislocation line we could also just move the atoms locally to fit the lattice E in a ball of radius R expanding outwards. This creates a cost at every point in 2λ distance from the surface of the ball.

$$E_{sur} = C_W \lambda R^{d-1} \quad . \tag{3.3.69}$$

On the other hand we gain a reduction in F energy for every point that is inside this ball.

$$E_{sur} = -C_F \left(F(A_R) - F(E)\right) R^d \quad . \tag{3.3.70}$$

We get an radius of maximal energy

$$R_{max} = \frac{(d-1) C_W}{d C_F \left(F(A_R) - F(E)\right)} \lambda \quad . \tag{3.3.71}$$

Furthermore, we get an energy barrier

$$E_{Bar} = -\frac{C_W^d}{\left(C_F\left(F(A_R) - F(E)\right)\right)^{d-1}}\lambda^d \quad . \tag{3.3.72}$$

For $d = 2$ the upper bound for the nucleation has the same scaling in λ as the dislocation. For $d = 3$ the barrier of the upper bound for the nucleation has a better scaling in λ. This is another sign that the core energy is too high in our model.

We also note that we want to study relaxation of lattices close to $SO_d(\mathbb{R})$. Our potential is convex there. Hence, $\nabla F_{av}\left(A_R^{-1}\right) = O(\text{dist}(A, SO_d(\mathbb{R})))$ but $(F(A_R) - F(E)) = O(\text{dist}(A, SO_d(\mathbb{R})))$ Therefore, in dimension two relaxation via dislocations is better than via nucleation, for configurations close to the groundstate.

Chapter 4

Lagrangian coordinates

4.1 Discrete Lagrangian coordinates

In this section we will develop a method to identify topological defects and later explain how this leads us to an estimate of the energy cost of such defects: For this we first prove that all points in a λ-ball around a regular point are regular with modified coefficients and a smaller $\tilde{\lambda}$. So, if we have two regular points with distance less than 2λ, the point between them will be regular for smaller λ. This way we can use Lemma 2.3.5 to show that the change of A between different regular points is a reparametrisation plus a small difference controlled by $\lambda^{-1}\sqrt{\epsilon_J}$, and that the change of τ between the points are given by $A\delta x$ a reparametrisation and a small difference controlled by $\sqrt{\epsilon_J}$. Therefore, for a sequence of regular points with $|y_{j+1} - y_j| < 1.5\lambda$ we get a reparametrisation in every point. If the sequence goes back to its starting point the composition of these reparametrisations will give us a topological invariant, which we call the generalized burgers vector. We use this to characterize topological defects, especially dislocations in the framework of our model. Furthermore, we get an upper bound on the possible changes of A and τ as sequence of regular points in terms of $\sum_j \sqrt{\epsilon_J}(y_j)$. So we can calculate how long a chain has to be to reach a certain change in the lattice parameters. We will conclude that a barrier between different crystal structures consists of irregular points and needs a width of at least λ or we can jump over it and expect that the crystal structure on both side of the barrier is essentially the same. On the other hand we can interpret this inequality as a lower bound for the sum of the $\sqrt{\epsilon_J}$ at the position of the chain. If we move a chain on a curve we can get an estimate of the average ϵ_J on the curve. In particular we can get an estimate for the average ϵ_J on a curve around a dislocation and can calculate the cost for the core energy of a dislocation.

The basic idea of our first lemma is that x is a regular point means the configuration looks like a lattice in a λ ball around the point x. Therefore, a point y close to x has to be regular too, if one uses a smaller $\tilde{\lambda}$, such that the $\tilde{\lambda}$

ball around x is a subset of the λ ball around x.

Lemma 4.1.1. *For all $C_A > 0$ there exists $\hat{\lambda} > 0$ and $\hat{\epsilon} > 0$ such that for all $\lambda > \hat{\lambda}$, $A \in Gl_d(\mathbb{R})$ with $\|A^{-1}\| < C_A$, $\tau \in R^d$ and $x, y \in B_{2\lambda}(\Omega)$ we have If x is $(\epsilon_\rho, \epsilon_J, C_A)$-regular with (A, τ) and $|x - y| < \lambda$, then y is $(\tilde{\epsilon}_\rho, \tilde{\epsilon}_J, C_A)$-regular with $(A, \tau + A(y - x))$ using the smaller $\tilde{\lambda} = \lambda - |x - y|$ where*

$$J_{\tilde{\lambda}}(A, \tau, \chi, y) \leq \left(\frac{\lambda}{\tilde{\lambda}}\right)^d J_\lambda(A, \tau, \chi, x) \quad ,$$
$$\tilde{\epsilon}_\rho = \left(\frac{\lambda}{\tilde{\lambda}}\right)^{d/2} \frac{C + O(\lambda^{-1})}{\lambda}(1 + \epsilon_\rho)\epsilon_J + \left(\frac{\lambda}{\tilde{\lambda}}\right)^d \epsilon_\rho \quad ,$$
$$\tilde{\epsilon}_J = \left(\frac{\lambda}{\tilde{\lambda}}\right)^d \frac{1 + \tilde{\epsilon}_\rho}{1 - \epsilon_\rho}\epsilon_J \quad . \tag{4.1.1}$$

Proof. We claim that for every atom $x_i \in \chi$ it holds

$$\varphi\left(\frac{|x_i - y|}{\tilde{\lambda}}\right) \leq \varphi\left(\frac{|x_i - x|}{\lambda}\right) \quad . \tag{4.1.2}$$

Because if $\|x_i - x\| \leq \lambda$, we have $\varphi\left(\frac{|x_i - y|}{\tilde{\lambda}}\right) \leq 1 = \varphi\left(\frac{|x_i - x|}{\lambda}\right)$ because 1 is the maximum of φ. x_i is outside $B_\lambda(x)$ and y is inside the ball. line segment between

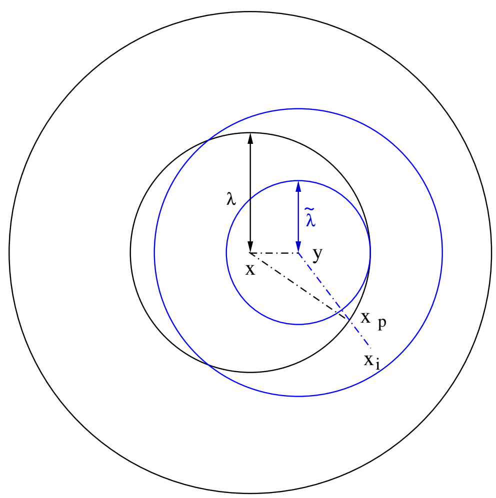

Figure 4.1: Geometric setting

y and x_i is intersecting with the surface of the ball in one point. We call this point x_p. (See picture 4.1). We get

$$|x - x_p| \leq |x - y| + |y - x_p| \quad ,$$
$$|y - x_p| \geq |x - x_p| - |x - y| = \lambda - |x - y| \geq \tilde{\lambda} \quad . \tag{4.1.3}$$

and

$$\begin{aligned}|x_i - y| =& |x_i - x_p| + |x_p - y| \geq |x_i - x_p| + \tilde{\lambda} \\ \geq& \frac{\tilde{\lambda}}{\lambda}|x_i - x_p| + \tilde{\lambda} \geq \frac{|x_i - x_p| + \lambda}{\lambda}\tilde{\lambda} \\ \geq& \frac{|x_i - x|}{\lambda}\tilde{\lambda} \quad .\end{aligned} \tag{4.1.4}$$

Since φ is monotone decreasing, we have

$$\varphi\left(\frac{|x_i - y|}{\tilde{\lambda}}\right) \leq \varphi\left(\frac{|x_i - x|}{\lambda}\right) \quad . \tag{4.1.5}$$

It holds

$$\begin{aligned}&J_{\tilde{\lambda}}(y, A, \tau + A(y-x), \chi) \\ =&\frac{\|A^{-1}\|^2}{C_\varphi \tilde{\lambda}^d}\sum_i W(A(x_i - y) + \tau + A(y-x))\varphi\left(\tilde{\lambda}^{-1}|x_i - y|\right) \\ \leq&\frac{\lambda^d}{\tilde{\lambda}^d}\frac{\|A^{-1}\|^2}{C_\varphi \lambda^d}\sum_i W(A(x_i - x) + \tau)\varphi\left(\lambda^{-1}|x_i - x|\right) \\ \leq& \frac{\lambda^d}{\tilde{\lambda}^d}J_{\tilde{\lambda}}(x, A, \tau + A(y-x)) \quad .\end{aligned} \tag{4.1.6}$$

We now want to achieve a lower bound on $\rho_{\tilde{\lambda}}(\chi, y)$. We start at a Bravais lattice $\chi = \chi_{\mathcal{A}} + x = A^{-1}(\mathbb{Z}^d - \tau) + x$ as a configuration. This configuration has $\epsilon_J = 0$ For this lattice we have $\rho_{\tilde{\lambda}}(\chi, y) = \det A + O(\lambda^{-2})$. There are different ways to reduce the density.
On the one hand one can take atoms away. This decreases $\rho_{\tilde{\lambda}}(\chi, y)$ but because of equation (4.1.5) it also decreases $\rho_\lambda(\chi, x)$ at least by

$$\delta\rho_{\tilde{\lambda}}(\chi, y) < \frac{\lambda^d}{\tilde{\lambda}^d}\delta\rho \quad . \tag{4.1.7}$$

Another possibility is to move atoms to positions of lower $\varphi((\lambda^{-1}|x_i - x|))$ this does not have to reduce $\rho_\lambda(\chi, x)$ at all but it will increase J_λ. If we shift the i'th atom for a distance δx_i we maximally reduce $\rho_{\tilde{\lambda}}(\chi, y)$ by

$$\delta\tilde{\rho}_i = \frac{1}{C_\varphi \tilde{\lambda}^d}\frac{|\nabla\varphi(\lambda^{-1}|x_i - y|)|}{\lambda}\delta x_i + O(\delta x_i \lambda^{-1}) \quad , \tag{4.1.8}$$

we get a minimal cost per atom of

$$\delta J_i < C_0^W \frac{1}{C_\varphi \tilde{\lambda}^d}\delta x_i^2 \varphi\left(\lambda^{-1}|x_i - x|\right) + O(\lambda^{-1}(\delta x_i)^2) \quad . \tag{4.1.9}$$

Furthermore, we have for $x_i \in B_{2\tilde{\lambda}}(y)$

$$\begin{aligned} |x_i - x| \leq& |x_i - y| + |y - x| \\ \leq& 2\tilde{\lambda} + \lambda - \tilde{\lambda} \\ <& 2\lambda \quad , \\ \varphi\left(\frac{|x_i - x|}{\lambda}\right) >& 0 \quad . \end{aligned} \tag{4.1.10}$$

Up to higher order we are in the case of a quadratic potential with linear constraint. This case is treated in Lemma B.1.5. We get

$$J_\lambda > \left(\frac{\tilde{\lambda}}{\lambda}\right)^d \left(\frac{1}{C_\varphi \tilde{\lambda}^d} \sum_{x_i \in B_{2\tilde{\lambda}}(y)} \frac{|\nabla\varphi(\lambda^{-1}|x_i - y|)|^2}{\varphi(\lambda^{-1}|x_i - x|)} + 0(\lambda^{-1})\right)^{-1} \lambda^2 \delta\rho^2. \tag{4.1.11}$$

We can make a discrete continuum transition using 2.1.2 with $m = 2$. We create an error-term in the transition that is proportional to the second derivative. With every derivatives of φ we get a factor λ^{-1} Therefore, the error is $O(\lambda^{-2})$ that means negligible compared to the error we already made.

$$\begin{aligned} J_\lambda >& \left(\frac{\tilde{\lambda}}{\lambda}\right)^d \left(\frac{1}{C_\varphi \tilde{\lambda}^d} \int_{\mathbb{R}^3} \frac{\left|\nabla\varphi(\tilde{\lambda}^{-1}|z - y|)\right|^2}{\varphi(\lambda^{-1}|z - x|)} \det A dz + 0(\lambda^{-1})\right)^{-1} \lambda^2 \delta\rho^2 \\ \delta\rho <& \left(\frac{\lambda}{\tilde{\lambda}}\right)^{d/2} \left(\frac{1}{C_\varphi} \int_{\mathbb{R}^3} \frac{|\nabla\varphi(|z - y|)|^2}{\varphi\left(|z - x| \frac{\tilde{\lambda}}{\lambda}\right)} dz + 0(\lambda^{-1})\right)^{\frac{1}{2}} \sqrt{\det A} \frac{\sqrt{J_\lambda(A, \tau, \chi, x)}}{\lambda} \\ \delta\rho <& \tilde{C}_\rho \left(\frac{\lambda}{\tilde{\lambda}}\right)^{d/2} \frac{\sqrt{J_\lambda(A, \tau, \chi, x)}}{\lambda} \quad . \end{aligned} \tag{4.1.12}$$

The $\rho_\lambda(\chi, x)$ we can estimate from above with $\rho < (1 + \epsilon_\rho) \det A$ If we summarize (4.1.7) and (4.1.12) We get

$$\det A - \rho_{\tilde{\lambda}}(\chi, y) < \left(\left(\frac{\lambda}{\tilde{\lambda}}\right)^{d/2} \frac{C + 0(\lambda^{-1})}{\lambda} (1 + \epsilon_\rho)\epsilon_J + \left(\frac{\lambda}{\tilde{\lambda}}\right)^d \epsilon_\rho\right) \det A \quad . \tag{4.1.13}$$

Starting from a lattice the density $\rho_{\tilde{\lambda}}(\chi, y)$ of the configuration can increase in two ways. On the one hand one can shift atoms to positions of higher φ. This leads to the same increase of J_λ as in the reduction case. On the other hand one can add more atoms, that will lead to the same increase as in of $\rho_\lambda(\chi, x)$ additionally it will increase J_λ because new atoms can not be placed in the minima because all minima are occupied. We get the same estimate for the upper bound of $\rho_{\tilde{\lambda}}(\chi, y)$

$$|\det A - \rho_{\tilde{\lambda}}(\chi, y)| < \left(\left(\frac{\lambda}{\tilde{\lambda}}\right)^{d/2} \frac{C + 0(\lambda^{-1})}{\lambda}(1+\epsilon_\rho)\epsilon_J + \left(\frac{\lambda}{\tilde{\lambda}}\right)^{d} \epsilon_\rho\right) \det A \quad . \tag{4.1.14}$$

Finally, we estimate

$$\begin{aligned} J_{\tilde{\lambda}}(A, \tau, \chi, y) &\leq \left(\frac{\lambda}{\tilde{\lambda}}\right)^{d} J_\lambda(A, \tau, \chi, x) \quad , \\ &\leq \left(\frac{\lambda}{\tilde{\lambda}}\right)^{d} \epsilon_J \rho_\lambda(\chi, x) \quad , \\ &\leq \left(1 + \tilde{\epsilon}_\rho \left(\frac{\lambda}{\tilde{\lambda}}\right)^{d} \epsilon_J \det A\right) \quad , \\ &\leq \left(\frac{\lambda}{\tilde{\lambda}}\right)^{d} \frac{1+\tilde{\epsilon}_\rho}{1-\epsilon_\rho} \epsilon_J \rho_{\tilde{\lambda}}(\chi, y) \quad . \end{aligned} \tag{4.1.15}$$

□

According to Lemma 4.1.1 points close to regular points need to be regular with smaller $\tilde{\lambda}$. If we have two regular points that are close enough, this means that the midpoints between them needs to be regular with the lattice parameters of both of these points, According to theorem 2.3.5 the lattice parameters have to be equal up to a reparametrisation and the change of τ due to the change of the x position and a small difference. The small difference in A is controlled by $\lambda^{-1}\sqrt{J_\lambda}$. The small difference in τ is controlled by $\sqrt{J_\lambda}$.

Theorem 4.1.2. *For all $C_A > s_o$ there exists $\hat{\lambda} \in \mathbb{R}$ and $\epsilon_J > 0$ such that for all $\lambda > \hat{\lambda}$, $A_1, A_2 \in Gl_d(\mathbb{R})$, $\tau_1, \tau_2 \in \mathbb{R}^d$ and $x_1, x_2 \in B_{2\lambda}(\Omega)$ the following holds. If x_1 is $(2^{-3-2d}, \epsilon_J, C_A)$-regular with $\mathcal{A}_1$ and x_2 is $(2^{-3-2d}, \epsilon_J, C_A)$ with $\mathcal{A}_2$ and $|x_1 - x_2| \leq \frac{3}{2}\lambda$, then there exists a unique reparametrisation $B \in Gl_d(\mathbb{Z})$, $t \in Z^d$such that*

$$\begin{aligned} \|id - A_1^{-1}BA_2\| &< \frac{c_J^A}{\sqrt{\det A_2}} \left(\frac{2\lambda}{2\lambda - |x_1 - x_2|}\right)^{d/2} \frac{\sqrt{J_\lambda}}{\lambda} \quad , \\ \left|B\tau_2 + t - \tau_1 - \frac{BA_2 + A_1}{2}(x_2 - x_1)\right| &< \frac{c_J^\tau \|A_1|}{\sqrt{\det A_2}} \left(\frac{2\lambda}{2\lambda - |x_1 - x_2|}\right)^{d/2} \sqrt{J_\lambda}, \end{aligned} \tag{4.1.16}$$

where

$$
\begin{aligned}
J_\lambda &:= \max\left\{J_\lambda(\mathcal{A}_1,\chi,x_1), J_\lambda(\mathcal{A}_2,\chi,x_2)\right\} \quad ,\\
c_J^A &:= \frac{3}{2}\left(\frac{C_{\varphi 2}}{8dC_\varphi}C_0^W\right)^{-\frac{1}{2}} \quad ,\\
c_J^\tau &:= \left(\frac{1}{10}C_0^W\right)^{-\frac{1}{2}} \quad .
\end{aligned}
\tag{4.1.17}
$$

Proof.

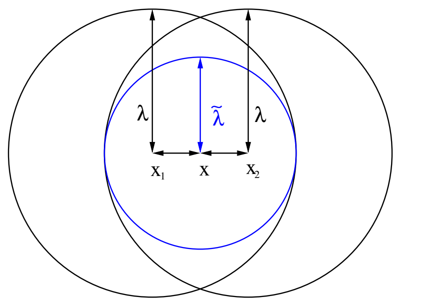

Figure 4.2: Geometric setting.

Existence We consider $\bar{x} = (x_1 + x_2)/2$ and get

$$
|x_1 - \bar{x}| = |x_2 - \bar{x}| = |x_1 - x_2|/2 < \lambda \tag{4.1.18}
$$

We apply Lemma 4.1.1 twice, one time with x_1 as x and $\bar{x}$ as y and the other time with x_2 as x and $\bar{x}$ as y. $\bar{x}$ is $(\tilde{\epsilon}_J, \tilde{\epsilon}_\rho, C_A)$ regular with $\tilde{\mathcal{A}}_1 := (A_1, \tau_1 + A_1(x_2 - x_1)/2)$ and $\tilde{\mathcal{A}}_2 := (A_2, \tau_2 + A_2(x_1 - x_2)/2)$. Therefore, we get

$$
\begin{aligned}
J_\lambda(\tilde{\mathcal{A}}_j,\chi,\bar{x}) &= \left(\frac{2\lambda}{2\lambda - |x_1 - x_2|}\right)^d J_{\tilde{\lambda}}(x, A, \tau + A(\bar{x} - x_j)) \quad ,\\
\tilde{\epsilon}_\rho &= \left(\frac{2\lambda}{2\lambda - |x_1 - x_2|}\right)^{d/2} \frac{C + 0(\lambda^{-1})}{\lambda}(1+\epsilon_\rho)\epsilon_J + \left(\frac{2\lambda}{2\lambda - |x_1 - x_2|}\right)^d \epsilon_\rho.
\end{aligned}
\tag{4.1.19}
$$

Since we have two regular lattices, we can apply Lemma 2.3.5 and get $B \in \mathrm{GL_d}(\mathbb{Z})$ and $t \in \mathbb{Z}^d$ such that

$$
\begin{aligned}
\|1 - A_1^{-1}BA_2\| &< \frac{C_J^A}{\sqrt{\det A_2}}\left(\frac{2\lambda}{2\lambda - |x_1 - x_2|}\right)^{d/2} \frac{\sqrt{J_\lambda}}{\lambda} \quad ,\\
\left|B\tau_2 - \tau_1 + \frac{BA_2 + A_1}{2}(x_2 - x_1) + t\right| &< \frac{c_J^\tau \|A_1\|}{\sqrt{\det A_2}}\left(\frac{2\lambda}{2\lambda - |x_1 - x_2|}\right)^{d/2} \sqrt{J_\lambda}.
\end{aligned}
\tag{4.1.20}
$$

Uniqueness Suppose there are $B_1, B_2 \in Gl_d(\mathbb{Z})$ with

$$\|1 - A_1^{-1} B_j A_2\| \leq \frac{c_J^A}{\sqrt{\det A_2}} \left(\frac{2\lambda}{2\lambda - |x_1 - x_2|} \right)^{d/2} \frac{\sqrt{\epsilon_J}}{\lambda} < \tilde{C}_J^A 2^d \frac{\sqrt{J_\lambda}}{\lambda} \quad , \quad (4.1.21)$$

then we get

$$\begin{aligned} \left|A_1^{-1}(B_2 - B_1)A_2\right| \leq& \left|A_1^{-1} B_2 A_2 - 1 + 1 - A_1^{-1} B_1 A_2\right| \\ \leq& \left|A_1^{-1} B_2 A_2 - 1\right| + \left|1 - A_1^{-1} B_1 A_2\right| \\ \leq& \|A_1^{-1} B_2 A_2 - 1\| + \|1 - A_1^{-1} B_1 A_2\| \\ \leq& 2 c_J^A 2^d \frac{\sqrt{J_\lambda}}{\lambda \sqrt{\det A_2}} \quad . \end{aligned} \quad (4.1.22)$$

Due to $\left|A_1^{-1}\right| \leq C_A$ and Remark 2.3.2 we get

$$\begin{aligned} |B_2 - B_1| \leq& |A_1| \left|A_1^{-1}(B_2 - B_1)A_2\right| \left|A_1^{-1}\right| \\ \leq& 2 C_{|A|} C_A c_J^A 2^d \frac{\sqrt{J_\lambda}}{\lambda \sqrt{\det A_2}} \quad . \end{aligned} \quad (4.1.23)$$

Since $B_1, B_2 \in Gl_d(\mathbb{Z})$ and $Gl_d(\mathbb{Z})$ is a discrete set, they are equal if the norm of there difference is smaller than 1. Therefore, if it holds

$$J_\lambda < \left(C_{|A|} c_J^A 2^{d+1} C_A \lambda\right)^2 \det A_2 \quad , \quad (4.1.24)$$

then B will be uniquely defined. Since it holds $|A_1^{-1}|, |A_2^{-1}| \leq C_A$, the matrix derivative of $\det A$ is bounded (see Lemma B.2.3). Additionally, it holds $\det A_2 < (1 - \epsilon_\rho)^{-1} \rho_d^{max}$. Hence, the estimate (4.1.21) implies that we can estimate

$$\det A_1 = \det A_2 + O\left(\frac{\sqrt{J_\lambda}}{\lambda}\right) \quad . \quad (4.1.25)$$

Due to the regularity condition on the density we get

$$\begin{aligned} \rho_\lambda(\chi, x_1) <& (1 + \epsilon_\rho) \det A_1 \quad , \\ \rho_\lambda(\chi, x_2) <& (1 + \epsilon_\rho) \det A_2 \quad . \end{aligned} \quad (4.1.26)$$

Therefore, we get for small enough ϵ_J

$$\begin{aligned} J_\lambda =& \max\left\{J_\lambda(\mathcal{A}_1, \chi, x_1), J_\lambda(\mathcal{A}_2, \chi, x_2)\right\} \\ \leq& \epsilon_J \max\left\{\rho_\lambda(\chi, x_1), \rho_\lambda(\chi, x_2)\right\} \\ \leq& \epsilon_J (1 + \epsilon_\rho) \max\left\{\det A_1, \det A_2\right\} \\ \leq& \epsilon_J (1 + \epsilon_\rho) \left(1 + O\left(\frac{\sqrt{J_\lambda}}{\lambda}\right)\right) \det A_2 \quad . \end{aligned} \quad (4.1.27)$$

Hence, the condition (4.1.24) is satisfied for sufficiently small ϵ_J and B is unique. Assume we have $t_1, t_2 \in Z^d$, we get

$$\begin{aligned}\left|B\tau_2 + t_j - \tau_1 - \frac{BA_2 + A_1}{2}(x_2 - x_1)\right| <& c_J^\tau \|A_j\| \left(\frac{2\lambda}{2\lambda - |x_1 - x_2|}\right)^{d/2} \frac{\sqrt{J_\lambda}}{\sqrt{\det A_2}} \\ <& c_J^\tau \sqrt{d} C_{|A|} 2^d \frac{\sqrt{J_\lambda}}{\sqrt{\det A_2}} \quad , \end{aligned} \tag{4.1.28}$$

We set

$$X := B\tau_2 - \tau_1 - \frac{BA_2 + A_1}{2}(x_2 - x_1) \quad , \tag{4.1.29}$$

and obtain

$$\begin{aligned}|t_2 - t_1| \leq& |t_2 - X + X - t_1| \\ \leq& |t_2 - X| + |X - t_1| < 2c_J^\tau \sqrt{d} C_{|A|} 2^d \frac{\sqrt{J_\lambda}}{\sqrt{\det A_2}} \quad . \end{aligned} \tag{4.1.30}$$

Since $t_1, t_2 \in Gl_d(\mathbb{Z})$ and $Gl_d(\mathbb{Z})$ is a discrete set they are equal if the norm of there difference is smaller than 1. Hence, if $J_\lambda < (2c_J^\tau \sqrt{d} C_{|A|} 2^d)^{-2} \det A_2$, then t will be uniquely defined. Therefore, we get uniqueness of t with the help of (4.1.27). □

Definition 4.1.3. *We call a point $x \in \Omega$ connecting-regular if*

1) x is $(2^{-3-2d}, \hat{\epsilon}_J, C_A)$-regular to $\mathcal{A}$,

2) $\frac{1}{2} \det E < \det A$

where $\hat{\epsilon}_J := \left(\left((4C_A c_{|A|} + 6)c_J^\tau + 18c_J^A\right) 2^d C_{|A|}\right)^{-2}$ is chosen to meet the conditions of Theorem 4.1.2 and of Theorem 4.1.8. The set of all connecting-regular point is called Ω_{reg}

We state a simplified version of Theorem 4.1.2. The main modification is that we use a uniform estimate for the det A.

Corollary 4.1.4. *For all $C_A > s_o$ there exists $\hat{\lambda} \in \mathbb{R}$ and $\epsilon_J > 0$ such that for all $\lambda > \hat{\lambda}$, $A_1, A_2 \in Gl_d(\mathbb{R})$, $\tau_1, \tau_2 \in \mathbb{R}^d$ and $x_1, x_2 \in B_{2\lambda}(\Omega)$ the following holds. If x_1 is connecting-regular with $\mathcal{A}_1$ and x_2 is connecting-regular with $\mathcal{A}_2$ and $|x_1 - x_2| \leq \frac{3}{2}\lambda$, then there exists a unique reparametrisation $B \in Gl_d(\mathbb{Z})$, $t \in Z^d$such that*

$$\begin{aligned}\|id - A_1^{-1} B A_2\| <& C_J^A \left(\frac{2\lambda}{2\lambda - |x_1 - x_2|}\right)^{d/2} \frac{\sqrt{J_\lambda}}{\lambda} \quad , \\ \left|B\tau_2 + t - \tau_1 - \frac{BA_2 + A_1}{2}(x_2 - x_1)\right| <& C_J^\tau \|A_1\| \left(\frac{2\lambda}{2\lambda - |x_1 - x_2|}\right)^{d/2} \sqrt{J_\lambda}, \end{aligned} \tag{4.1.31}$$

where

$$
\begin{aligned}
J_\lambda :=& \max\left\{J_\lambda(\mathcal{A}_1,\chi,x_1), J_\lambda(\mathcal{A}_2,\chi,x_2)\right\} \quad ,\\
C_J^A :=& \frac{3}{2}\left(\frac{C_{\varphi 2}}{16 d C_\varphi} C_0^W \det E\right)^{-\frac{1}{2}} \quad ,\\
C_J^\tau :=& \left(\frac{1}{20} C_0^W \det E\right)^{-\frac{1}{2}}
\end{aligned}
\tag{4.1.32}
$$

Proof. Just compare Theorem 4.1.2 with Definition 4.1.3. □

Corollary 4.1.5. *There exists λ_{JP} and $\epsilon_{JP} > 0$ such that for $\lambda > \lambda_{JP}$ all x with $\hat{h}_\lambda(x,\chi) < \epsilon_{JP}$ are connecting regular.*

Proof. We compare Definition 4.1.3 with Theorem 2.4.3. According to Theorem 2.4.3 the parameters satisfy $\epsilon_J = O(\epsilon) + O(\lambda^{-2})$ and $\epsilon_\rho = O(\epsilon) + O(\lambda^{-2})$. Hence, for large enough λ and small enough ϵ the assumptions will be fulfilled. □

We want to apply Theorem 4.1.2 iteratively on a sequence of connecting-regular point. We introduce some definition to describe this compactly.

Definition 4.1.6. *1) We call a series of points $y_j \in B_{2\lambda}(\Omega)$ with $j = 0...K$ connecting chain if all y_j are connecting-regular and $|y_{j+1} - y_j| < 3/2\lambda$ for all $j = 0...K$*

2) We call the series $(y_j, A_j, \tau_j) \in B_{2\lambda}(\Omega) \times Gl_d(\mathbb{R}) \times \in \mathbb{R}^d$ with $j = 0...N$ a connecting $\mathcal{A}$-chain if x_j is connecting-regular with (A_j, τ_j) for all $j = 1...N$

3) We call a connecting $\mathcal{A}$-chain closed, if $y_N = y_0$ and $\mathcal{A}_N = \mathcal{A}_0$.

4) For a connecting $\mathcal{A}$-chain we call the sequence of $\mathcal{B}_j = (B_j, t_j) \in (Gl_d\mathbb{Z}, \mathbb{Z}^d)$ uniquely defined by Theorem 4.1.2 the associated reparametrisation sequence.

Definition 4.1.7. *For a connecting $\mathcal{A}$-chain and the associated reparametrisation sequence $\mathcal{B}_j = (B_j, t_j) \in (Gl_d\mathbb{Z}, \mathbb{Z}^d)$, we define the product reparametrisation $(\boldsymbol{B}, \boldsymbol{t}) \in Gl_d(\mathbb{R}) \times \mathbb{Z}^d$ as composition of the affine maps given by the reparametrisations*

$$
\begin{aligned}
\mathcal{B} =& \mathcal{B}_1 ... \mathcal{B}_N = \prod_{j=1}^{N} \mathcal{B}_j \quad ,\\
\boldsymbol{B} =& B_1 .... B_N = \prod_{j=1}^{N} B_j \quad ,\\
\boldsymbol{t} =& \sum_{k=1}^{N} \left(\prod_{j=1}^{k-1} B_j\right) t_k \quad .
\end{aligned}
\tag{4.1.33}
$$

For a closed connecting chain we call the product of reparametrisations the generalized burgers vector. If $\boldsymbol{B} \neq Id$ we say the chain goes around a topological defect in A. If $\boldsymbol{t} \neq 0$ we say the chain goes around a topological defect in τ. We also call a topological defect in τ a dislocation.

If we have a connecting $\mathcal{A}$-chain, we can add and leave out intermediate steps without changing the product of reparametrisations. In particular this is not changing the generalized burgers vector. Hence, the generalized burgers vector is a topological quantity.

Theorem 4.1.8. *If we have a connecting $\mathcal{A}$-chain $(y_j, A_j, \tau_j) \in (B_{2\lambda}(\Omega) \times Gl_d(\mathbb{R}) \times \mathbb{R}^d$ with $j = 0...N$, and if we have a second connecting $\mathcal{A}$-chain $(\tilde{x}_j, \tilde{A}_j, \tilde{\tau}_j) \in (B_{2\lambda}(\Omega) \times Gl_d(\mathbb{R}) \times \in \mathbb{R}$ with $j = 0...N-1$ such that there is a $n \in \mathbb{Z}$ with $1 < n < N$ such that it holds*

$$
\begin{aligned}
j < n \Rightarrow & (y_j, A_j, \tau_j) = (\tilde{y}_j, \tilde{A}_j, \tilde{\tau}_j) \quad , \\
j > n \Rightarrow & (y_j, A_j, \tau_j) = (\tilde{y}_{j-1}, \tilde{A}_{j-1}, \tilde{\tau}_{j-1}) \quad ,
\end{aligned}
\tag{4.1.34}
$$

then the reparametrisation products of both sequences are the same

$$
\begin{aligned}
\prod_{j=1}^{N} B_j = & \prod_{j=1}^{N-1} \tilde{B}_j \quad , \\
\sum_{k=1}^{N} \left(\prod_{j=1}^{k} B_i \right) t_k = & \sum_{k=1}^{N-1} \left(\prod_{j=1}^{k} \tilde{B}_i \right) \tilde{t}_k \quad ,
\end{aligned}
\tag{4.1.35}
$$

where $\mathcal{B}_j = (B_j, \tau_j)$ denotes the associated reparametrisation sequence to (y_j, A_j, τ_j) and $\tilde{\mathcal{B}}_j(\tilde{B}_j, \tilde{\tau}_j)$ denotes the associated reparametrisation sequence to $(\tilde{y}_j, \tilde{A}_j, \tilde{\tau}_j)$

Proof. **Equality of the B products** Because of the uniqueness of the reparametrisation proved in Theorem 4.1.2, we know $B_j = \tilde{B}_j$ for $j = 1...n-1$ and $B_j = \tilde{B}_{j-1}$ for
$j = n+2...N$. Therefore, the two products are equal, if $B_n B_{n+1} = \tilde{B}_n$. Furthermore, we estimate

$$
\begin{aligned}
J_\lambda(k) = & \max \{ J_\lambda(\mathcal{A}_{k-1}, \chi, x_{k-1}), J_\lambda(\mathcal{A}_k, \chi, x_k) \} \quad , \\
\leq & \epsilon_J \max \{ \rho_\lambda(\chi, x_{k-1}), \rho_\lambda(\chi, x_k) \} \quad , \\
\leq & \epsilon_J (1 + \epsilon_\rho) \max \{ \det A_{k-1}, \det A_k \} \\
\leq & \epsilon_J (1 + \epsilon_\rho) \left(1 + O\left(\frac{\sqrt{J_\lambda}}{\lambda} \right) \right) \det A_k
\end{aligned}
\tag{4.1.36}
$$

Hence for sufficiently large λ we have with Theorem 4.1.2 for the longer chain

$$
\begin{aligned}
\| id - A_{n-1}^{-1} B_n A_n \| < & c_J^A 2^{d+1} \frac{\epsilon_J}{\lambda} \quad , \\
\| id - A_n^{-1} B_{n+1} A_{n+1} \| < & c_J^A 2^{d+1} \frac{\epsilon_J}{\lambda} \epsilon_J \quad .
\end{aligned}
\tag{4.1.37}
$$

We calculate for ϵ_J small enough

$$\begin{aligned}
&\left|id - A_{n-1}^{-1} B_j B_{n+1} A_{n+1}\right| \\
\leq &\left|id - A_{n-1}^{-1} B_n A_n + A_{n-1}^{-1} B_n A_n \left(1 - A_n^{-1} B_{n+1} A_{n+1}\right)\right| \\
\leq &\left|id - A_{n-1} B_n A_n + A_{n-1} B_n A_n\right| + \left|A_{n-1}^{-1} B_n A_n\right| \left|id - A_n^{-1} B_{n+1} A_{n+1}\right| \\
\leq &6 c_J^A 2^d \frac{\epsilon_J}{\lambda} \quad . \qquad (4.1.38)
\end{aligned}$$

We know from Theorem 4.1.2 for the shorter chain

$$\begin{aligned}
\|id - \tilde{A}_{n-1}^{-1} \tilde{B}_n \tilde{A}_n\| <&2 c_J^A 2^d \frac{\sqrt{\epsilon_J}}{\lambda} \quad , \\
\|id - A_{n-1}^{-1} \tilde{B}_n A_{n+1}\| <&2 c_J^A 2^d \frac{\sqrt{\epsilon_J}}{\lambda} \quad .
\end{aligned} \qquad (4.1.39)$$

We get for $\epsilon_J < \lambda^2 (8 C_A C_{|A|} C_J^A 2^d)^{-2}$

$$\begin{aligned}
\left|\tilde{B}_n - B_n B_{n+1}\right| \leq |A_{n-1}| &\left|A_{n-1}^{-1} \left(\tilde{B}_n - B_n B_{n+1}\right) A_{n+1}\right| \left|A_{n+1}^{-1}\right| \\
\leq &C_A C_{|A|} \left|A_{n-1}^{-1} \tilde{B}_{n-1+1} - A_{n-1}^{-1} B_n B_{n+1} A_{n+1}\right| \\
\leq &C_A C_{|A|} \left|A_{n-1}^{-1} \tilde{B}_{n-1}\right| + \left|1 - A_{n-1}^{-1} B_n B_{n+1} A_{n+1}\right| \\
\leq &8 c_J^A C_A C_{|A|} 2^d \frac{\sqrt{\epsilon_J}}{\lambda} < 1 \quad . \qquad (4.1.40)
\end{aligned}$$

The distance between $\tilde{B}_n$ and $B_n B_{n+1}$ will be smaller than one and they have to be equal because they are both elements of the discrete set $Gl_d(\mathbb{Z})$. We have

$$\begin{aligned}
\prod_{j=1}^{N-1} \tilde{B}_j =& \left(\prod_{j=1}^{n-1} \tilde{B}_j\right) B_n \prod_{j=n+1}^{N-1} \tilde{B}_j \\
=& \left(\prod_{j=1}^{n-1} B_j\right) B_n B_{n+1} \prod_{j=n+1}^{N-1} \tilde{B}_{j+1} \quad , \\
=& \prod_{j=1}^{N} B_j \quad . \qquad (4.1.41)
\end{aligned}$$

Equality of the τ-product: Because of the uniqueness of the reparametrisation proved in Theorem 4.1.2, we know $t_j = \tilde{t}_j$ for $j = 1...n-1$ and $t_j = \tilde{t}_{j-1}$ for $j = n+2...N$. Together with our calculation for B we get $(\prod_{j=1}^{k-1} B_j) t_k = (\prod_{j=1}^{k-1} \tilde{B}_j) \tilde{t}_k$ for $k = 1...n-1$ and $(\prod_{j=1}^{k-1} B_j) t_k = (\prod_{j=1}^{k-2} \tilde{B}_j) \tilde{t}_{k-1}$ for $k = n+1...N$.

So we need still to prove

$$\begin{aligned} \left(\prod_{j=1}^{n-1} B_j\right) t_n + \left(\prod_{j=1}^{n} B_j\right) t_{n+1} = & \left(\prod_{j=1}^{n-1} \tilde{B}_j\right) \tilde{t}_n \quad , \\ t_n + B_n t_{n+1} = & \tilde{t}_n \quad . \end{aligned} \tag{4.1.42}$$

If we apply Theorem 4.1.2 on the first chain, we get

$$\begin{aligned} \delta\tau_n := & B_n\tau_n + t_n - \tau_{n-1} - \frac{B_n A_n + A_{n-1}}{2}(y_n - y_{j-n}) \quad , \\ |\delta\tau_n| < & 2c_J^\tau C_{|A|} 2^d \sqrt{\epsilon_J} \quad , \\ \delta\tau_{n+1} := & B_{n+1}\tau_{n+1} + t_{n+1} - \tau_n - \frac{B_{n+1}A_{n+1} + A_n}{2}(y_{n+1} - y_n) \quad , \\ |\delta\tau_{n+1}| < & 2c_J^\tau C_{|A|} 2^d \sqrt{\epsilon_J} \quad . \end{aligned} \tag{4.1.43}$$

We calculate with the help of Theorem 4.1.2 for $\epsilon_J < \lambda^2 (c_J^A 2^d)^{-2}$ that it holds

$$\begin{aligned} |B_n A_n - A_{n-1}| \leq & \left|A_{n-1}^{-1} B_n A_n - id\right| |A_n| \\ \leq & C_{|A|} C_J^A 2^d \frac{\sqrt{\epsilon_J}}{\lambda} \quad , \\ |B_n A_n - B_n B_{n+1} A_{n+1}| \leq & |B_n A_n| \left|id - A_n^{-1} B_{n+1} A_{n+1}\right| \\ \leq & 2\,|A_{n-1}| \left|A_{n-1}^{-1} B_n A_n\right| c_J^A 2^d \frac{\sqrt{\epsilon_J}}{\lambda} \\ \leq & 2C_{|A|}\left(1 + 2c_J^A 2^d \frac{\sqrt{\epsilon_J}}{\lambda}\right) c_J^A 2^d \frac{\sqrt{\epsilon_J}}{\lambda} \leq C_{|A|} C_J^A 2^d \frac{\sqrt{\epsilon_J}}{\lambda} \quad , \end{aligned} \tag{4.1.44}$$

We also get

$$\begin{aligned} |B_n| \leq & |A_{n-1}| \left|A_{n-1}^{-1} B_n A_n\right| \left|A_n^{-1}\right| \\ \leq & C_A C_{|A|}\left(1 + 2c_J^A 2^d \frac{\sqrt{\epsilon_J}}{\lambda}\right) \leq C_A C_{|A|} \quad . \end{aligned} \tag{4.1.45}$$

We obtain

$$\begin{aligned}
&\left|B_nB_{n+1}\tau_{n+1}+B_nt_{n+1}+t_n-\tau_{n-1}-\frac{B_nB_{n+1}A_{n+1}+A_{n-1}}{2}\left(y_{n+1}-y_{n-1}\right)\right|\\
=&\left|B_n\delta\tau_{n+1}+\delta\tau_n+\frac{B_nA_n+A_{n-1}}{2}\left(y_n-y_{n-1}\right)+B_n\frac{B_{n+1}A_{n+1}+A_n}{2}\left(y_{n+1}-y_n\right)\right|\\
&+\left|-\frac{B_nB_{n+1}A_{n+1}+A_{n-1}}{2}\left(y_{n+1}-y_{n-1}\right)\right|\\
\leq&\left|B_n\delta\tau_{n+1}\right|+\left|\delta\tau_n\right|+\frac{1}{2}\left|\left(B_nA_n-A_{n-1}\right)\left(y_{n+1}-y_n\right)\right|\\
&+\frac{1}{2}\left|\left(B_nA_n-B_nB_{n+1}A_{n+1}\right)\left(y_n-y_{n-1}\right)\right|\\
\leq&\left|B_n\right|\left|\delta\tau_{n+1}\right|+\left|\delta\tau_n\right|+\frac{3\lambda}{4}\left|B_nA_n-A_{n-1}\right|+\frac{3\lambda}{4}\left|B_nA_n-B_nB_{n+1}A_{n+1}\right| \quad .
\end{aligned} \tag{4.1.46}$$

We use the estimates (4.1.43), (4.1.44) and (4.1.45).

$$\begin{aligned}
&\left|B_nB_{n+1}\tau_{n+1}+B_nt_{n+1}+t_n-\tau_{n-1}-\frac{B_nB_{n+1}A_{n+1}+A_{n-1}}{2}\left(y_{n+1}-y_{n-1}\right)\right|\\
&\leq 2(C_AC_{|A|}+1)c_J^\tau C_{|A|}+18c_J^AC_{|A|}2^{d-2}\sqrt{\epsilon_J}\\
&\leq\left((4C_AC_{|A|}+2)2_J^\tau+18C_J^A\right)2^dc_{|A|}\sqrt{\epsilon_J} \quad .
\end{aligned} \tag{4.1.47}$$

On the other hand, if we apply Theorem 4.1.2 to the second chain, we get

$$\begin{aligned}
\left|\tilde{B}_n\tilde{\tau}_n+\tilde{t}_n-\tilde{\tau}_{n-1}-\frac{\tilde{B}_n\tilde{A}_n+\tilde{A}_{n-1}}{2}\left(\tilde{x}_n-\tilde{x}_{n-1}\right)\right| &< 2c_J^\tau C_{|A|}2^d\sqrt{\epsilon_J}\\
\left|B_nB_{n+1}\tau_{n+1}+\tilde{t}_n-\tau_{n-1}-\frac{B_nB_{n+1}A_{n+1}+A_{n-1}}{2}\left(y_{n+1}-y_{n-1}\right)\right| &< 2c_J^\tau C_{|A|}2^d\sqrt{\epsilon_J} \quad .
\end{aligned} \tag{4.1.48}$$

Hence, if we call $X=B_nB_{n+1}\tau_{n+1}-\tau_{n-1}-\frac{B_nB_{n+1}A_{n+1}+A_{n-1}}{2}\left(y_{n+1}-y_{n-1}\right)$, we finally get with the estimates (4.1.47) and (4.1.48)

$$\begin{aligned}
\left|B_nt_{n+1}+t_n-\tilde{t}_n\right| &\leq \left|B_nt_{n+1}+t_n+X\right|+\left|X-\tilde{t}_n\right|\\
&\leq\left((2C_AC_{|A|}+3)c_J^\tau+18c_J^A\right)2^dC_{|A|}\sqrt{\epsilon_J} \quad .
\end{aligned} \tag{4.1.49}$$

For $\epsilon_J<\left(\left((4C_Ac_{|A|}+6)c_J^\tau+18c_J^A\right)2^dC_{|A|}\right)^{-2}$ the difference between $B_nt_{n+1}+t_n$ and $\tilde{t}_n$ is smaller than 1 and since both belong to the discrete set $\mathbb{Z}^d$, they have to be equal. □

Corollary 4.1.9. *Replacing in one step in the connecting sequence* $(y_j,\tilde{A}_j,\tilde{\tau}_j)$ *by* (y_j,A_j,τ_j) *does not change the product reparametrisation of the chain.*

Proof. We consider a chain, that goes from $(y_{j-1}, A_{j-1}, \tau_{j-1})$ over (y_j, A_j, τ_j) to $(y_{j+1}, A_{j+1}, \tau_{j-+1})$. Now, we add a point $(y_j, \tilde{A}_j, \tilde{\tau}_j)$. By Theorem 4.1.8 we know that the new chain still has the same reparametrisation product. Now, we leave out (y_j, A_j, τ_j) and by Theorem 4.1.8 we know the reparametrisation product is still the same. □

Next, we calculate upper bounds for the change of A and τ in a connecting chain.

Lemma 4.1.10. *For all $C_A > 0$ there exists $\hat{\lambda}$ such that for all $\lambda > \hat{\lambda}$ the following holds: If $(\mathcal{A}_j, y_j)$ with $j = 0...N$ is a connecting $\mathcal{A}$-chain and $\mathcal{B}_j = (B_j, t_j)$ denote the associated reparametrisation sequence to $\mathcal{A}_j$, then it holds for $1 \leq k_1 < k_2 \leq N$*

$$\left|A_{k_1-1}^{-1}\left(\prod_{k_1}^{k_2} B_j^{-1}\right)A_{k_2}\right| \leq \exp\left(\frac{C_J^A}{\lambda}\sum_{j=k_1}^{k_2}\hat{b}_j\right) \quad ,$$
$$\left|1 - A_0^{-1}\left(\prod_{j=1} B_j\right)A_N\right| \leq \frac{C_J^A}{\lambda}\sum_{j=1}^{N}\hat{b}_j \exp\left(\frac{C_J^A}{\lambda}\sum_{j=1}^{N}\hat{b}_j\right) \quad . \tag{4.1.50}$$

with

$$J_j = J_\lambda(\mathcal{A}_j, \chi, y_j) \quad ,$$
$$\hat{b}_j = \left(\frac{2\lambda}{2\lambda - |y_j - y_{j-1}|}\right)^{d/2} \max\left\{\sqrt{J_j}, \sqrt{J_{j-1}}\right\} \quad . \tag{4.1.51}$$

Proof. Because y_j with $j = 0...N$ is a connecting chain. And $(A_j, \tau_j) \in Gl_d(\mathbb{R})$ is an associated $\mathcal{A}$-sequence. We use the notation

$$a_j = A_{j-1}^{-1} B_j^{-1} A_j \quad ,$$
$$b_j = 1 - A_{j-1}^{-1} B_j^{-1} A_j = 1 - a_j \quad . \tag{4.1.52}$$

We can use Corollary 4.1.4 and get for every $j = 1...N$

$$|b_j| \leq \|b_j\| < \hat{b}_j \frac{C_J^A}{\lambda} \quad ,$$
$$\hat{b}_j = \left(\frac{2\lambda}{2\lambda - |y_j - y_{j-1}|}\right)^{d/2} \max\left\{\sqrt{J_j}, \sqrt{J_{j-1}}\right\} \quad . \tag{4.1.53}$$

Using this upper bound for $|b_j|$ we derive an upper bound for general products of a_j

$$\left|\prod_{j=k_1}^{k_2} a_j\right| = \left|\prod_{j=k_1}^{k_2}(1 - b_j)\right| \leq \prod_{j=k_1}^{k_2}(1 + |b_j|)$$
$$\leq \prod_{j=k_1}^{k_2} \exp(|b_j|) \leq \exp\left(\sum_{j=k_1}^{k_2}|b_j|\right) \quad . \tag{4.1.54}$$

Furthermore, we get

$$\prod_{j=k_1}^{k_2} a_j = \prod_{k_1}^{k_2} \left(A_{j-1}^{-1} B_j^{-1} A_j\right) = A_{k_1-1}^{-1} \left(\prod_{k_1}^{k_2} B_j^{-1}\right) A_{k_2} \quad . \tag{4.1.55}$$

We derive a bound on $1 - \prod a_j$

$$\begin{aligned}
\left|1 - \prod_{j=1}^{N} a_j\right| &\leq \left|1 - a_1 + \sum_{j=2}^{N} \prod_{j=1}^{j-1} a_j (1 - a_j)\right| \\
&\leq |1 - a_1| + \sum_{j=2}^{N} |1 - a_j| \left|\prod_{j=1}^{j-1} a_j\right| \\
&\leq |b_1| + \sum_{j=2}^{N} |(b_j)| \exp\left(\sum_{k=1}^{j-1} |b_k|\right) \\
&\leq \sum_{j=1}^{N} |(b_j)| \exp\left(\sum_{k=1}^{N} |b_k|\right) \\
&\leq \sum_{j=1}^{N} |(b_j)| \exp\left(\sum_{k=1}^{N} |b_k|\right) \quad .
\end{aligned} \tag{4.1.56}$$

We make use of the upper bound for $|b_j|$ and get

$$\left|1 - \prod_{j=1}^{N} a_j\right| \leq \sum_{j=1}^{N} \frac{C_J^A}{\lambda} \hat{b}_j \exp\left(\frac{C_J^A}{\lambda} \sum_{k=1}^{N} \hat{b}_k\right) \quad . \tag{4.1.57}$$

□

Now, we calculate an upper bound for the change of the lattice parameters τ in a connecting $\mathcal{A}$-chain.

Lemma 4.1.11. *For all $C_A > 0$ exists a $\hat{\lambda}$ such that for all $\lambda > \hat{\lambda}$ the following holds If $(y_j, \mathcal{A}_j)$ with $j = 0...N$ is a connecting $\mathcal{A}$-chain and $\mathcal{B}_j = (B_j, t_j)$ denotes the associated reparametrisation sequence to $\mathcal{A}_j$, then it holds for all $1 \leq k_1 < k_2 \leq N$*

$$\begin{aligned}
&\left|\sum_{k=1}^{N} \hat{B}_{k-1} t_k + \hat{B}_N \tau_N - \tau_0 + \frac{\hat{B}_N A_N + A_0}{2} (y_N - y_0)\right| \\
&\leq \left(C_A C_{|A|} C_J^\tau + \frac{C_J^A}{\lambda} \sum_{j=1}^{N} |y_{j+1} - y_j|\right) |A_0| \sum_{j=1}^{N} \hat{b}_j \exp\left(\frac{C_A}{\lambda} \sum_{k=1}^{N} \hat{b}_k\right) \quad ,
\end{aligned} \tag{4.1.58}$$

where

$$\begin{aligned}
\hat{B}_k =& \prod_{j=1}^{k} B_j \quad , \\
J_j =& J_\lambda(\mathcal{A}_j, \chi, y_j) \quad , \\
\hat{b}_j =& \left(\frac{2\lambda}{2\lambda - |y_j - y_{j-1}|} \right)^{d/2} \max\left\{ \sqrt{J_j}, \sqrt{J_{j-1}} \right\} \quad .
\end{aligned} \tag{4.1.59}$$

Proof. We denote

$$\begin{aligned}
\delta\tau :=& \sum_{k=1}^{N} \hat{B}_{j-1} t_j + \hat{B}_N \tau_N - \tau_0 + \frac{\hat{B}_N A_N + A_0}{2} (y_N - y_0) \quad , \\
\delta\tau_j :=& t_j + B_j \tau_j - \tau_{j-1} + \frac{B_j A_j + B_{j-1} A_{j-1}}{2} (y_{j+1} - y_j) \quad , \\
a_j :=& A_{j-1}^{-1} B_j^{-1} A_j \quad .
\end{aligned} \tag{4.1.60}$$

Since (y_j, A_j, τ_j) with $j = 0...N$ is a connecting $\mathcal{A}$-chain, we can use Corollary 4.1.4 and get for every $j = 1...N$

$$\begin{aligned}
\|1 - a_j\| <& \frac{C_J^A}{\lambda} \hat{b}_j \quad , \\
|\delta\tau_j| <& C_J^\tau \|A_{j-1}\| \hat{b}_j \quad .
\end{aligned} \tag{4.1.61}$$

Hence, we have bounds for $\delta\tau_j$ and want a bound for $\delta\tau$

$$\begin{aligned}
|\delta\tau| =& \left| \sum_{j=1}^{N} \hat{B}_{j-1} t_j + \hat{B}_j \tau_j - \hat{B}_{j-1} \tau_{j-1} + \frac{\hat{B}_N A_N + A_0}{2} (y_j - y_{j-1}) \right| \\
=& \left| \sum_{j=1}^{N} \hat{B}_{j-1} \delta\tau_j + \frac{1}{2} \left(\hat{B}_N A_N - \hat{B}_j A_j + A_0 - \hat{B}_{j-1} A_{j-1} \right) (y_{j+1} - y_j) \right| \\
=& C_J^\tau \sum_{j=1}^{N} \left| \hat{B}_{j-1} \right| \|A_{j-1}\| \hat{b}_j \\
&+ \frac{1}{2} \sum_{j=1}^{N} \left(\left| \hat{B}_N A_N - \hat{B}_j \right| + \left| A_0 - \hat{B}_{j-1} A_{j-1} \right| \right) |y_{j+1} - y_j| \quad .
\end{aligned} \tag{4.1.62}$$

Using Lemma 4.1.10 we can estimate

$$\begin{aligned}
\left| \hat{B}_{j-1} \right| \le |A_0| \left| A_0^{-1} \hat{B}_{j-1} A_{j-1} \right| \left| A_{j-1}^{-1} \right| \le& C_A |A_0| \exp\left(\frac{C_J^A}{\lambda} \sum_{k=1}^{j-1} \hat{b}_k \right) \\
\le& C_A |A_0| \exp\left(\frac{C_J^A}{\lambda} \sum_{k=1}^{N} \hat{b}_k \right) \quad .
\end{aligned} \tag{4.1.63}$$

We calculate

$$\begin{aligned}\left|A_0 - \hat{B}_{n-1}A_{n-1}\right| &\le \sum_{j=1}^{n-1}\left|\hat{B}_jA_j - \hat{B}_{j-1}A_{j-1}\right| \\ &\le \sum_{j=1}^{n-1}\left|\hat{B}_{j-1}A_{j-1}\right|\left|A_{j-1}^{-1}B_jA_j - id\right| \\ &\le \sum_{j=1}^{n-1}|A_0|\left|A_0^{-1}\hat{B}_{j-1}A_{j-1}\right|\left|A_{j-1}^{-1}B_jA_j - id\right| \\ &\le \sum_{j=1}^{n-1}|A_0|\left|\prod_{k=1}^{j-1}a_k\right||a_j - id| \quad . \end{aligned} \tag{4.1.64}$$

Due to Lemma 4.1.10 we get

$$\begin{aligned}\left|A_0 - \hat{B}_{n-1}A_{n-1}\right| &\le |A_0|\sum_{j=1}^{n-1}\exp\left(\frac{C_J^A}{\lambda}\sum_{k=1}^{n-1}\hat{b}_j\right)\frac{C_J^A}{\lambda}\hat{b}_j \\ &\le |A_0|\sum_{j=1}^{n-1}\frac{C_J^A}{\lambda}\hat{b}_j\exp\left(\frac{C_J^A}{\lambda}\sum_{k=1}^{N}\hat{b}_k\right) \quad . \end{aligned} \tag{4.1.65}$$

We estimate $\left|\hat{B}_NA_N - \hat{B}_nA_n\right|$ in the same way and obtain

$$\begin{aligned}\left|\hat{B}_NA_N - \hat{B}_nA_n\right| &\le \sum_{j=n+1}^{N}\left|\hat{B}_jA_j - \hat{B}_{j-1}A_{j-1}\right| \\ &\le \sum_{j=n+1}^{N}|A_0|\left|A_0^{-1}\hat{B}_{j-1}A_{j-1}\right|\left|A_{j-1}^{-1}B_jA_j - id\right| \\ &\le \sum_{j=n+1}^{N}|A_0|\left|\prod_{k=1}^{j-1}a_k\right||a_j - id| \\ &\le |A_0|\sum_{j=n+1}^{N}\frac{C_J^A}{\lambda}\hat{b}_j\exp\left(\frac{C_J^A}{\lambda}\sum_{k=1}^{N}\hat{b}_k\right) \quad . \end{aligned} \tag{4.1.66}$$

A combination of the estimates (4.1.65) and (4.1.66) leads to

$$\left|A_0 - \hat{B}_{n-1}A_{n-1}\right| + \left|\hat{B}_NA_N - \hat{B}_nA_n\right| \le |A_0|\sum_{j=1}^{N}\frac{C_J^A}{\lambda}\hat{b}_j\exp\left(\frac{C_J^A}{\lambda}\sum_{k=1}^{N}\hat{b}_k\right) \quad . \tag{4.1.67}$$

Using the estimates (4.1.61), (4.1.63) and (4.1.67) results in

$$
\begin{aligned}
|\delta\tau| \leq & \sum_{j=1}^{N} C_{|A|} C_J^{\tau} C_A \, |A_0| \, \hat{b_j} \exp\left(\frac{C_J^A}{\lambda} \sum_{k=1}^{N} \hat{b}_k \right) \\
& + |A_0| \sum_{j=1}^{N} \frac{C_J^A}{\lambda} \hat{b}_j \exp\left(\frac{C_J^A}{\lambda} \sum_{k=1}^{N} \hat{b}_k \right) \sum_{j=1}^{N} |y_{j+1} - y_j| \\
\leq & \left(C_A C_{|A|} C_J^{\tau} + \frac{C_J^A}{\lambda} \sum_{j=1}^{N} |y_{j+1} - y_j| \right) |A_0| \sum_{j=1}^{N} \hat{b}_j \exp\left(\frac{C_A}{\lambda} \sum_{k=1}^{N} \hat{b}_k \right) \quad .
\end{aligned}
$$

□

A closed connecting $\mathcal{A}$-chain that has a topological defect in A, meaning $\prod_{j=1}^{N} B_j \neq Id$, has a minimal length $O(\lambda^2)$.

Lemma 4.1.12. *For all C_A exists $\hat{\lambda}$ such that for all $\lambda > \hat{\lambda}$ holds If $(y_j, \mathcal{A}_j) \in B_{2\lambda}(\Omega) \times Gl_d(\mathbb{R}) \times \mathbb{R}^d$ with $j = 0...N$ is a closed connecting $\mathcal{A}$-chain. and has a topological defect, then we have*

$$
\sum_{j=1}^{N} |y_j - y_{j-1}| \geq \frac{3}{8} \lambda^2 \left(C_J^A 2^d \sqrt{\hat{\epsilon}_J \rho_d^{max}} \right)^{-1} f^{-1} \left(\frac{1}{|A_0| \left| A_0^{-1} \right|} \right) \quad , \tag{4.1.68}
$$

where $f(x) := x \exp(x)$ and

$$
\hat{\epsilon}_J := \left(\left((4 C_A c_{|A|} + 6) c_J^{\tau} + 18 c_J^A \right) 2^d C_{|A|} \right)^{-2} \tag{4.1.69}
$$

Proof. If we have $|y_{k+1} - y_{k-1}| < 1.5\lambda$ for the connecting chain $\mathcal{A}$-chain (y_j, A_j, τ_j) with $j = 1...N$, then we can leave out y_k in the chain. According to Lemma 4.1.8 the chain have then the same burgers vector. Hence, we can find a modified closed connecting $\mathcal{A}$-chain $(\tilde{x}_j, \tilde{A}_j, \tilde{\tau}_j)$ for $j = 1...\tilde{N}$ with $|\tilde{x}_{i+1} - \tilde{x}_{j-1}| \geq 1.5\lambda$ that still has the same Burgers vector. We denote the associated reparametrisation chain (B_j, t_j). We realize that, because of the triangle inequality, it holds

$$
\sum_{j=1}^{N} |y_j - y_{j-1}| \geq \sum_{j=1}^{\tilde{N}} |\tilde{x}_j - \tilde{x}_{j-1}| \geq \sum_{j=0}^{\tilde{N}/2} |\tilde{x}_{2i+2} - \tilde{x}_{2i}| \geq \frac{3}{4} \lambda \tilde{N} \quad . \tag{4.1.70}
$$

Now, we study the term $\left| 1 - A_0^{-1} \left(\prod_{j=1}^{\tilde{N}} B_j \right) A_0 \right|$. On the one hand, we have a topological defect, i.e. $\prod_{j=1}^{\tilde{N}} B_j \neq Id$. Since $\prod_{j=1} B_j$ and Id are both in the discrete set $Gl_d(\mathbb{Z})$, their distance has to be at least 1. Since the chain is closed, it holds

$$
\begin{aligned}
1 \leq & \left| 1 - \left(\prod_{j=1}^{\tilde{N}} B_j \right) \right| \\
\leq & |A_0| \left| 1 - A_0^{-1} \left(\prod_{j=1}^{\tilde{N}} B_j \right) A_0 \right| \left| A_0^{-1} \right| \quad .
\end{aligned} \tag{4.1.71}
$$

On the other hand we know due to Lemma 4.1.10

$$
\left| 1 - A_0^{-1} \left(\prod_{j=1} B_j \right) A_0 \right| \leq \frac{C_J^A}{\lambda} \sum_{j=1}^{\tilde{N}} \hat{b}_j \exp \left(\frac{C_J^A}{\lambda} \sum_{k=1}^{\tilde{N}} \hat{b}_j \right) \quad , \tag{4.1.72}
$$

where

$$
\begin{aligned}
\hat{b}_j = & \left(\frac{2\lambda}{2\lambda - |\tilde{x}_j - \tilde{x}_{j-1}|} \right)^{d/2} \max \left\{ \sqrt{J_j}, \sqrt{J_{j-1}} \right\} \\
\leq & 2^d \sqrt{\hat{\epsilon}_J \rho_d^{max}} \quad .
\end{aligned} \tag{4.1.73}
$$

. Combining (4.1.71) ,(4.1.72) and (4.1.73) we get

$$
\frac{1}{|A_0| \left| A_0^{-1} \right|} \leq \frac{C_J^A}{\lambda} \tilde{N} 2^d \sqrt{\hat{\epsilon}_J \rho_d^{max}} \exp \left(\frac{C_J^A}{\lambda} \tilde{N} 2^d \sqrt{\hat{\epsilon}_J \rho_d^{max}} \right) \quad . \tag{4.1.74}
$$

By observing that $x \to f(x) := x \exp(x)$ is a strictly monoton function, we can solve the inequality (4.1.74) for N, and obtain

$$
\tilde{N} \geq \lambda \left(C_J^A 2^d \sqrt{\hat{\epsilon}_J \rho_d^{max}} \right)^{-1} f^{-1} \left(\frac{1}{|A_0| \left| A_0^{-1} \right|} \right) \tag{4.1.75}
$$

The final result follows by linking the last inequality with 4.1.70

$$
\sum_{j=1}^{N} |y_j - y_{j-1}| \geq \frac{3}{4} \lambda \tilde{N} \geq \frac{3}{4} \lambda^2 \left(C_J^A 2^d \sqrt{\hat{\epsilon}_J \rho_d^{max}} \right)^{-1} f^{-1} \left(\frac{1}{|A_0| \left| A_0^{-1} \right|} \right) \quad . \tag{4.1.76}
$$

□

We observed that a chain with a topological defect in A has a length scaling like λ^2. This means that the chain can not have short cuts. From here we conclude, that there must be a 1.5λ-barrier of not connecting-regular points. Hence, any topological defect has an irregular core with an area scaling at least like $O(\lambda^3)$. According to Corollary 4.1.5 all points that are not connecting-regular needs to have an energy of at least ϵ_{JP}. Therefore, the core energy cost of an topological defect in A scales at least like λ^3 times the length of the defect.

In the next lemma we prove an lower bound for the average J_λ of a curve of length L arround a dislocation. The generalized burgers vector is a topological quantity.

Therefore, if a dislocation is present in one connecting chain, then the dislocation is present in all connecting chains, which can be obtained by replacing single steps in the chain. We can divide the curve into N parts of equal length $L/N \leq 1.5\lambda$ with a sequence of of points y_j. There are two possibilities: First, all points y_j are regular. In this case, the sequence is a connecting chain and has to show a dislocation. We use Lemma 4.1.11 to get an estimate for the average J_λ of the endpoints. The second possibility is, that at least one point is irregular. We can shift the starting point of our sequence to get two connected estimates; one for the measure of the set of irregular points and one for the average J_λ of the regular points.

Lemma 4.1.13. *For all $C_A > 0$ exists $\hat{\lambda}$ such that for all $\lambda > \hat{\lambda}$ the following hold: For any curve $u \in C^1([0,1],\Omega)$ with $u(0) = u(1)$ with length S and for a closed connecting $\mathcal{A}$-chain $(\tilde{x}_j, \tilde{\mathcal{A}}_j) \in B_{2\lambda}(\Omega) \times Gl_d(\mathbb{R}) \times \mathbb{R}^d$, $j = 0...N$,such that $y_j \in u([0,1])$ and $(y_j, \tilde{\mathcal{A}}_j)$ has a dislocation but no topological defect in A and for every $N \in \mathbb{N}$ with $S < 1.5\lambda N$ we have*

$$\int_{u[0,1]\cap\Omega_{reg}} J_\lambda(\mathcal{A}(x),\chi,x)dx \geq (S/N - S_{irr})N^{-1}\frac{\lambda^2}{(C_J^A)^2}\left(\frac{2\lambda - S/N}{2\lambda}\right)^d \times \left(f^{-1}\left(\left(|A_0|\left(C_{\delta S}\lambda + S\right)\right)^{-1}\right)\right)^2 \quad , \tag{4.1.77}$$

where

$$\begin{aligned} S_{irr} :=& \int_{u[0,1]\cap\Omega_{irr}} dx \quad , \\ f(\alpha) :=& \alpha\exp(\alpha) \quad , \\ C_{\delta S} :=& \frac{C_A C_J^\tau C_{|A|}}{C_J^A} \quad . \end{aligned} \tag{4.1.78}$$

Proof. We consider $\delta x \in [0, S/N]$ and take t_j such that

$$\begin{aligned} \delta x =& \int_0^{t_0} |\nabla u(s)|\, ds \quad , \\ S/N =& \int_{t_j}^{t_{j+1}} |\nabla u(s)|\, ds \quad . \end{aligned} \tag{4.1.79}$$

Therefore, we have for $y_j = u(t_j)$ and can estimate

$$|y_{j+1} - y_j| = \left|\int_{t_{j+1}}^{t_j} \nabla u(s) ds\right| \leq \int_{t_{j+1}}^{t_N} \|\nabla u(s)\| ds \leq S/N \leq 1.5\lambda \quad .$$

Hence, there are two possibilities. Either the y_j are a connecting chain and we can find a connecting $\mathcal{A}$-chain (y_j, A_j, τ_j) to them. Or at least one of the positions y_j is not connecting-regular. We denote the set of $\delta x \in [0, S/N]$ for which all y_j are connecting-regular R and the set of $\delta x \in [0, S/N]$ for which one y_j is not connecting-regular I. If they are a connecting chain they have a Burgers vector because it is a topological quantity according to Lemma 4.1.8. We will now study the term

$$\delta\tau = \sum_{k=1}^{N} \hat{B}_{k-1} t_k + \hat{B}_N \tau_N - \tau_0 + \frac{\hat{B}_N A_N + A_0}{2} (y_N - y_0) \quad . \tag{4.1.80}$$

First we realize that in our case $y_N = y_0$ and since the chain is closed, we have $\tau_N = \tau_0$. Furthermore, there is no topological defect in A and therefore $\hat{B}_N = id$. On the other $\sum_{k=1}^{N} \hat{B}_{k-1} t_k \neq 0$, because there is a dislocation. Additionally, $\sum_{k=1}^{N} \hat{B}_{k-1} t_k$ is an element of the discrete set $\mathbb{Z}^d$, and it holds

$$|\delta\tau| = \left| \sum_{k=1}^{N} \hat{B}_{k-1} t_k \right| \geq 1 \quad . \tag{4.1.81}$$

Next, we use use Lemma 4.1.11 to get

$$\begin{aligned} &|\delta\tau| \\ &\quad \leq \left(C_A C_J^\tau C_{|A|} + \frac{C_J^A}{\lambda} \sum_{j=1}^{N} |y_{j+1} - y_j| \right) |A_0| \sum_{j=1}^{N} \hat{b}_j \exp\left(\frac{C_A}{\lambda} \sum_{k=1}^{N} \hat{b}_k \right) \\ &\hat{b}_j = \left(\frac{2\lambda}{2\lambda - |y_j - y_{j-1}|} \right)^{d/2} \max\left\{ \sqrt{J(y_j)}, \sqrt{J(y_{j-1})} \right\} \\ &\quad \leq \left(\frac{2\lambda}{2\lambda - S/N} \right)^{d/2} \max\left\{ \sqrt{J(y_j)}, \sqrt{J(y_{j-1})} \right\} \quad . \end{aligned} \tag{4.1.82}$$

We notice that

$$\begin{aligned} \max\left\{ \sqrt{J(y_j)}, \sqrt{J(y_{j-1})} \right\} &\leq \sqrt{J(y_j)} + \sqrt{J(y_{j-1})} \\ \sum_{j=1}^{N} \max\left\{ \sqrt{J(y_j)}, \sqrt{J(y_{j-1})} \right\} &\leq 2 \sum_{j=0}^{N} \sqrt{J(y_j)} \quad , \end{aligned} \tag{4.1.83}$$

and that

$$\sum_{j=1}^{N} |y_{j+1} - y_j| \leq S \quad . \tag{4.1.84}$$

We summarize

$$
\begin{aligned}
1 \leq& |\delta\tau| \\
\leq& \left(C_A C_J^\tau C_{|A|} + \frac{C_J^A}{\lambda} S \right) |A_0| \left(\frac{2\lambda}{2\lambda - S/N} \right)^{d/2} \\
&\times 2 \sum_{j=0}^{N-1} \sqrt{J(y_j)} \exp\left(\frac{C_J^A}{\lambda} \left(\frac{2\lambda}{2\lambda - S/N} \right)^{d/2} 2 \sum_{k=1}^{N} \sqrt{J(y_k)} \right) \quad . \qquad (4.1.85)
\end{aligned}
$$

We solve the inequality for $\sum_{k=1}^N \sqrt{J(y_j)}$ using $f(x) = x\exp(x)$ and we obtain

$$
1 \leq |A_0| \left(\frac{C_A C_J^\tau C_{|A|}}{C_J^A} \lambda + S \right) f \left(\frac{C_J^A}{\lambda} \left(\frac{2\lambda}{2\lambda - S/N} \right)^{d/2} 2 \sum_{j=1}^{N} \sqrt{J(y_j)} \right) \quad ,
$$

$$
\sum_{j=1}^{N} \sqrt{J(y_j)} \geq \frac{\lambda}{C_J^A} \left(\frac{2\lambda - S/N}{2\lambda} \right)^{d/2} f^{-1} \left(\left(|A_0| \left(\frac{C_A C_J^\tau C_{|A|}}{2C_J^A} \lambda + S \right) \right)^{-1} \right) =: X \quad . \qquad (4.1.86)
$$

Hence, we have the constraint $\sum_{j=1}^N \sqrt{J(y_j)} \geq X$. With this restriction we minimize $\sum_{j=1}^N J(y_j)$ with $\sqrt{J(y_j)}$ as variable. This is the case of minimizing many quadratic potential with a linear constrain described in Lemma B.1.5. We get

$$
\sum_{j=1}^{N} J(y_j) \geq \frac{X^2}{N} \qquad (4.1.87)
$$

We integrate this estimate over R

$$
\begin{aligned}
|R| N^{-1} X^2 &= \int_R N^{-1} X^2 d\delta x \\
&\leq \int_R \sum_{j=1}^{N-1} J(y_j) d\delta x \\
&\leq \int_{u[0,1]\cap\Omega_{\mathrm{reg}}} J dx \quad . \qquad (4.1.88)
\end{aligned}
$$

We resubstitute X

$$
\begin{aligned}
\int_{u[0,1]\cap\Omega_{\mathrm{reg}}} \epsilon_J dx \geq& |R| N^{-1} X^2 \\
\geq& \frac{|R|}{N} \frac{\lambda^2}{(C_J^A)^2} \left(\frac{2\lambda - S/N}{2\lambda} \right)^{d} \\
&\times \left(f^{-1} \left(\left(|A_0| \left(\frac{C_A C_J^\tau C_{|A|}}{C_J^A} \lambda + S \right) \right)^{-1} \right) \right)^2 \quad . \qquad (4.1.89)
\end{aligned}
$$

On the other hand, for every δx that is not in R there is at least one y_j that is not connecting-regular and we obtain

$$\int_{u[0,1]\cap\Omega_{\mathrm{irr}}} dx \geq |I| = S/N - |R| \quad . \tag{4.1.90}$$

□

Next, we calculate a lower bound scaling like λ^2 for the energy in the core region of an isolated dislocation. Isolated dislocation means that all closed connecting chains that run around a point y_0 on the boundary of a circle $\partial B_r(y_0)$ with $r < R$ have up to reparametrisation the same Burgers vector. We apply Lemma 4.1.13 to these circles. This will give us a combined estimate on the irregular points and the average J_λ. According to Lemma 2.4.3 we can bound the energy density from below with a term linear in J_λ. Due to Corollary 4.1.5, irregular points have a minimal energy density. Hence, we get an estimate for the average energy density of these circles and therefore for the core energy of the dislocation.

Theorem 4.1.14. *There exists $\hat{\lambda}$ such that for all $\lambda \geq \hat{\lambda}$, $b \in \mathbb{Z}^d$, $b \neq 0$, $x_b \in \Omega$ and $R > \frac{3\sqrt{2}}{4}\lambda$ such that $B_R(x_b) \in \Omega$ the following holds: If all $r \in [\frac{3\sqrt{2}}{4}\lambda, R]$ and all closed connecting $\mathcal{A}$-chain (A_j, τ_j, y_j) with $j = 1...N$ satisfying*

- $y_j = x_b + r(\cos\phi_j, \sin\phi_j)$,
- $0 < \phi_{j+1} - \phi_j \leq \frac{pi}{2}$
- $\phi_N - \phi_j = 2\pi$,

have up to reparametrisation the same generalized Burgers vector $(0, b)$, then there exists $\hat{r} = O(\lambda)$, such that for $R \leq \hat{r}$ it holds

$$\int_{\frac{3\sqrt{2}}{4}\lambda}^{R} \int_{u_r[0,1]} \hat{h}_\lambda(\chi, x) dx dr = \geq \qquad \frac{6}{5}\lambda\epsilon_{JP}\left(R - \frac{3\sqrt{2}}{4}\lambda\right) \quad . \tag{4.1.91}$$

and for $R > \hat{r}$ we have

$$\begin{aligned}
&\int_{\frac{3\sqrt{2}}{4}\lambda}^{r} \int_{u_r[0,1]} \hat{h}_\lambda(\chi, x) dx dr \\
&\geq \frac{6}{5}\lambda\epsilon_{JP}\left(\hat{r} - \frac{3\sqrt{2}}{4}\lambda\right) - \pi\frac{\vartheta\mu_1}{4C_\phi^W\lambda^2}\det A_0\left(R^2 - \hat{r}^2\right) \\
&+ \frac{18}{25}\frac{\mu_1 - \vartheta}{\mu_1}\frac{\lambda^4}{4^d\left(C_J^A\right)^2|A_0|^2}\left((C_{\delta S}\lambda + 2\pi\hat{r})^{-2} - (C_{\delta S}\lambda + 2\pi R)^{-2}\right) \quad .
\end{aligned} \tag{4.1.92}$$

where

$$2\pi\hat{r} := \left(C_{\delta S}\lambda + \left(\frac{4\left(\mu_1 - \vartheta\right)}{5\ 4^d \mu_1 \left(C_J^A\right)^2 \epsilon_{JP} \left|A_0\right|^{-2}} \right)^{1/3} \right) \lambda \quad ,$$

$$C_{\delta S} := \frac{C_A C_J^\tau C_{|A|}}{C_J^A} \quad . \tag{4.1.93}$$

Proof. We consider $\partial B_r(x_b)$. If there exists no connecting $\mathcal{A}$-chain on $\partial B_r(x_b)$, there is at least a 1.5λ-barrier of irregular points that prevents connecting over it. According to Corollary 4.1.5 all points with $\hat{h}_\lambda(x,\chi) < \epsilon_{JP}$ are connecting-regular Hence, the integral over the energy density over $\partial B_r(x_b)$ has to fulfill

$$\int_{\partial B_r(x_b)} \hat{h}_\lambda(x,\chi)\, dx \geq 1.5\lambda\epsilon_{JP} \quad . \tag{4.1.94}$$

If there is a closed connecting $\mathcal{A}$-chain, then it has up to reparametrisation the same generalized burgers vector $(0,b)$ like all others. Hence, Lemma 4.1.13 says that for every $N \in \mathbb{Z}$ such that $2\pi r < 1.5\lambda N$ there exists $S_{irr} \in [0, S/N]$ such that

$$\int_{\partial B_r(x_b)\cap\Omega_{\mathrm{irr}}} dx = S_{irr} \quad , \tag{4.1.95}$$

and

$$\int_{u_r[0,1]\cap\Omega_{\mathrm{reg}}} J_\lambda(\mathcal{A}(x),\chi,x)dx \geq (2\pi r/N - S_{irr})N^{-1}\frac{\lambda^2}{\left(C_J^A\right)^2}\left(\frac{2\lambda - 2\pi r/N}{2\lambda}\right)^d \times \left(f^{-1}\left(\left(\left|A_0\right|\left(C_{\delta S}\lambda + S\right)\right)^{-1}\right)\right)^2 \quad . \tag{4.1.96}$$

We choose

$$N := \left\lceil 4/3\pi r\lambda^{-1} \right\rceil \quad . \tag{4.1.97}$$

Since, it holds $r > \frac{3\sqrt{2}}{4}\lambda$, we can estimate the discretization error made in (4.1.97)

$$\frac{4}{3}\pi r\lambda^{-1} \leq N \leq \frac{4}{3}\pi r\lambda^{-1} + 1 \leq \frac{5}{3}\pi r\lambda^{-1} \quad . \tag{4.1.98}$$

According to Lemma 4.1.5 all points with $\hat{h}_\lambda(x,\chi) < \epsilon_{JP}$ are connecting-regular. Hence, we get

$$\int_{u[0,1]\cap\Omega_{\mathrm{irr}}} \hat{h}_\lambda(x,\chi)\, dx \geq \epsilon_{JP} S_{irr} \quad . \tag{4.1.99}$$

In the estimate (4.1.96) for the regular part we realize that the argument of $f(x)$ is very small. Therefore, it holds

$$\left(f^{-1}\left(\left|A_0\right|^{-1}\left(C_{\delta S}\lambda + S\right)^{-1}\right)\right)^2 = \left|A_0\right|^{-2}\left(C_{\delta S}\lambda + 2\pi r\right)^{-2} + O(r^{-3}) \quad . \tag{4.1.100}$$

Furthermore, we can estimate because of $2\pi r N^{-1} < 1.5\lambda$

$$\left(\frac{2\lambda - 2\pi r/N}{2\lambda}\right)^d \geq 4^{-d} \quad . \tag{4.1.101}$$

This turns the estimate (4.1.96) into

$$\begin{aligned}&\int_{u_r[0,1]\cap\Omega_{\mathrm{reg}}} J_\lambda(\mathcal{A}(x),\chi,x)dx \\ \geq&(\frac{2\pi r}{N} - S_{irr})\frac{6}{5\;4^d\left(C_J^A\right)^2|A_0|^2}\lambda^3\left(C_{\delta S}\lambda + 2\pi r\right)^{-3} + O(\lambda^4 r^{-4}) \quad .\end{aligned} \tag{4.1.102}$$

For the regular area, we can use equation (2.4.38) from Theorem 2.4.3.

$$\begin{aligned}J_\lambda \leq&\epsilon + \frac{\vartheta}{\mu_1 - \vartheta}\left(\epsilon + \frac{\mu_1^2}{4C_\phi^W\lambda^2}\det A\right) \quad , \\ \epsilon \geq&\frac{\mu_1 - \vartheta}{\mu_1}J_\lambda - \frac{\vartheta\mu_1}{4C_\phi^W\lambda^2}\det A_0 + O(\lambda^3) \quad .\end{aligned} \tag{4.1.103}$$

Because of Lemma 4.1.10 and because reparametrisations are not changing the determinant and the additional changes of A are $O(r\lambda^{-2})$, $\det A$ is constant up to order $O(r\lambda^{-2})$. We get for the integral

$$\begin{aligned}\int_{u_r[0,1]\cap\Omega_{\mathrm{reg}}}\hat{h}_\lambda(\chi,x)dx \geq&\frac{\mu_1 - \vartheta}{\mu_1}\int_{u_r[0,1]\cap\Omega_{\mathrm{reg}}} J_\lambda\left(\mathcal{A}(x),\chi,x\right)dx - 2\pi r\frac{\vartheta\mu_1}{4C_\phi^W\lambda^2}\det A \\ \geq&(2\pi r/N - S_{irr})\frac{\mu_1 - \vartheta}{\mu_1}\frac{6\lambda^3}{5\;4^d\left(C_J^A\right)^2|A_0|^2}\left(C_{\delta S}\lambda + 2\pi r\right)^{-3} \\ &+ O(\lambda^4 r^{-4}) - 2\pi r\frac{\vartheta\mu_1}{4C_\phi^W\lambda^2}\det A_0 \quad .\end{aligned} \tag{4.1.104}$$

This term has the structure

$$\int_{u_r[0,1]\cap\Omega_{\mathrm{reg}}}\hat{h}_\lambda(\chi,x)dx = (2\pi r/N - S_{irr})O(\lambda^3 r^{-3}) - O(r\lambda^{-2}) \quad . \tag{4.1.105}$$

Together with the estimate (4.1.99) for the irregular part, we arrive at

$$\begin{aligned}\int_{u_r[0,1]\cap\Omega_{\mathrm{reg}}}\hat{h}_\lambda(\chi,x)dx =&\int_{u_r[0,1]\cap\Omega_{\mathrm{reg}}}\hat{h}_\lambda(\chi,x)dx + \int_{u[0,1]\cap\Omega_{\mathrm{irr}}}\hat{h}_\lambda\left(x,\chi\right)dx \\ \geq&(2\pi r/N - S_{irr})O(\lambda^3 r^{-3}) + \epsilon_{JP}S_{irr} \quad .\end{aligned} \tag{4.1.106}$$

Since both terms depending on S_{irr} are linear, the minimum is attained either at $S_{irr} = 0$ or at $S_{irr} = 2\pi r/N$, depending on the coefficients. The coefficient that favoring $S_{irr} = 0$ is $O(\lambda^3 r^3)$ and the other is $O(1)$. We get $\hat{r} = O(\lambda)$, where the minimum changes from $S_{irr} = 0$ to $S_{irr} = 2\pi r/N$. If we use the estimate (4.1.104), we get

$$2\pi\hat{r}\left(\frac{4\lambda^3\left(\mu_1-\vartheta\right)}{5\,4^d\mu_1\left(C_J^A\right)^2\epsilon_{JP}\left|A_0\right|^2}\right)^{1/3} - C_{\delta S}\lambda \quad . \tag{4.1.107}$$

Furthermore, we realize that the energy of the second estimate is lower than the estimate for the case that there is connecting $\mathcal{A}$-chain at all. Hence, for $r \geq \hat{r}$ the estimate for the regular part is better. We have

$$\begin{aligned}&\int_{\hat{r}}^{r}\int_{u_r[0,1]\cap\Omega_{\mathrm{reg}}}\hat{h}_\lambda(\chi,x)dxdr\\ &\geq\frac{18}{25}\frac{\mu_1-\vartheta}{\mu_1}\frac{\lambda^4}{4^d\left(C_J^A\right)^2\left|A_0\right|^2}\left((C_{\delta S}\lambda+2\pi\hat{r})^{-2}-(C_{\delta S}\lambda+2\pi r)^{-2}\right)\\ &-\pi\frac{\vartheta\mu_1}{4C_\phi^W\lambda^2}\det A_0\left(r^2-\hat{r}^2\right)\quad .\end{aligned} \tag{4.1.108}$$

For $r \leq \hat{r}$ we use and $6/5\lambda \leq S_{irr} = 2\pi r/N$ to estimate independent of whether there is a connecting $\mathcal{A}$-chain or not. Hence, we obtain with the estimate 4.1.98

$$\int_{\frac{3\sqrt{2}}{4}\lambda}^{r}\int_{u_r[0,1]\cap\Omega_{\mathrm{reg}}}\hat{h}_\lambda(\chi,x)dxdr = \geq \qquad \frac{6}{5}\lambda\epsilon_{JP}\left(r-\frac{3\sqrt{2}}{4}\lambda\right) \quad . \tag{4.1.109}$$

This two estimates imply the conclusion. □

Remark 4.1.15. 1) The structure of the second estimate is

$$\int_{B_R(x_b)}\hat{h}_\lambda(\chi,x)dx = O(\lambda^2) - O(\lambda^4R^2) - O(\lambda^{-2}R) \quad . \tag{4.1.110}$$

This estimate reaches it maximum at some r of order $O(\lambda^{3/2})$ for higher r the conditions are getting stronger with growing R but the result is not getting better. Furthermore, if we compare this energy with the energy of a lattice with $0 \leq F(A) \leq \epsilon_{JP}$, there will be $R = O(\lambda)$ such that for $r < R$ the energy density must be higher in case of a dislocation but not for $r > R$. Nevertheless in this case we still have an core energy of $O(\lambda^2)$.

2) The conditions of this lemma can be even fulfilled, if there is no dislocation at all, but enough irregularities to prevent any connecting chains on the circles. The statement of the lemma holds true in this case but is not a very good estimate

3) If there is a connecting chain on the circle of radius r_1 and a connecting chain on the circle of radius r_2 and $|r_1 - r_2| \leq 5/4\lambda$, they have up to reparametrisation the same burgers vector since every point of one chain is in connecting-distance from at least on point of the other chain. If some of the connecting

chains would have different burgers vectors this means that between them there is a large irregular object.

4.2 Continuous Lagrangian coordinates

Heuristic overview In this section we will construct continuous Lagrangian coordinates for areas of regular points. Finally, we will obtain a lower bound depending only on these coordinates. We will calculate this estimate for positions x that have an energy density lower than some bound $\hat{\epsilon}$. According to Lemma 2.2.7 for every x there exists $\hat{A}(x) \in Gl_d(\mathbb{R})$ and $\hat{\tau}(x) \in \mathbb{R}^d$ such that

$$\begin{aligned} \hat{h}_\lambda(\chi, x) =& h_\lambda\left(\hat{\mathcal{A}}(x), \chi, x\right) \\ =& J_\lambda\left(\hat{\mathcal{A}}(x), \chi, x\right) + F\left(\hat{A}(x)\right) + \vartheta \det \hat{A}(x) - \vartheta\rho_\lambda \quad . \end{aligned} \tag{4.2.1}$$

We remember that $\hat{\mathcal{A}}(x)$ is defined point wise . Hence, $\hat{\mathcal{A}}(x)$ does not need to be a continuous function, but it may jump between the different reparametrisations. However we prove in Lemma 4.2.1 that $J_\lambda(\cdot, \chi, x)$ and $h_\lambda(\cdot, \chi, x)$ are locally convex for regular points. Using this we prove in Theorem 4.2.3 with the help of implicit function theorem to prove that there are branches of local minimizers of $J_\lambda(\cdot, \chi, x)$ and $h_\lambda(\cdot, \chi, x)$ that are differentiable functions of the position x and the atom positions χ. The same strategy has been used by S.Luckhaus and L.Mugnai in [7] on nearly the same model. However our version these results are improvements that will be explained for every lemma separately. Most important was to improve the estimates for the gradients of the local minimizers of J_λ in Corollary 4.2.4 so that we can use them to bound $J_\lambda\left(\tilde{\mathcal{A}}_J, \chi, x\right)$. We get:

$$J_\lambda\left(\tilde{\mathcal{A}}_J, \chi, x\right) \geq \frac{C_{con}^2\left\|\tilde{A}_g^{-1}\right\|^2}{\alpha_\nabla 2^d \|\nabla\sqrt{\tilde{\varphi}}\|_\infty^2} \frac{\rho_\lambda^2}{\rho_{2\lambda}} \lambda^2\left(\lambda^2\|\nabla\tilde{A}_g\|^2 + \|\nabla\tilde{\tau}_g - \tilde{A}_g\|^2\right) \tag{4.2.2}$$

We can also apply the same procedure to the second gradients

$$J_\lambda\left(\tilde{\mathcal{A}}_J, \chi, x\right) \geq C_{\nabla 2}\left(\frac{\rho_{2\lambda}}{\rho_\lambda}\right)\left\|\tilde{A}^{-1}\right\|^2 \rho_\lambda \lambda^4\left(\lambda^2\|\nabla^2\tilde{A}_J\|^2 + \|\nabla^2\tilde{\tau}_J - \nabla\tilde{A}_J\|^2\right) \quad , \tag{4.2.3}$$

These improved estimates will finally allow us bound the energy density from below with a functional only depending on τ_J of the form

$$\hat{h}_\lambda(\chi, y) \geq F_C\left(\nabla\tilde{\tau}_B(y)\right) + \frac{1}{5}\tilde{C}_\nabla\left(\frac{\rho_{2\lambda}}{\rho_\lambda}\right)\left\|\nabla\tilde{\tau}_B^{-1}(y)\right\|^2 \lambda^4\|\nabla^2\tilde{\tau}_B(y)\|^2 \det\left(\nabla\tilde{\tau}_B\right) \quad , \tag{4.2.4}$$

where

$$F_C(A) = \min\left\{F(BA)|B \in Gl_d(\mathbb{Z}^d)\right\} + O(\lambda^{-2}) \tag{4.2.5}$$

First, we concentrate on proving the local convexity of h_λ and J_λ for regular points similar to Proposition 5.10 and Corollary 5.11 from [7]. However our methods works with lower particle density. If we have a regular point, then this implies a certain number of regular atoms. Regular atoms have to sit near lattice positions. If we choose the parameters right, there can be only one regular atom near any lattice position. Hence, for a large enough density not all regular atoms can sit on a plain . This is sufficient to prove local convexity even if the density is relatively low.

Lemma 4.2.1. *For all C_A there exists $\hat{\lambda}, \epsilon_J$ such that for all $\lambda > \hat{\lambda}$, $x \in B_{2\lambda}(\Omega)$ that are $(C_A, \epsilon_\rho, \epsilon_J)$-regular with $\mathcal{A} \in Gl_d(\mathbb{R}) \times \mathbb{R}^d$ and all test matrices $\mathcal{M} = (M, \mu) \in \mathbb{R}^{d\times d} \times \mathbb{R}^d$ it holds*

$$\partial^2_{\mathcal{A}} J_\lambda(\mathcal{A}, \chi, x)[\mathcal{M}] \geq C_{Con} \left\|A^{-1}\right\|^2 \rho_\lambda \|\mathcal{M}\|^2_\lambda \quad , \tag{4.2.6}$$

$$\partial^2_{\mathcal{A}} h_\lambda(\mathcal{A}, \chi, x)[\mathcal{M}] \geq C_{Con} \left\|A^{-1}\right\|^2 \rho_\lambda \|\mathcal{M}\|^2_\lambda \quad , \tag{4.2.7}$$

where C_{con} is defined by

$$C_{con} := c^0_\Theta \min\left\{\frac{1}{12}, \frac{c^0_\Theta C^2_\varphi}{4\,(9+d)\, w^2_{d-1} 4^d} \frac{\rho^2_\lambda}{\det A^2}\right\} \quad . \tag{4.2.8}$$

Proof. The second derivative $\partial^2_{\mathcal{A}} J_\lambda$ tested by $\mathcal{M} = (M, \mu) \in \mathbb{R}^{d\times d}(\mathbb{R}) \times \mathbb{R}^d$ is given by

$$\begin{aligned}
&\partial^2_{\mathcal{A}} J_\lambda(\mathcal{A}, \chi, x)[\mathcal{M}] \\
=&\frac{\|A^{-1}\|^2}{C_\varphi \lambda^d} \sum_i \nabla^2 W(A\,(x_i - x) + \tau)[M(x_i - x) + \mu]\varphi \\
&+ 2\frac{\partial_{\mathcal{A}} \|A^{-1}\|^2 [M]}{C_\varphi \lambda^d} \sum_i \left\langle \nabla W(A\,(x_i - x) + \tau), M(x_i - x) + \mu \right\rangle \varphi \\
&+ \frac{\partial^2_{\mathcal{A}} \|A^{-1}\|^2 [M]}{C_\varphi \lambda^d} \sum_i W(A\,(x_i - x) + \tau)\varphi \quad .
\end{aligned} \tag{4.2.9}$$

The two last terms lower are of order $O(\lambda^{-1})\|\mathcal{M}\|_\lambda$. Furthermore, we can split the first sum into one sum over the regular atoms $\chi^{reg}_{\mathcal{A},\beta,x}$ with $\beta = \min\{|A|^{-1}\Theta_W, s_o/3\}$ and one sum over the irregular atoms, and get

$$\begin{aligned}
\partial^2_{\mathcal{A}} J_\lambda(\mathcal{A}, \chi, x)[\mathcal{M}] =&\frac{\|A^{-1}\|^2}{C_\varphi \lambda^d} \sum_{x_i \in \chi^{reg}_{\mathcal{A},\beta,x}} \nabla^2 W(A\,(x_i - x) + \tau)[M(x_i - x) + \mu]\varphi \\
&+ \frac{\|A^{-1}\|^2}{C_\varphi \lambda^d} \sum_{x_i \in \chi^{irr}_{\mathcal{A},\beta,x}} \nabla^2 W(A\,(x_i - x) + \tau)[M(x_i - x) + \mu]\varphi \\
&- O(\lambda^{-1})\|\mathcal{M}\|^2_\lambda \quad .
\end{aligned} \tag{4.2.10}$$

On the one hand all the regular atoms satisfie

$$\begin{aligned} dist(x_i, \chi_{\mathcal{A}} + x) \leq& \beta \quad , \\ dist(A(x_i - x) + \tau\mathbb{Z}^d) \leq& \beta|A| \leq \Theta_W \quad , \\ c^0_\Theta (M(x_i - x) + \mu)^2 \leq& (M(x_i - x) + \mu)\nabla^2 W(A(x_i - x) + \tau) \quad . \end{aligned} \tag{4.2.11}$$

Since W is two times differentiable and periodic, there is an upper bound for its second derivative, which we can use to bound the contribution of the irregular atoms. Hence, we get

$$\begin{aligned} \partial^2_{\mathcal{A}} J_\lambda(\mathcal{A}, \chi, x)(\mathcal{M}, \mathcal{M}) \geq& c^0_\Theta \frac{\|A^{-1}\|^2}{C_\varphi \lambda^d} \sum_{x_i \in \chi^{reg}_{\mathcal{A},\beta,x}} (M(x_i - x) + \mu)^2 \varphi\left(\lambda^{-1}|x_i - x|\right) \\ &- 8\left\|A^{-1}\right\|^2 \|\nabla^2 W\|_\infty \rho^{irr}_{\mathcal{A},\beta}(x) \|\mathcal{M}\|^2_\lambda - O(\lambda^{-1})\|\mathcal{M}\|^2_\lambda \quad . \end{aligned} \tag{4.2.12}$$

We define the average particle position by

$$\bar{x} := \left(\rho^{reg}_{\mathcal{A},\beta}(x)\right)^{-1} \frac{1}{C_\varphi \lambda^d} \sum_{x_i \in \chi^{reg}_{\mathcal{A},\beta,x}} x_i \varphi\left(\lambda^{-1}|x_i - x|\right) \quad . \tag{4.2.13}$$

Using this definition we get

$$\begin{aligned} \partial^2_{\mathcal{A}} J_\lambda(\mathcal{A}, \chi, x)[\mathcal{M}] \geq& c^0_\Theta \frac{\|A^{-1}\|^2}{C_\varphi \lambda^d} \sum_{x_i \in \chi^{reg}_{\mathcal{A},\beta,x}} (M(x_i - \bar{x})^2 + (M(\bar{x} - x) + \mu)^2)\varphi \\ &- \left\|A^{-1}\right\|^2 \|\nabla^2 W\|_\infty \rho^{irr}_{\mathcal{A},\beta}(x) + O(\lambda^{-1})\|\mathcal{M}\|^2_\lambda \quad . \end{aligned} \tag{4.2.14}$$

Because $(M(\bar{x} - x) + \mu)^2$ is independent of i, this sum can be expressed with the density of regular points. If we denote by e_M the eigenvector the largest eigenvalue of $M^T M$, we get

$$\begin{aligned} \partial^2_{\mathcal{A}} J_\lambda(\mathcal{A}, \chi, x)[\mathcal{M}] \geq& c^0_\Theta \frac{\|A^{-1}\|^2}{C_\varphi \lambda^d} \sum_{x_i \in \chi^{reg}_{\mathcal{A},\beta,x}} (e_m(x_i - \bar{x}))^2 |M|^2 \varphi \\ &+ c^0_\Theta \left\|A^{-1}\right\|^2 (M(\bar{x} - x) + \mu)^2 \rho^{reg}_{\mathcal{A},\beta}(x) \\ &- 8\left\|A^{-1}\right\|^2 \|\nabla^2 W\|_\infty \rho^{irr}_{\mathcal{A},\beta}(x) \|\mathcal{M}\|^2_\lambda + O(\lambda^{-1})\|\mathcal{M}\|^2_\lambda \quad . \end{aligned} \tag{4.2.15}$$

We concentrate on the calculation of

$$X := \frac{1}{C_\varphi \lambda^d} \sum_{x_i \in \chi^{reg}_{\mathcal{A},\beta,x}} (e_m(x_i - \bar{x}))^2 \varphi\left(\lambda^{-1}|x_i - x|\right) \quad . \tag{4.2.16}$$

Because of $\beta \leq s_o/3$ there can be only one regular atom in $B_\beta(A^{-1}(z_i - \tau) + x)$ for any z_i Therefore, the regular atoms can not sit all on the plain $P := \{y \in R^d | e_m(y - \bar{x}) = 0\}$. We call h the minimal distance to the plain P up to which we have to fill atoms to reach the density $\rho^{reg}_{\mathcal{A},\beta}(x)$. We define the cylinder

$$Z_P := \{y || \langle e_M, y - x\rangle | \leq 2\lambda\} \quad . \tag{4.2.17}$$

The characteristic function 1_{Z_P} of this set satisfies:

$$1_{Z_P}(x) \geq \varphi\left(\lambda^{-1} |x_i - x|\right) \quad . \tag{4.2.18}$$

Hence, it holds

$$\begin{aligned} \rho^{reg}_{\mathcal{A},\beta}(x) =& \frac{1}{C_\varphi \lambda^d} \sum_{x_i \in \chi^{reg}_{\mathcal{A},\beta,x}} \varphi\left(\lambda^{-1} |x_i - x|\right) \\ \leq& \frac{1}{C_\varphi \lambda^d} \sum_{x_i \in \chi^{reg}_{\mathcal{A},\beta,x}} 1_{Z_P}(x_i) \\ \leq& 2w_{d-1} 2\lambda^{d-1} \det Ah \quad . \end{aligned} \tag{4.2.19}$$

and we get

$$h \geq \frac{C_\varphi \lambda \rho^{reg}_{\mathcal{A},\beta}(x)}{w_{d-1} 2^d \det A} \quad . \tag{4.2.20}$$

Since for any valley with distance less then h from the plain P, that does not have a regular atom, there needs to be an regular atom with larger distance to reach the same density. Filling the whole cylinder gives us a lower bound for X

$$\begin{aligned} X \geq& \frac{1}{C_\varphi \lambda^d} \int_0^h 2\tilde{h}^2 w_{d-1} (2\lambda)^{d-1} \det A d\tilde{h} \\ \geq& \frac{C_\varphi^2}{3w_{d-1}^2 4^d} \lambda^2 \det A^{-2} \left(\rho^{reg}_{\mathcal{A},\beta}\right)^3 \quad . \end{aligned} \tag{4.2.21}$$

We insert this into estimate (4.2.15)

$$\begin{aligned} \partial^2_{\mathcal{A}} J_\lambda(\mathcal{A}, \chi, x)[\mathcal{M}] \geq& c^0_\Theta \left\|A^{-1}\right\|^2 |M|^2 \frac{C_\varphi^2}{3w_{d-1}^2 4^d} \lambda^2 \det A^{-2} \left(\rho^{reg}_{\mathcal{A},\beta}\right)^3 \\ &+ c^0_\Theta \left\|A^{-1}\right\|^2 (M(\bar{x} - x) + \mu)^2 \rho^{reg}_{\mathcal{A},\beta}(x) \\ &- \left\|A^{-1}\right\|^2 \|\nabla^2 W\|_\infty \rho^{irr}_{\mathcal{A},\beta}(x) + O(\lambda^{-1}) \|\mathcal{M}\|^2_\lambda \quad . \end{aligned} \tag{4.2.22}$$

We treat two cases. In case one holds $|\mu| < 3\lambda|M|$. In case two holds $|\mu| \geq 3\lambda|M|$. For case one we calculate

$$(9 + d)\lambda^2 |M|^2 \geq d\lambda^2 |M|^2 + |\mu|^2 = \lambda^2 \|M\|^2 + |\mu|^2 = \|\mathcal{M}\|^2_\lambda \quad . \tag{4.2.23}$$

We apply this to the estimate (4.2.22) and get

$$\partial^2_{\mathcal{A}} J_\lambda(\mathcal{A},\chi,x)[\mathcal{M}] \geq \frac{c^0_\Theta C^2_\varphi}{3\,(9+d)\,w^2_{d-1}4^d} \left\|A^{-1}\right\|^2 \det A^{-2} \left(\rho^{reg}_{\mathcal{A},\beta}\right)^3 \|\mathcal{M}\|^2_\lambda$$
$$- 8 \left\|A^{-1}\right\|^2 \|\nabla^2 W\|_\infty \rho^{irr}_{\mathcal{A},\beta}(x) + O(\lambda^{-1})\|\mathcal{M}\|^2_\lambda \quad . \quad (4.2.24)$$

Since every atom contributing to the average $\bar{x}$ is in $B_{2\lambda}(x)$ also $\bar{x}$ itself has to be in $B_{2\lambda}(x)$. Therefore, we obtain for case two

$$(M(\bar{x}-x)+\mu)^2 \geq (|\mu| - |M||\bar{x}-x|)^2 \geq (|\mu| - |M|2\lambda)^2 \geq \frac{1}{9}|\mu|^2 \quad . \quad (4.2.25)$$

With estimate (4.2.22), we get

$$\partial^2_{\mathcal{A}} J_\lambda(\mathcal{A},\chi,x)[\mathcal{M}] \geq c^0_\Theta \left\|A^{-1}\right\|^2 \|M\|^2 \frac{dC^2_\varphi}{3dw^2_{d-1}4^d} \lambda^2 \det A^{-2} \left(\rho^{reg}_{\mathcal{A},\beta}\right)^3$$
$$+ \frac{c^0_\Theta}{9} \left\|A^{-1}\right\|^2 |\mu|^2 \rho^{reg}_{\mathcal{A},\beta}(x)$$
$$- \left\|A^{-1}\right\|^2 \|\nabla^2 W\|_\infty \rho^{irr}_{\mathcal{A},\beta}(x) + O(\lambda^{-1})\|\mathcal{M}\|^2_\lambda \quad . \quad (4.2.26)$$

We summarize (4.2.24) and (4.2.26) to get

$$\partial^2_{\mathcal{A}} J_\lambda(\mathcal{A},\chi,x)[\mathcal{M}] \leq c^0_\Theta \left\|A^{-1}\right\|^2 \rho^{reg}_{\mathcal{A},\beta}(x)\alpha\|\mathcal{M}\|^2_\lambda - \left\|A^{-1}\right\|^2 \|\nabla^2 W\|_\infty \rho^{irr}_{\mathcal{A},\beta}(x)$$
$$+ O(\lambda^{-1})\|\mathcal{M}\|^2_\lambda \quad . \quad (4.2.27)$$

where α is defined by

$$\alpha := \min\left\{\frac{1}{9}, \frac{c^0_\Theta C^2_\varphi}{3\,(9+d)\,w^2_{d-1}4^d} \frac{\left(\rho^{reg}_{\mathcal{A},\beta}\right)^2}{(\det A)^2}\right\} \quad . \quad (4.2.28)$$

We know from Lemma 2.2.5 with $\beta := \min\{|A|^{-1}\Theta_W, s_o/3\}$ that it holds

$$\rho^{irr}_{\mathcal{A},\beta}(x) \leq \frac{1}{C^W_0 \min\{|A|^{-1}\Theta_W, s_o/3\}^2} J_\lambda(\mathcal{A},\chi,x) \quad , \quad (4.2.29)$$

$$\rho^{reg}_{\mathcal{A},\beta}(x) \geq \rho_\lambda(\chi,x) - \frac{1}{C^W_0 \min\{|A|^{-1}\Theta_W, s_o/3\}^2} J_\lambda(\mathcal{A},\chi,x) \quad . \quad (4.2.30)$$

Therefore, we can control $\rho^{irr}_{\mathcal{A},\beta}$ and $\rho_\lambda - \rho^{reg}_{\mathcal{A},\beta}(x)$ for sufficiently low ϵ_J and large λ arriving at

$$\partial^2_{\mathcal{A}} J_\lambda(\mathcal{A},\chi,x)[\mathcal{M}] \geq \frac{7}{8}\alpha c^0_\Theta \left\|A^{-1}\right\|^2 \rho_\lambda(x)\|\mathcal{M}\|^2_\lambda \quad . \quad (4.2.31)$$

Furthermore, we know that

$$\partial^2_{\mathcal{A}} h_\lambda(\mathcal{A},\chi,x)[\mathcal{M}] = \partial^2_{\mathcal{A}} J_\lambda(\mathcal{A},\chi,x)[\mathcal{M}] + \partial^2_{\mathcal{A}} F(A)[\mathcal{M}] + \vartheta \det A[\mathcal{M}]$$
$$\geq \frac{7}{8}\alpha c^0_\Theta \left\|A^{-1}\right\|^2 \rho_\lambda(x)\|\mathcal{M}\|^2_\lambda + O(\lambda^2)\|\mathcal{M}\|^2_\lambda$$
$$\geq C_{Con} \left\|A^{-1}\right\|^2 \rho_\lambda \|\mathcal{M}\|^2_\lambda \quad . \quad (4.2.32)$$

□

Next, we prove as small technical lemma. that looks rather unmotivated. However it will be necessary in the proofs of Theorem 4.2.3 and Corollary 4.2.4

Lemma 4.2.2. *For all configurations* χ *and all* $\mathcal{A} \in Gl_d(\mathbb{R}) \times \mathbb{R}^d$ *we have*

$$J_\lambda(\mathcal{A}, \tilde{\chi}, x) \geq \alpha_\nabla^{-1} \left\| \tilde{A}^{-1} \right\|^2 C_\varphi^{-1} \lambda^{-d} \sum_i |\nabla W|^2 (A\,(x_i - x) + \tau) \varphi \left(\lambda^{-1} |x - x_i| \right) \quad , \tag{4.2.33}$$

where

$$\alpha_\nabla := 64 \max \left\{ \frac{\|\nabla W\|_\infty^2}{C_0^W \Theta_W^2}, \frac{|c_\Theta^1|^2}{c_\Theta^0} \right\} \quad . \tag{4.2.34}$$

Proof. We bound $W(\tilde{A}\,(x_i - x) + \tilde{\tau})$ from below with $(\nabla W)^2 (\tilde{A}\,(x_i - x) + \tilde{\tau})$. We define for every atom

$$\delta z_i := \operatorname{dist} \left(\tilde{A}(x_i - x) + \tilde{\tau}, \mathbb{Z}^d \right) \quad . \tag{4.2.35}$$

Due to the bounds on the second derivative of W in the convex region we get for atoms with $\delta z_i \leq \Theta_W$

$$(\nabla W)^2 (\delta z_i) \leq |c_\Theta^1|^2 |\delta z_i|^2 \leq \frac{2 |c_\Theta^1|^2}{c_\Theta^0} W(\delta z_i) \quad . \tag{4.2.36}$$

Due to the general bound $\|W\|_\infty$ we get for atoms with $\delta z_i \geq \Theta_W$

$$(\nabla W)^2 (\delta z_i) \leq \|\nabla W\|_\infty^2 \leq \frac{2 \|\nabla W\|_\infty^2}{C_0^W \Theta_W^2} W(\delta z_i) \quad . \tag{4.2.37}$$

Hence, for the maximum $\alpha_\nabla := 64 \max \left\{ \frac{\|\nabla W\|_\infty^2}{C_0^W \Theta_W^2}, \frac{|c_\Theta^1|^2}{c_\Theta^0} \right\}$ we get for all atoms

$$\begin{aligned} (\nabla W)^2 (\delta z_i) \leq & \alpha_\nabla W(\delta z_i) \quad , \\ J_\lambda(\mathcal{A}, \tilde{\chi}, x) \geq & \alpha_\nabla^{-1} \left\| \tilde{A}^{-1} \right\|^2 C_\varphi^{-1} \lambda^{-d} \sum_i |\nabla W|^2 (\tilde{A}\,(x_i - x) + \tilde{\tau}) \varphi \quad . \end{aligned} \tag{4.2.38}$$

□

In theorem 4.2.3 we prove that, if x_0 is $(C_A, \epsilon_\rho, \epsilon_J)$-regular with $\mathcal{A}_0$, then there exist a unique local minimizer of $J_\lambda(\cdot, \chi, x)$ and a unique minimizer of $h_\lambda(\cdot, \chi, x)$ in the neighborhood of $\mathcal{A}_0$. These results are a consequence of the local convexity shown in Lemma 4.2.1. Furthermore, we can prove with implicit function theorem that these minimizers are differentiable functions of x and χ. The statement of this theorem is very close to the first part of Theorem 4.5 from [7]. However we additionally prove that the local minimizers are also differentiable functions of the configuration.

Theorem 4.2.3. *For all C_A and $\epsilon_\rho > 0$ there exists $\hat{\lambda} > 0$, $\epsilon_J > 0$, $\delta_{\mathcal{A}} > 0$ such that for all $\lambda > \hat{\lambda}$, $x_0 \in \Omega$ and $\mathcal{A}_0 \in Gl_d(\mathbb{R}) \times \mathbb{R}^d$ the following holds: If x_0 is $(C_A, \epsilon_\rho, \epsilon_J)$-regular with $\mathcal{A}_0(x)$, then holds using g_λ as a placeholder for J_λ and h_λ*

1) There exists a local minimizer of g_λ

$$\tilde{\mathcal{A}}_g = \arg\min\{g_\lambda(\mathcal{A},\chi,x) | \mathcal{A} \in Gl_d(\mathbb{R}) \times \mathbb{R}^d \text{with } \|\mathcal{A}-\mathcal{A}_0\|_\lambda < \delta_{\mathcal{A}}\} \quad , \tag{4.2.39}$$

2) The local minimizer fulfills

$$\begin{aligned} \left\|\mathcal{A}_0 - \tilde{\mathcal{A}}_J\right\|_\lambda &\leq \left(\frac{1}{2} C_{Con} \|A_0^{-1}\|^2 \rho_\lambda\right)^{-1/2} \sqrt{J_\lambda}(\mathcal{A}_0,\chi,x) \quad , \\ \left\|\tilde{\mathcal{A}}_J - \tilde{\mathcal{A}}_h\right\|_\lambda &\leq 2\left(\lambda C_{Con} \|A_0^{-1}\|^2 \rho_\lambda\right)^{-1} \left(\|\partial_A F(A_0)\| + \|\vartheta \partial_A \det A_0\|\right) + O(\lambda^{-2}) \quad . \end{aligned} \tag{4.2.40}$$

3) We have the estimate

$$J_\lambda(\mathcal{A}_0,\chi,x) \geq J_\lambda(\tilde{\mathcal{A}}_J,\chi,x) + \frac{1}{2} C_{Con} \left(\|A_0^{-1}\|^2 + O(\lambda^{-1})\right) \rho_\lambda \left\|\mathcal{A}_0 - \tilde{\mathcal{A}}_J\right\|_\lambda^2 \quad . \tag{4.2.41}$$

4) For every differentiable curve $(x(s),\chi(s))$ with $x(0) = x$ and $\chi(s) = \chi$ there exists a neighborhood of $s = 0$ such that $\mathcal{A}_g(s)$ inside this neighborhood there is a differentiable function $\mathcal{A}_g(s)$ that is a local minimizer of g_λ for all s and fulfills

$$\begin{aligned} \left\|\frac{d\tilde{\mathcal{A}}_g}{ds}\right\|_\lambda \leq & C_{Con}^{-1} \sqrt{8} |\tilde{A}_g| \left(\|\nabla^2 W\|_\infty + O(\lambda^{-1})\right) \left(\left|\frac{dx}{ds}\right| + \frac{1}{C_\varphi \lambda^d \rho_\lambda} \sum_i \left|\frac{dx_i}{ds}\right| \varphi\right) \\ & + C_{Con}^{-1} O(\lambda^{-1}) \|\mathcal{M}\|_\lambda \left(\frac{1}{C_\varphi \lambda^d \rho_\lambda} \sum_i \left(\left|\frac{dx_i}{ds}\right| + \left|\frac{dx}{ds}\right| |\nabla| \tilde{\varphi}\right)\right) \quad . \end{aligned} \tag{4.2.42}$$

Proof. Since $\|A_0^{-1}\| < C_A$ and since the expressions $\|A^{-1}\|$, $|A|$ and $\det A$ are uniformly continuous functions of A, we can find $\delta_{\mathcal{A}} > 0$ independent of λ and A such that for $\lambda\|A - A_0\| \leq \delta_{\mathcal{A}}$ holds

$$\begin{aligned} \|A^{-1}\| &< C_A + O(\lambda^{-1}) \quad , \\ |\rho_\lambda(\chi,x) - \det A| &< \left(\epsilon_\rho + O(\lambda^{-1})\right) \det A \quad . \end{aligned} \tag{4.2.43}$$

Furthermore, we estimate

$$\begin{aligned}
&\left|\partial_{\mathcal{A}} J_\lambda\left(\mathcal{A}_0,\chi,x\right)[\mathcal{M}]\right| \\
\leq&\left|\frac{\left\|A_0^{-1}\right\|^2}{C_\varphi\lambda^d}\sum_i\left\langle\nabla W(A_0\left(x_i-x\right)+\tau), M(x_i-x)+\mu\right\rangle\varphi\right| \\
&+\left|\frac{\partial_A\left\|A_0^{-1}\right\|^2[M]}{C_\varphi\lambda^d}\sum_i W(A_0\left(x_i-x\right)+\tau)\varphi\right| \\
\leq&\left|\frac{\left\|A_0^{-1}\right\|^2}{C_\varphi\lambda^d}\sum_i\left\langle\nabla W(A_0\left(x_i-x\right)+\tau), M(x_i-x)+\mu\right\rangle\varphi\right|+O(\lambda^{-1}J_\lambda)\|\mathcal{M}\|_\lambda \quad .
\end{aligned} \tag{4.2.44}$$

We can use Cauchy-Schwarz inequality on the scalar product $\langle X,Y\rangle_*=\sum_i\langle X_i,Y_i\rangle$ to get

$$\begin{aligned}
&\left|\partial_{\mathcal{A}} J_\lambda\left(\mathcal{A}_0,\chi,x\right)[\mathcal{M}]\right| \\
\leq&\frac{\left\|A_0^{-1}\right\|^2}{C_\varphi\lambda^d}\left(\sum_i\left(\nabla W\right)^2\varphi\right)^{\frac{1}{2}}\left(\sum_i\left(M(x_i-x)+\mu\right)^2\varphi\right)^{\frac{1}{2}} \\
&+O(\lambda^{-1})\|\mathcal{M}\|_\lambda J_\lambda\left(\mathcal{A}_0,\chi,x\right) \quad .
\end{aligned} \tag{4.2.45}$$

Due to Lemma 4.2.2 to obtain the bound:

$$\left|\partial_{\mathcal{A}} J_\lambda\left(\mathcal{A}_0,\chi,x\right)[\mathcal{M}]\right|\leq O(\sqrt{J}_\lambda\left(\mathcal{A}_0,\chi,x\right)\|\mathcal{M}\|_\lambda) \quad . \tag{4.2.46}$$

Therefore, if we choose $\tilde{\epsilon_J}$ fulfilling the conditions of Lemma 4.2.1, then for sufficiently small ϵ_J exists $\delta_{\mathcal{A}}$ such that x is $(C_A+O(\lambda^{-1}),\epsilon_\rho+O(\lambda^{-1}),\tilde{\epsilon}_J)$ regular with $\mathcal{A}$ for $\|\mathcal{A}-\mathcal{A}_0\|_\lambda\leq\delta_{\mathcal{A}}$. Hence, for sufficiently small ϵ_J all the conditions of Lemma 4.2.1 are satisfied. Furthermore $J_\lambda(\tilde{\mathcal{A}}_J,\chi,x)$ is for $\|\mathcal{A}-\mathcal{A}_0\|_\lambda\leq\delta_{\mathcal{A}}$ a strictly convex function of $\mathcal{A}$

$$\partial^2_{\mathcal{A}} J_\lambda(\mathcal{A},\chi,x)[\mathcal{M}]\geq C_{Con}\|A^{-1}\|^2\rho_\lambda\|\mathcal{M}\|^2_\lambda \quad . \tag{4.2.47}$$

The estimates (4.2.46) and (4.2.47) fulfill the conditions of Lemma B.1.1. Hence, there exists a unique minimizer local minimizer $\tilde{\mathcal{A}}_J$ of J_λ with $\|\tilde{\mathcal{A}}_J-\mathcal{A}_0\|_\lambda\leq\delta_{\mathcal{A}}$. Since for the local minimizer holds $\frac{\partial J_\lambda}{\partial\mathcal{A}}=0$, we get

$$J_\lambda(\mathcal{A}_0,\chi,x)\geq J_\lambda(\tilde{\mathcal{A}}_J,\chi,x)+\frac{1}{2}C_{Con}\left(\|A_0^{-1}\|^2+O(\lambda^{-1})\right)\rho_\lambda\|\mathcal{A}_0-\tilde{\mathcal{A}}_J\|^2_\lambda \quad . \tag{4.2.48}$$

Since $J_\lambda\geq 0$, we estimate

$$\left\|\mathcal{A}_0-\tilde{\mathcal{A}}_J\right\|_\lambda\leq\left(\frac{1}{2}\|A_0^{-1}\|^2C_{Con}\rho_\lambda\right)^{-1/2}\sqrt{J}_\lambda(\mathcal{A}_0,\chi,x) \quad . \tag{4.2.49}$$

For h_λ we calculate

$$\left|\partial_{\mathcal{A}} h_\lambda\left(\tilde{\mathcal{A}}_J, \chi, x\right)[\mathcal{M}]\right| \leq |\partial_A F(A)[M] + \vartheta \partial_A \det A[M]| = O(\lambda^{-1}\|\mathcal{M}\|_\lambda) \quad . \tag{4.2.50}$$

Additionally, for $\|\mathcal{A} - \mathcal{A}_0\|_\lambda \leq \delta_{\mathcal{A}}$ we have

$$\partial_{\mathcal{A}}^2 h_\lambda(\tilde{\mathcal{A}}_J, \chi, x)[\mathcal{M}] \geq C_{Con}\|A^{-1}\|^2 \rho_\lambda \|\mathcal{M}\|_\lambda^2 \quad . \tag{4.2.51}$$

Hence, the conditions of Lemma B.1.1 are fulfilled, and we get a unique local minimizer $\tilde{\mathcal{A}}_h$ satisfying

$$\left\|\tilde{\mathcal{A}}_J - \tilde{\mathcal{A}}_h\right\|_\lambda \leq 2\left(\lambda C_{Con}\|A^{-1}\|^2\rho_\lambda\right)^{-1}\left(\|\partial_A F(A)\| + \|\vartheta\partial_A \det A_0\|\right) + O(\lambda^{-2}) \quad . \tag{4.2.52}$$

Finally, we calculate estimates for $x_i(s)$ and $x(s)$

$$\begin{aligned}
&C_\varphi \lambda^d \frac{d}{ds}\partial_{\mathcal{A}} J_\lambda(\tilde{\mathcal{A}}_J(x), \chi(s), x(s))[\mathcal{M}] \\
=& -\left\|\tilde{A}_J^{-1}\right\|^2 \sum_i \left\langle \nabla^2 W\left(M(x_i - x) + \mu\right), \tilde{A}_J\left(\frac{dx_i}{ds} - \frac{dx}{ds}\right)\right\rangle \varphi \\
&- \left\|\tilde{A}_J^{-1}\right\|^2 \sum_i \left\langle \nabla W, M\left(\frac{dx_i}{ds} - \frac{dx}{ds}\right)\right\rangle \varphi \\
&+ \partial_A \left\|\tilde{A}_J^{-1}\right\|^2 [M] \sum_i \left\langle \nabla W, A\left(\frac{dx_i}{ds} - \frac{dx}{ds}\right)\right\rangle \varphi \\
&+ \lambda^{-1}\left\|\tilde{A}_J^{-1}\right\|^2 \sum_i \langle \nabla W, M(x_i - x) + \mu\rangle \left\langle \nabla\tilde{\varphi}, \left(\frac{dx_i}{ds} - \frac{dx}{ds}\right)\right\rangle \\
&+ \lambda^{-1}\partial_A \left\|\tilde{A}_J^{-1}\right\|^2 [M] \sum_i W \left\langle \nabla\tilde{\varphi}, \left(\frac{dx_i}{ds} - \frac{dx}{ds}\right)\right\rangle \quad .
\end{aligned} \tag{4.2.53}$$

Hence, we estimate

$$\begin{aligned}
&\left|C_\varphi \lambda^d \frac{d}{ds}\partial_{\mathcal{A}} J_\lambda(\tilde{\mathcal{A}}_J, \chi, x)[\mathcal{M}]\right| \\
\leq& \sqrt{8}\left\|\tilde{A}_J^{-1}\right\|^2 |\tilde{A}_J| \left(\|\nabla^2 W\|_\infty + O(\lambda^{-1})\right)\|\mathcal{M}\|_\lambda \left(\left|\frac{dx}{ds}\right| C_\varphi \lambda^d \rho_\lambda + \sum_i \left|\frac{dx_i}{ds}\right| \varphi\right) \\
&+ O(\lambda^{-1})\|\mathcal{M}\|_\lambda \left(\sum_i \left(\left|\frac{dx_i}{ds}\right| + \left|\frac{dx}{ds}\right| |\nabla| \tilde{\varphi}\right)\right) \quad .
\end{aligned} \tag{4.2.54}$$

Therefore, the conditions of the second part of Lemma B.1.1 are fulfilled and we obtain

$$\begin{aligned}\left\|\frac{d\mathcal{A}}{ds}\right\|_\lambda \leq & C_{Con}^{-1}\rho_\lambda^{-1}\sqrt{8}|\tilde{A}_J|\left(\|\nabla^2 W\|_\infty + O(\lambda^{-1})\right)\left(\left|\frac{dx}{ds}\right| + \frac{1}{C_\varphi \lambda^d \rho_\lambda}\sum_i \left|\frac{dx_i}{ds}\right|\varphi\right)\\ & + C_{Con}^{-1}O(\lambda^{-1})\|\mathcal{M}\|_\lambda\left(\frac{1}{C_\varphi\lambda^d\rho_\lambda}\sum_i\left(\left|\frac{dx_i}{ds}\right| + \left|\frac{dx}{ds}\right|\right)|\nabla\tilde{\varphi}|\right) \quad .\end{aligned} \tag{4.2.55}$$

Finally, we note

$$\begin{aligned}\partial_x\partial_{\mathcal{A}}h_\lambda(\mathcal{A},\chi,x) =& \partial_x\partial_{\mathcal{A}}J_\lambda(\mathcal{A},\chi,x) \quad ,\\ \partial_{x_i}\partial_{\mathcal{A}}h_\lambda(\mathcal{A},\chi,x) =& \partial_{x_i}\partial_{\mathcal{A}}J_\lambda(\mathcal{A},\chi,x) \quad ,\end{aligned} \tag{4.2.56}$$

and therefore get, the corresponding estimates for the local minimizer of $\tilde{A}_j$. □

Now, we improve the estimate for the gradients of the local minimizers. The basic idea is that $\nabla\tau_J$ has to be very similar to A_J. Hence, if we do not estimate $\|\nabla\tau_J\|$ but $\|\nabla\tau_J - A_J\|$, we can get a much better estimate. The result is similar to the final estimate in Theorem 4.5 from [7]. However we improve the estimate so that we can use the gradient of the local minimizers to bound J_λ from below. Furthermore, we use the same technique to get an estimate for the second gradient of the local minimizer $\mathcal{A}_J$.

Corollary 4.2.4. *For all C_A and $\epsilon_\rho > 0$ there exists $\hat{\lambda} > 0$, $\epsilon_J > 0$, $\delta_{\mathcal{A}} > 0$ such that for all $\lambda > \hat{\lambda}$, $x_0 \in \Omega$ and $\mathcal{A}_0 \in Gl_d(\mathbb{R}) \times \mathbb{R}^d$ the following holds: If x_0 is $(C_A, \epsilon_\rho, \epsilon_J)$-regular with $\mathcal{A}_0(x)$, then gradients of the local minimizers $\tilde{\mathcal{A}}_g$ (see Theorem 4.2.3) satisfy*

$$J_\lambda\left(\tilde{\mathcal{A}}_g,\chi,x\right) \geq \frac{C_{con}^2\left\|\tilde{A}_g^{-1}\right\|^2}{\alpha_\nabla 2^d\|\nabla\sqrt{\tilde{\varphi}}\|_\infty^2}\frac{\rho_\lambda^2}{\rho_{2\lambda}}\lambda^2\left(\lambda^2\|\nabla\tilde{A}_g\|^2 + \|\nabla\tilde{\tau}_g - \tilde{A}_g\|^2\right) \quad . \tag{4.2.57}$$

Furthermore, if W is three times differentiable, we get:

$$J_\lambda\left(\tilde{\mathcal{A}}_J,\chi,x\right) \geq C_{\nabla 2}\left(\frac{\rho_{2\lambda}}{\rho_\lambda}\right)\left\|\tilde{A}^{-1}\right\|^2\rho_\lambda\lambda^4\left(\lambda^2\|\nabla^2\tilde{A}_J\|^2 + \|\nabla^2\tilde{\tau}_J - \nabla\tilde{A}_J\|^2\right) \quad , \tag{4.2.58}$$

where

$$\begin{aligned}(C_{\nabla 2}(X))^{-\frac{1}{2}} =& \frac{\sqrt{\alpha_\nabla}}{C_{con}}\left(\|\nabla\sqrt{\tilde{\varphi}}\|_\infty^2 + \|\nabla^2\sqrt{\tilde{\varphi}}\|_\infty + 2\infty\|\nabla\sqrt[4]{\tilde{\varphi}}\|^2\right)d\sqrt{2^d X}\\ & + \frac{\sqrt{\alpha_\nabla}}{C_{con}^2}\left(2^d\|\nabla\sqrt{\tilde{\varphi}}\|_\infty^2\right)^{\frac{1}{2}}\left(16\ 2^{\frac{d}{2}}X + \sqrt{8d}\sqrt{X}\right) \quad .\end{aligned} \tag{4.2.59}$$

Proof. **Step 1: The first derivative:** Since the same conditions as in Theorem B.1.1 are fulfilled, we get the minimizers $\tilde{\mathcal{A}}_J$ and $\tilde{\mathcal{A}}_h$. The proof of the first part is the same for both and we will just call them $\tilde{\mathcal{A}}$ in the calculation. We have the equation

$$0 = \partial_{\mathcal{A}} g(\tilde{\mathcal{A}}, \chi, x) \quad . \tag{4.2.60}$$

In particular for all test matrices $\mathcal{M} = (M, \mu) \in \mathbb{R}^{d\times d} \times \mathbb{R}^d$ holds

$$0 = \partial_{\mathcal{A}} g(\tilde{\mathcal{A}}(x), \chi, x)[\mathcal{M}] \quad . \tag{4.2.61}$$

On the one hand this implies for the τ derivative

$$0 = \sum_i \nabla W(\tilde{A}\,(x_i - x) + \tilde{\tau})\varphi\left(\lambda^{-1}\,|x_i - x|\right) \quad . \tag{4.2.62}$$

On the other hand, the total derivative of $\partial_{\mathcal{A}} g(\tilde{\mathcal{A}}(x), \chi, x)[\mathcal{M}]$ in every direction e_j is zero, because we know that $\partial_{\mathcal{A}} g(\tilde{\mathcal{A}}(x), \chi, x)[\mathcal{M}]$ is constant.

$$\begin{aligned} 0 =& \frac{d}{dx^j}\left(\partial_{\mathcal{A}} g(\tilde{\mathcal{A}}(x), \chi, x)[\mathcal{M}]\right) \\ =& \partial^2_{\mathcal{A}} g(\tilde{\mathcal{A}}(x), \chi, x)\left(\mathcal{M}, \nabla_j \tilde{\mathcal{A}}(x)\right) + \nabla_j\left(\partial_{\mathcal{A}} g(\tilde{\mathcal{A}}(x), \chi, x)[\mathcal{M}]\right) \quad . \end{aligned} \tag{4.2.63}$$

We realize that J_λ is the only term in h_λ, that explicitly depends on x and on $\mathcal{A}$. Therefore, we get

$$0 = \partial^2_{\mathcal{A}} g(\tilde{\mathcal{A}}(x), \chi, x)\left(\mathcal{M}, \nabla_j \tilde{\mathcal{A}}(x)\right) + \nabla_j\left(\partial_{\mathcal{A}} J(\tilde{\mathcal{A}}(x), \chi, x)[\mathcal{M}]\right) \quad . \tag{4.2.64}$$

Furthermore, J_λ is the only part of h_λ that depends on τ. Hence, it holds

$$\partial_{\tau_j}\left(\partial_{\mathcal{A}} g_\lambda[\mathcal{M}]\right) = \partial_{\tau_j}\left(\partial_{\mathcal{A}} J_\lambda[\mathcal{M}]\right) \quad . \tag{4.2.65}$$

We compare $\partial_{\tau_j}\left(\partial_{\mathcal{A}} J_\lambda[\mathcal{M}]\right)$ with $\nabla_j \partial_{\mathcal{A}} J_\lambda[\mathcal{M}]$. First, we calculate the τ-derivative and then use equation (4.2.62).

$$\begin{aligned} & C_\varphi \lambda^d \partial_{\tau_j} \partial_{\mathcal{A}} J_\lambda(\tilde{\mathcal{A}}, \chi, x)[\mathcal{M}] \\ =& \left\|\tilde{A}^{-1}\right\|^2 \sum_i \left\langle \nabla_j \nabla W(\tilde{A}\,(x_i - x) + \tilde{\tau}), M(x_i - x) + \mu \right\rangle \varphi \\ & + \partial_A \left\|\tilde{A}^{-1}\right\|^2 [M] \sum_i \nabla_j W(\tilde{A}\,(x_i - x) + \tilde{\tau})\varphi \\ =& \left\|\tilde{A}^{-1}\right\|^2 \sum_i \left\langle \nabla_j \nabla W(\tilde{A}\,(x_i - x) + \tilde{\tau}), M(x_i - x) + \mu \right\rangle \varphi \quad . \end{aligned} \tag{4.2.66}$$

Now, we calculate the partial derivative $\nabla_j \partial_{\mathcal{A}} J_\lambda(\tilde{\mathcal{A}}, \chi, x)[\mathcal{M}]$ and get

$$\begin{aligned}
&C_\varphi \tilde{\lambda^d} \nabla_j \partial_{\mathcal{A}} J_\lambda(\tilde{\mathcal{A}}(x), \chi, x)[\mathcal{M}] \\
&= - \left\| \tilde{A}^{-1} \right\|^2 \sum_i \left(\left\langle \nabla^2 W \left(M(x_i - x) + \mu \right), \tilde{A} e_j \right\rangle + \langle \nabla W, M e_j \rangle \right) \varphi \\
&\quad + \partial_A \left\| \tilde{A}^{-1} \right\|^2 [M] \sum_i \langle \nabla W, A e_j \rangle \varphi + \left\| \tilde{A}^{-1} \right\|^2 \sum_i \langle \nabla W, M(x_i - x) + \mu \rangle \nabla_j \tilde{\varphi} \\
&\quad + \partial_A \left\| \tilde{A}^{-1} \right\|^2 [M] \sum_i W \nabla_j \tilde{\varphi} \quad .
\end{aligned} \tag{4.2.67}$$

The second and the third term are zero due to equation (4.2.62). We compare equation (4.2.66) with equation (4.2.67) and see that the first term of $\nabla_j \left(\partial_{\mathcal{A}} J_\lambda[\mathcal{M}] \right)$ equals $- \left\langle \partial_x \left(\partial_{\mathcal{A}} J_\lambda[\mathcal{M}] \right), A e_j \right\rangle$. We summarize the last two terms into a linear map $D : \mathbb{R}^{d \times d} \times \mathbb{R}^d \to \mathbb{R}^d$.

$$\nabla_j \partial_{\mathcal{A}} J_\lambda(\tilde{\mathcal{A}}(x), \chi, x)[\mathcal{M}] = - \left\langle \partial_\tau \partial_{\mathcal{A}} J_\lambda(\tilde{\mathcal{A}}(x), \chi, x)[\mathcal{M}], \tilde{A} e_j \right\rangle - D_j[\mathcal{M}] \quad , \tag{4.2.68}$$

where $D[\mathcal{M}]$ is defined by

$$\begin{aligned}
D[\mathcal{M}] := &- \frac{\left\| \tilde{A}^{-1} \right\|^2}{\lambda C_\varphi \lambda^d} \sum_i \left\langle \nabla W(\tilde{A}\,(x_i - x) + \tilde{\tau}), M(x_i - x) + \mu \right\rangle \nabla \tilde{\varphi} \\
&- \frac{\partial_A \left\| \tilde{A}^{-1} \right\|^2 [M]}{\lambda C_\varphi \lambda^d} \sum_i W(\tilde{A}\,(x_i - x)\,\tilde{A} + \tilde{\tau}) \nabla \tilde{\varphi} \quad .
\end{aligned} \tag{4.2.69}$$

Using equation (4.2.68) we can reformulate equation (4.2.64) as follows

$$D_j[\mathcal{M}] = \partial^2_{\mathcal{A}} g(\tilde{\mathcal{A}}(x), \chi, x) \left(\mathcal{M}, \left(\nabla_j \tilde{A}, \nabla_j \tilde{\tau} - \tilde{A} e_j \right) \right) \quad . \tag{4.2.70}$$

We test this equation with $\mathcal{M} = (\nabla_j \tilde{A}, \nabla_j \tilde{\tau} - \tilde{A} e_j)$ and sum over j to obtain

$$\sum_j D_j \left[\left(\nabla \tilde{A}, \nabla_j \tilde{\tau} - \tilde{A} e_j \right) \right] = \partial^2_{\mathcal{A}} g(\tilde{\mathcal{A}}(x), \chi, x) \left[\left(\nabla_j \tilde{A}, \nabla_j \tilde{\tau} - \tilde{A} e_j \right) \right] \quad . \tag{4.2.71}$$

Because of Lemma 4.2.1, we get:

$$\sum_j D_j \left(\nabla_j \tilde{A}, \nabla_j \tilde{\tau} - \tilde{A} e_j \right) \geq C_{con} \rho_\lambda \| \tilde{A}^{-1} \|^2 \left(\lambda^2 \| \nabla \tilde{A}(x) \|^2 + \| \nabla \tilde{\tau}(x) - \tilde{A} \|^2 \right) \quad . \tag{4.2.72}$$

We rewrite the left side of the last inequality

$$\begin{aligned} &C_\varphi \lambda^d \sum_j D_j \left[\left(\nabla_j \tilde{A}, \nabla_j \tilde{\tau} - A e_j \right) \right] \\ =& -\lambda^{-1} \left\| \tilde{A}^{-1} \right\|^2 \sum_{i,j} \langle \nabla W, \nabla_j A(x_i - x) + \nabla_j \tilde{\tau} \rangle \nabla_j \tilde{\varphi} \\ & - \lambda^{-1} \sum_{i,j} \partial_A \left\| \tilde{A}^{-1} \right\|^2 [\nabla_j A] W \nabla_j \tilde{\varphi} \quad . \end{aligned} \tag{4.2.73}$$

Moreover, we have

$$\nabla \tilde{\varphi}(x) = 2 \sqrt{\tilde{\varphi}} \nabla \sqrt{\tilde{\varphi}} \quad , \tag{4.2.74}$$

and

$$\begin{aligned} (\nabla_j A(x_i - x) + \nabla_j \tau - A e_j)^2 \leq & 2 |\nabla_j A|^2 |x_i - x|^2 + 2 |\nabla_j \tau - A e_j|^2 \\ & 8 \lambda^2 \|\nabla_j A\|^2 + 2 |\nabla_j \tau - A e_j|^2 \quad . \end{aligned} \tag{4.2.75}$$

Therefore, we use Cauchy-Schwarz inequality to estimate

$$\begin{aligned} & C_\varphi \lambda^{d+1} \sum_j D_j \left(\nabla_j \tilde{A}, \nabla_j \tilde{\tau} - A e_j \right) \\ =& -2 \left\| \tilde{A}^{-1} \right\|^2 \sum_{i,j} \langle \nabla W, \nabla_j A(x_i - x) + \nabla_j \tau - A_{.j} \rangle \sqrt{\tilde{\varphi}} \nabla_j \sqrt{\tilde{\varphi}} \\ & - 2 \sum_{i,j} \partial_A \left\| \tilde{A}^{-1} \right\|^2 [\nabla_j A] W \sqrt{\tilde{\varphi}} \nabla_j \sqrt{\tilde{\varphi}} \\ =& 2 \left\| \tilde{A}^{-1} \right\|^2 \sum_j \left(\sum_i (\nabla W)^2 \left(8 \lambda^2 \|\nabla \tilde{A}_j\|^2 + 2 |\nabla_j \tilde{\tau} - \tilde{A} e_j|^2 \right) \tilde{\varphi}^2 \right)^{\frac{1}{2}} \left(\sum_i |\nabla \sqrt{\tilde{\varphi}}|^2 \right)^{\frac{1}{2}} \\ & + 2 \left| \partial_A \left\| \tilde{A}^{-1} \right\|^2 \right| \|\nabla \tilde{A}\| \left(\sum_i W^2 \tilde{\varphi} \right)^{\frac{1}{2}} \left(\sum_i |\nabla \sqrt{\tilde{\varphi}}|^2 \right)^{\frac{1}{2}} \quad . \end{aligned} \tag{4.2.76}$$

Since we have $\varphi(z) = 1$ for $z \leq 1$, we estimate

$$\begin{aligned} \sum_i |\nabla \sqrt{\tilde{\varphi}}|^2 \left(\lambda^{-1} |x_i - x| \right) =& \sum_i |\nabla \sqrt{\tilde{\varphi}}|^2 \left(\lambda^{-1} |x_i - x| \right) \varphi \left((2\lambda)^{-1} |x_i - x| \right) \\ \leq & C_\varphi (2\lambda)^d \|\nabla \sqrt{\tilde{\varphi}}\|_\infty^2 \rho_{2\lambda}(\chi, x) \quad . \end{aligned} \tag{4.2.77}$$

We want to bound $\sum W^2 \varphi$ and $\sum \nabla^2 \varphi$ from above with J_λ. We get

$$W^2(\tilde{A}\,(x_i - x) + \tilde{\tau}) \leq \|W\|_\infty W(\tilde{A}\,(x_i - x) + \tilde{\tau}) \quad . \tag{4.2.78}$$

In the second term we have $(\nabla W)^2(\tilde{A}\,(x_i - x) + \tilde{\tau})$ instead of $W(\tilde{A}\,(x_i - x) + \tilde{\tau})$. We use Lemma 4.2.2 and the estimate (4.2.78) on the inequality (4.2.76) and get

$$\begin{aligned}&\sum_j D_j\left(\nabla_j \tilde{A}, \nabla_j \tilde{\tau} - \tilde{A}\right)\\ \leq &\left((\alpha_\nabla)^{\frac{1}{2}}\left\|\tilde{A}^{-1}\right\| + 2\lambda^{-1}\|W\|_\infty \frac{\left|\partial_A \left\|\tilde{A}^{-1}\right\|^2\right|}{\left\|\tilde{A}^{-1}\right\|}\right)\left(2^d\|\nabla\sqrt{\tilde{\varphi}}\|^2_\infty \rho_{2\lambda}(\chi, x)\right)^{\frac{1}{2}}\\ &\times \lambda^{-1}\sqrt{J}_\lambda\left(\tilde{\mathcal{A}}, \chi, x\right)\left(\lambda^2|\nabla A\|^2 + \|\nabla\tilde{\tau} - A\|^2\right)^{\frac{1}{2}} \quad . \end{aligned} \tag{4.2.79}$$

If we apply this on the estimate (4.2.71), we get

$$\begin{aligned}&C_{con}\rho\|\tilde{A}^{-1}\|^2\left(\lambda^2\|\nabla\tilde{A}(x)\|^2 + \|\nabla\tau(x) - \tilde{A}\|^2\right)^{\frac{1}{2}}\\ \leq &\left((\alpha_\nabla)^{\frac{1}{2}}\left\|\tilde{A}^{-1}\right\| + O(\lambda^{-1})\right)\left(2^d\|\nabla\sqrt{\tilde{\varphi}}\|^2_\infty\rho_{2\lambda}(\chi, x)\right)^{\frac{1}{2}}\lambda^{-1}\sqrt{J}_\lambda\left(\tilde{\mathcal{A}}, \chi, x\right).\end{aligned} \tag{4.2.80}$$

We solve this for J_λ and obtain for large enough λ

$$J_\lambda\left(\tilde{\mathcal{A}}, \chi, x\right) \geq \frac{C^2_{con}\left\|\tilde{A}^{-1}\right\|^2}{\alpha_\nabla 2^d\|\nabla\sqrt{\tilde{\varphi}}\|^2_\infty}\frac{\rho^2_\lambda}{\rho_{2\lambda}}\lambda^2\left(\lambda^2\|\nabla\tilde{A}\|^2 + \|\nabla\tilde{\tau} - \tilde{A}\|^2\right) \quad . \tag{4.2.81}$$

Step two: Additional derivative for the local minimizer of J_λ: We start with equation (4.2.70):

$$\partial^2_{\mathcal{A}} J(\tilde{\mathcal{A}}(x), \chi, x)\left(\mathcal{M}, \left(\nabla_j\tilde{A}, \nabla_j\tilde{\tau} - \tilde{A}e_j\right)\right) = D_j[\mathcal{M}] \quad .$$

We apply the total derivative $\frac{d}{dx^k}$ on both sides, and get

$$\frac{d}{dx^k}\left(\partial^2_{\mathcal{A}} J(\tilde{\mathcal{A}}(x), \chi, x)\left(\mathcal{M}, \left(\nabla_j\tilde{A}, \nabla_j\tilde{\tau} - \tilde{A}e_j\right)\right)\right) = \frac{d}{dx^k} D_j[\mathcal{M}] \quad . \tag{4.2.82}$$

We apply the product rule and separate the second derivatives of $\mathcal{A}$ from the first derivatives

$$\begin{aligned}&\partial^2_{\mathcal{A}} J(\tilde{\mathcal{A}}(x), \chi, x)\left(\mathcal{M}, \left(\nabla_k\nabla_j\tilde{A}, \nabla_k\nabla_j\tilde{\tau} - \nabla_k\tilde{A}e_j\right)\right)\\ = &\frac{d}{dx^k}D_j[\mathcal{M}] - \left(\frac{d}{dx^k}\partial^2_{\mathcal{A}} g(\tilde{\mathcal{A}}(x), \chi, x)\right)\left([\mathcal{M}], \left(\nabla_j\tilde{A}, \nabla_j\tilde{\tau} - \tilde{A}e_j\right)\right) \quad .\end{aligned} \tag{4.2.83}$$

We test the equation with $\mathcal{M} = \left(\nabla_k \nabla_j \tilde{A}, \nabla_k \nabla_j \tilde{\tau} - \nabla_k \tilde{A} e_j\right)$, use the local convexity to estimate the left side and sum over all j and k to obtain

$$\begin{aligned}
&C_{con}\rho \|\tilde{A}^{-1}\|^2 \left(\lambda^2 \|\nabla^2 \tilde{A}\|^2 + \|\nabla^2 \tilde{\tau} - \nabla \tilde{A}\|^2\right) \\
\leq &- \sum_{j,k} \left(\frac{d}{dx^k} \partial^2_{\mathcal{A}} J)\right) \left(\left(\nabla_k \nabla_j \tilde{A}, \nabla_k \nabla_j \tilde{\tau} - \nabla_k \tilde{A} e_j\right), \left(\nabla_j \tilde{A}, \nabla_j \tilde{\tau} - \tilde{A} e_j\right)\right) \\
&+ \sum_{j,k} \frac{d}{dx^k} D_j \left(\nabla_k \nabla_j \tilde{A}, \nabla_k \nabla_j \tilde{\tau} - \nabla_k \tilde{A} e_j\right) \quad . \qquad (4.2.84)
\end{aligned}$$

First, we calculate $\left(\frac{d}{dx^k} \partial^2_{\mathcal{A}} J(\tilde{\mathcal{A}}(x), \chi, x)\right)(\mathcal{M}_1, \mathcal{M}_2)$, where we start with

$$\begin{aligned}
&C_\varphi \lambda^d \partial^2_{\mathcal{A}} J_\lambda(\mathcal{A}, \chi, x)(\mathcal{M}_1, \mathcal{M}_2) \\
= &\left\|\tilde{A}^{-1}\right\|^2 \sum_i \left\langle M_2(x_i - x) + \mu_2, \nabla^2 W(M_1(x_i - x) + \mu_1)\right\rangle \varphi \\
&+ \partial_{\mathcal{A}} \left\|\tilde{A}^{-1}\right\|^2 [M_1] \sum_i \langle \nabla W, M_2(x_i - x) + \mu_2\rangle \varphi \\
&+ \partial_{\mathcal{A}} \left\|\tilde{A}^{-1}\right\|^2 [M_2] \sum_i \nabla W(M_1(x_i - x) + \mu_1)\varphi \\
&+ \partial^2_{\mathcal{A}} \left\|\tilde{A}^{-1}\right\|^2 (M_1, M_2) \sum_i W\varphi \quad . \qquad (4.2.85)
\end{aligned}$$

We remember that a minimizer $\tilde{\mathcal{A}}$ of J_λ satisfies $\partial_{\mathcal{A}} J(\tilde{\mathcal{A}}(x), \chi, x) = 0$

$$\begin{aligned}
\frac{1}{C_\varphi \lambda^d} \sum_i \langle \nabla W, M(x_i - x) + \mu\rangle \varphi &= - \frac{\partial_A \left\|\tilde{A}^{-1}\right\|^2 [M]}{C_\varphi \lambda^d \left\|\tilde{A}^{-1}\right\|^2} \sum_i W\varphi \\
&= - \frac{\partial_A \left\|\tilde{A}^{-1}\right\|^2 [M]}{\left\|\tilde{A}^{-1}\right\|^4} J_\lambda(\tilde{\mathcal{A}}, \chi, x) \quad . \qquad (4.2.86)
\end{aligned}$$

Therefore, equation (4.2.85) turns into

$$\begin{aligned}
&\partial^2_{\mathcal{A}} J_\lambda(\mathcal{A}, \chi, x)(\mathcal{M}_1, \mathcal{M}_2) \\
= &\frac{\left\|\tilde{A}^{-1}\right\|^2}{C_\varphi \lambda^d} \sum_i \left\langle M_2(x_i - x) + \mu_2, \nabla^2 W(M_1(x_i - x) + \mu_1)\right\rangle \varphi \\
&+ \left\|\tilde{A}^{-1}\right\|^{-2} \partial^2_A \left\|\tilde{A}^{-1}\right\|^2 (M_1, M_2) J_\lambda(\tilde{\mathcal{A}}, \chi, x) \\
&- 2 \left\|\tilde{A}^{-1}\right\|^{-4} \partial_A \left\|\tilde{A}^{-1}\right\|^2 [M_1] \partial_A \left\|\tilde{A}^{-1}\right\|^2 [M_2] J_\lambda(\tilde{\mathcal{A}}, \chi, x) \quad . \qquad (4.2.87)
\end{aligned}$$

Now, we calculate $\frac{d}{dx}\partial^2_{\mathcal{A}} J_\lambda(\mathcal{A},\chi,x)(\mathcal{M}_1,\mathcal{M}_2)$. We realize that a derivative on one of the $\|\tilde{A}^{-1}\|$ terms will produce an inner derivative $\nabla A = O(\lambda^{-2}\sqrt{J_\lambda})$. Furthermore, $\partial_{\mathcal{A}}\left\|\tilde{A}^{-1}\right\|^2[M]$ is $O(\lambda^{-1})\|\mathcal{M}\|_\lambda$. Hence, we get for the derivative of the second line

$$\begin{aligned}&\left|2\frac{d}{dx}\left(\left\|\tilde{A}^{-1}\right\|^{-4}\partial_A\left\|\tilde{A}^{-1}\right\|^2(M_1)\partial_A\left\|\tilde{A}^{-1}\right\|^2(M_2)J_\lambda(\tilde{\mathcal{A}},\chi,x)\right)\right|\\ \le& O(\lambda^{-4}J_\lambda)\|\mathcal{M}_1\|_\lambda\|\mathcal{M}_2\|_\lambda + O(\lambda^{-2})\|\mathcal{M}_1\|_\lambda\|\mathcal{M}_2\|_\lambda\frac{d}{dx}\left|J_\lambda(\mathcal{A},\chi,x)\right| \quad . \end{aligned} \tag{4.2.88}$$

Since $\partial_{\mathcal{A}} J_\lambda = 0$, we get

$$C_\varphi\lambda^d\frac{d}{dx}J_\lambda(\mathcal{A},\chi,x) = -\left\|\tilde{A}^{-1}\right\|^2\sum_i\left(\nabla W A\varphi + 2\lambda^{-1}W\sqrt{\tilde{\varphi}}\nabla\sqrt{\tilde{\varphi}}\right) \quad . \tag{4.2.89}$$

According to equation (4.2.62) the first term is zero. We can apply Cauchy-Schwarz inequality as in the estimate (4.2.76) on the second term and obtain

$$\left|\frac{d}{dx}J_\lambda(\mathcal{A},\chi,x)\right| \le O(\lambda^{-1}J_\lambda) \quad . \tag{4.2.90}$$

Therefore, it holds

$$\begin{aligned}&\left(\frac{d}{dx^k}\partial^2_{\mathcal{A}}J_\lambda(\mathcal{A},\chi,x)\right)(\mathcal{M}_1,\mathcal{M}_2)\\ =&\frac{d}{dx^k}\left(\frac{\left\|\tilde{A}^{-1}\right\|^2}{C_\varphi\lambda^d}\sum_i\left\langle M_2(x_i-x)+\mu_2,\nabla^2W(M_1(x_i-x)+\mu_1)\right\rangle\varphi\right)\\ &+O(\lambda^{-3}J_\lambda)\|\mathcal{M}_1\|_\lambda\|\mathcal{M}_2\|_\lambda \quad . \end{aligned} \tag{4.2.91}$$

The x derivative can be applied on $\|\tilde{A}^{-1}\|$ producing an inner derivative $\nabla A = O(\lambda^{-2}\sqrt{J})$. A total x-derivative of the W will have an inner derivative

$$\frac{d}{dx}(\tilde{A}(x_i-x)+\tilde{\tau}) = \left(\nabla_k\tilde{A}(x_i-x)+\nabla_k\tilde{\tau}-\tilde{A}e_k\right) = O(\lambda^{-1}\sqrt{J}) \quad . \tag{4.2.92}$$

Hence, we get

$$\begin{aligned}&C_\varphi\lambda^d\left(\frac{d}{dx^k}\partial^2_{\mathcal{A}}J_\lambda(\tilde{\mathcal{A}},\chi,x)\right)(\mathcal{M}_1,\mathcal{M}_2)\\ =&2\lambda^{-1}\left\|\tilde{A}^{-1}\right\|^2\sum_i\left\langle M_2(x_i-x)+\mu_2,\nabla^2W(M_1(x_i-x)+\mu_1)\right\rangle\sqrt{\tilde{\varphi}}\nabla_k\sqrt{\tilde{\varphi}}\\ &-\left\|\tilde{A}^{-1}\right\|^2\sum_i\left\langle M_2e_k,\nabla^2W(M_1(x_i-x)+\mu_1)\right\rangle\tilde{\varphi}\\ &-\left\|\tilde{A}^{-1}\right\|^2\sum_i\left\langle M_1e_k,\nabla^2W(M_2(x_i-x)+\mu_2)\right\rangle\tilde{\varphi}\\ &+O(\lambda^{d-3}\sqrt{J_\lambda})\|\mathcal{M}_1\|_\lambda\|\mathcal{M}_2\|_\lambda \quad . \end{aligned} \tag{4.2.93}$$

We test with some $\mathcal{M}_1^{j,k}$ and $\mathcal{M}_1^j$ and sum over j and k. We estimate with the Cauchy Schwarz inequality

$$\begin{aligned}
&C_\varphi \lambda^d \left\|\tilde{A}^{-1}\right\|^{-2} \left|\sum_{j,k}\left(\frac{d}{dx^k}\partial_{\mathcal{A}}^2 J_\lambda(\tilde{\mathcal{A}},\chi,x)\right)(\mathcal{M}_1^{j,k},\mathcal{M}_2^j)\right| \\
\leq & 2\lambda^{-1}\left(\sum_{i,j,k}\left(\nabla^2 W\left(M_2^j(x_i-x)+\mu_2^j\right)\right)^2\left(\nabla_k\sqrt{\tilde{\varphi}}\right)^2\right)^{\frac{1}{2}} \\
&\times\left(\sum_{i,j,k}\left(M_1^{j,k}(x_i-x)+\mu_1^{j,k}\right)^2\tilde{\varphi}\right)^{\frac{1}{2}} \\
&+\left(\sum_{i,j,k}\left(\nabla^2 W(M_2^j e_k)\right)^2\tilde{\varphi}\right)^{\frac{1}{2}}\left(\sum_{i,j,k}\left(M_1^{j,k}(x_i-x)+\mu_1^{j,k}\right)^2\tilde{\varphi}\right)^{\frac{1}{2}} \\
&+\left(\sum_{i,j,k}\left(\left(M_2^j(x_i-x)+\mu_2^j\right)^2\nabla^2 W\right)^2\tilde{\varphi}\right)^{\frac{1}{2}}\left(\sum_{i,j,k}(M_1^{j,k}e_k)^2\tilde{\varphi}\right)^{\frac{1}{2}} \\
&+O(\lambda^{d-3}\sqrt{J_\lambda})\|\mathcal{M}_1\|_\lambda\|\mathcal{M}_2\|_\lambda \quad . \qquad (4.2.94)
\end{aligned}$$

Finally, it holds

$$\begin{aligned}
&\left|\sum_{j,k}\left(\frac{d}{dx^k}\partial_{\mathcal{A}}^2 J(\tilde{\mathcal{A}},\chi,x)\right)\left(\left(\nabla_k\nabla_j\tilde{A},\nabla_k\nabla_j\tilde{\tau}-\nabla_k\tilde{A}e_j\right),\left(\nabla_j\tilde{A},\nabla_j\tilde{\tau}-\tilde{A}e_j\right)\right)\right| \\
\leq & \left(16\sqrt{2^d\rho_{2\lambda}\rho_\lambda}+2\sqrt{8d}\rho_\lambda\right)\lambda^{-1}\left\|\tilde{A}^{-1}\right\|^2|\nabla^2 W|\left(\lambda^2\|\nabla^2\tilde{A}\|^2+\|\nabla^2\tilde{\tau}-\nabla\tilde{A}\|^2\right)^{\frac{1}{2}} \\
&\times\left(\lambda^2\|\nabla\tilde{A}\|^2+\|\nabla\tilde{\tau}-\tilde{A}\|^2\right)^{\frac{1}{2}} \quad . \qquad (4.2.95)
\end{aligned}$$

Next we consider $\frac{d}{dx^k}\left(\frac{d}{dx^k}D_j\right)[\mathcal{M}]$

$$\begin{aligned}
&C_\varphi\lambda^d\left(\frac{d}{dx^k}D_j\right)[\mathcal{M}] \\
=&\lambda^{-1}\frac{d}{dx^k}\left(\left\|\tilde{A}^{-1}\right\|^2\sum_i\left\langle\nabla W(\tilde{A}\,(x_i-x)+\tilde{\tau}),M(x_i-x)+\mu\right\rangle\nabla_j\tilde{\varphi}\right) \\
&-\lambda^{-1}\frac{d}{dx^k}\left(\partial_A\left\|\tilde{A}^{-1}\right\|^2[M]\sum_i W(\tilde{A}\,(x_i-x)+\tilde{\tau})\nabla_j\tilde{\varphi}\right) \quad . \qquad (4.2.96)
\end{aligned}$$

We know from our previous calculation that $W(\tilde{A}\,(x_i-x)+\tilde{\tau})$ gives a $O(J_\lambda)$-contribution and $\nabla W(\tilde{A}\,(x_i-x)\,\tilde{A}+\tilde{\tau})$ gives an $O(\sqrt{J}_\lambda)$-contribution. The inner derivative of the argument of W is

$$\nabla_k\left(\tilde{A}\,(x_i-x)+\tilde{\tau}\right)=(\nabla_k\tilde{A}\,(x_i-x)+\nabla_k\tilde{\tau}-Ae_k)=O(\lambda^{-1}\sqrt{J}_\lambda) \quad . \qquad (4.2.97)$$

Furthermore, a derivative on $\|\tilde{A}^{-1}\|$ will produce an inner derivative $\nabla A = O(\lambda^{-2}\sqrt{J_\lambda})$. Finally, $\partial_{\mathcal{A}} \left\|\tilde{A}^{-1}\right\|^2 [M]$ is $O(\lambda^{-1})\|\mathcal{M}\|_\lambda$. We obtain

$$\begin{aligned}
&C_\varphi \lambda^d \left\|\tilde{A}^{-1}\right\|^{-2} \left(\frac{d}{dx^k} D_j\right)[\mathcal{M}] \\
=&2\lambda^{-1}\sum_i \left\langle \nabla_k \tilde{A}\,(x_i - x) + \nabla_k \tilde{\tau} - \nabla_k A, \nabla^2 W\,(M(x_i - x) + \mu)\right\rangle \sqrt{\tilde{\varphi}}\nabla_j\sqrt{\tilde{\varphi}} \\
&+ \lambda^{-1}\sum_i \langle \nabla W, M(x_i - x) + \mu\rangle\,(\sqrt{\tilde{\varphi}}\nabla_k\nabla_j\sqrt{\tilde{\varphi}} + 2\nabla_k\sqrt{\tilde{\varphi}}\nabla_j\sqrt{\tilde{\varphi}}) \\
&- \lambda^{-1}\sum_i \langle \nabla W, M e_k\rangle \sqrt{\tilde{\varphi}}\nabla_j\sqrt{\tilde{\varphi}} + O(\lambda^{d-3}J_\lambda)\|\mathcal{M}\|_\lambda \quad .
\end{aligned} \tag{4.2.98}$$

With $\sqrt[4]{\tilde{\varphi}}$ we can rewirte

$$\nabla_k\sqrt{\tilde{\varphi}}\nabla_j\sqrt{\tilde{\varphi}} = 4\sqrt{\tilde{\varphi}}(X)\nabla_j\sqrt[4]{\tilde{\varphi}}\nabla_k\sqrt[4]{\tilde{\varphi}} \quad . \tag{4.2.99}$$

We denote

$$U_{j,k} := \nabla_k\nabla_j\tilde{A}\,(x_i - x) + \nabla_k\nabla_j\tilde{\tau} - \nabla_k A e_j \quad . \tag{4.2.100}$$

We test (4.2.98) with $\mathcal{M} = \left(\nabla_k\nabla_j\tilde{A}, \nabla_k\nabla_j\tilde{\tau} - \nabla_k\tilde{A}e_j\right)$ and sum over j and k. Applying the Cauchy Schwarz inequality we get

$$\begin{aligned}
&C_\varphi\lambda^d \left|\sum_{j,k}\left(\frac{d}{dx^k}D_j\right)\left(\nabla_k\nabla_j\tilde{A}, \nabla_k\nabla_j\tilde{\tau} - \nabla_k\tilde{A}e_j\right)\right| \\
\leq&\lambda^{-1}\left\|\tilde{A}^{-1}\right\|^2 |\nabla^2 W|_\infty \left(\sum_{i,j,k}\left(\nabla_k\tilde{A}\,(x_i - x) + \nabla_k\tilde{\tau} - Ae_k\right)^2 (\nabla_j\sqrt{\tilde{\varphi}})^2\right)^{\frac{1}{2}} \\
&\times\left(\sum_{i,j,k}U_{j,k}^2\tilde{\varphi}\right)^{\frac{1}{2}} \\
&+ \lambda^{-1}\left\|\tilde{A}^{-1}\right\|^2 |\left(\sum_i(\nabla W)^2\tilde{\varphi}\right)^{\frac{1}{2}}\sum_{j,k}\left(\sum_i\left(\nabla_k\nabla_j\tilde{A}e_k\right)^2(\nabla_j\sqrt{\tilde{\varphi}})^2\right)^{\frac{1}{2}} \\
&+ \lambda^{-2}\left\|\tilde{A}^{-1}\right\|^2\left(\sum_{i,j,k}(\nabla W)^2\tilde{\varphi}\right)^{\frac{1}{2}}\left(\sum_{i,j,k}(U_{j,k})^2(\nabla_k\nabla_j\sqrt{\tilde{\varphi}})^2\right)^{\frac{1}{2}} \\
&+ 8\lambda^{-2}\left\|\tilde{A}^{-1}\right\|^2\left(\sum_{i,j,k}(\nabla W)^2\tilde{\varphi}\right)^{\frac{1}{2}}\left(\sum_{i,j,k}U_{j,k}^2(\nabla_k\sqrt[4]{\tilde{\varphi}}\nabla_j\sqrt[4]{\tilde{\varphi}})^2\right)^{\frac{1}{2}} \quad .
\end{aligned} \tag{4.2.101}$$

We can use equation (4.2.38) to obtain

$$\begin{aligned}
&\left|\sum_j \sum_k \left(\frac{d}{dx^k} D_j\right) \left(\nabla_k \nabla_j \tilde{A}, \nabla_k \nabla_j \tilde{\tau} - \nabla_k \tilde{A} e_j\right)\right| \\
\leq & 16\lambda^{-1} \left\|\tilde{A}^{-1}\right\|^2 |\nabla^2 W|_\infty \|\nabla \sqrt{\tilde{\varphi}}\|_\infty \sqrt{2^d \rho_\lambda \rho_{2\lambda}} \\
&\times \left(\lambda^2 \|\nabla \tilde{A}\|^2 + \|\nabla \tilde{\tau} - \tilde{A}\|^2\right)^{\frac{1}{2}} \left(\lambda^2 \|\nabla^2 \tilde{A}\|^2 + \|\nabla^2 \tilde{\tau} - \nabla \tilde{A}\|^2\right)^{\frac{1}{2}} \\
&+ 2d\lambda^{-1} \left\|\tilde{A}^{-1}\right\| \alpha_\nabla \left(\|\nabla \sqrt{\tilde{\varphi}}\|_\infty + \|\nabla^2 \sqrt{\tilde{\varphi}}\|_\infty + 4\|\nabla \sqrt[4]{\tilde{\varphi}} \otimes \nabla \sqrt[4]{\tilde{\varphi}}\|_\infty\right) \sqrt{2^d \rho_{2\lambda}} \\
&\times \lambda^{-1} \sqrt{J_\lambda}(\tilde{\mathcal{A}}, \chi, x) \left(\lambda^4 \|\nabla^2 \tilde{A}\| + \|\nabla^2 \tilde{\tau} - \nabla \tilde{A}\|^2\right)^{\frac{1}{2}} \quad . \qquad (4.2.102)
\end{aligned}$$

Finally, we combine the estimates (4.2.102), (4.2.95) and (4.2.84) to get

$$\begin{aligned}
& C_{con} \rho_\lambda \|\tilde{A}^{-1}\|^2 \left(\lambda^2 \|\nabla^2 \tilde{A}\|^2 + \|\nabla^2 \tilde{\tau} - \nabla \tilde{A}\|^2\right)^{\frac{1}{2}} \\
\leq & 2d \|\tilde{A}^{-1}\| \sqrt{\alpha_\nabla} \left(\|\nabla \sqrt{\tilde{\varphi}}\|_\infty^2 + \|\nabla^2 \sqrt{\tilde{\varphi}}\|_\infty + 4\|\nabla \sqrt[4]{\tilde{\varphi}}\|_\infty^2\right) \sqrt{2^d \rho_{2\lambda}} \lambda^{-2} \sqrt{J_\lambda} \\
&+ \left(16\sqrt{2^d \rho_\lambda \rho_{2\lambda}} + \sqrt{8d} \rho_\lambda\right) |\nabla^2 W|_\infty \|\nabla \sqrt{\tilde{\varphi}}\|_\infty \\
& \lambda^{-1} \left\|\tilde{A}^{-1}\right\|^2 \left(\lambda^2 \|\nabla \tilde{A}\|^2 + \|\nabla \tilde{\tau} - A\|^2\right)^{\frac{1}{2}} \quad . \qquad (4.2.103)
\end{aligned}$$

We use the the upper bound (4.2.57) on $\lambda^2 \|\nabla \tilde{A}\|^2 + \|\nabla \tau - A\|^2$ to finally arrive at

$$\begin{aligned}
& C_{con} \rho_\lambda \|\tilde{A}^{-1}\|^2 \left(\lambda^2 \|\nabla^2 \tilde{A}\|^2 + \|\nabla^2 \tilde{\tau} - \nabla \tilde{A}\|^2\right)^{\frac{1}{2}} \\
\leq & \lambda^{-2} \|\tilde{A}^{-1}\| \alpha_\nabla^{\frac{1}{2}} \sqrt{J_\lambda}(\tilde{\mathcal{A}}, \chi, x) \\
&\times \left(\left(\|\nabla \sqrt{\tilde{\varphi}}\|_\infty^2 + \|\nabla^2 \sqrt{\tilde{\varphi}}\|_\infty + 2\infty \|\nabla \sqrt[4]{\tilde{\varphi}}\|^2\right) d\sqrt{2^d \rho_{2\lambda}} \right. \\
&\left. + C_{con}^{-1} \left(2^d \|\nabla \sqrt{\tilde{\varphi}}\|_\infty^2\right)^{\frac{1}{2}} \left(162^{\frac{d}{2}} \rho_\lambda^{-\frac{1}{2}} \rho_{2\lambda} + \sqrt{8d} \sqrt{\rho_{2\lambda}}\right)\right) \quad . \qquad (4.2.104)
\end{aligned}$$

□

Finally, we use the bounds from Theorem 4.2.4 to bound the energy from below with a functional only depending on τ_J of one local minimizer. According to Lemma 2.2.7 for every point x there is a global minimizer $\hat{\mathcal{A}}(x)$ such that

$$h_\lambda(\hat{\mathcal{A}}, \chi, x) = \hat{h}_\lambda(\chi, x) \quad . \qquad (4.2.105)$$

The global minimizer of h_λ does not have to be continuous. However the local minimizers of J_λ are differentiable. We denote one with $\mathcal{A}_B$. $\hat{\mathcal{A}}$ is regular and so we can find a reparametrisation $\mathcal{B}\hat{\mathcal{A}}$ that is close to $\mathcal{A}_B$. Due to (4.2.41) from Theorem 4.2.3 we then get:

$$J_\lambda(\hat{\mathcal{A}},\chi,x) \geq J_\lambda(\tilde{\mathcal{A}}_B,\chi,x) + \frac{1}{2}C_{Con}\left(\|A_0^{-1}\|^2 + (O\lambda^{-1})\right)\rho_\lambda \left\|\hat{\mathcal{A}} - \tilde{\mathcal{A}}_B\right\|_\lambda^2 \quad . \tag{4.2.106}$$

Next, we can bound $J_\lambda(\tilde{\mathcal{A}}_B,\chi,x)$ from below with the help of Lemma 4.2.4 and get an estimate of the form

$$\begin{aligned} J_\lambda\left(\tilde{\mathcal{A}}_g,\chi,x\right) \geq & C\lambda^4\|\nabla\tilde{A}_B\|^2 + C\lambda^2\|\nabla\tilde{\tau}_B - \tilde{A}_B\|^2 \\ & + C\lambda^6\left(\lambda^2\|\nabla^2\tilde{A}_B\|^2 + C\lambda^4\|\nabla^2\tilde{\tau}_B - \nabla\tilde{A}_B\|^2\right) \quad . \end{aligned} \tag{4.2.107}$$

Furthermore, we can use lemma 2.4.2 to estimate the difference between ρ_λ and $\det A$. Finally, we will take the minimum over all $\tilde{\tau}_B$ and $\hat{A}$. as a lower bound and arrive at an estimate of the form

$$\hat{h}_\lambda(\chi,y) \geq F_C\left(\nabla\tilde{\tau}_B(y)\right) + \frac{1}{5}\tilde{C}_\nabla\left(\frac{\rho_{2\lambda}}{\rho_\lambda}\right)\left\|\nabla\tilde{\tau}_B^{-1}(y)\right\|^2\lambda^4\|\nabla^2\tilde{\tau}_B(y)\|^2\det\left(\nabla\tilde{\tau}_B\right) \quad , \tag{4.2.108}$$

where

$$F_C\left(A\right) = \min\left\{F(BA)|B \in Gl_d(\mathbb{Z}^d)\right\} + O(\lambda^{-2}) \quad . \tag{4.2.109}$$

The main technical difficulty is to construct for every point x the correct $\mathcal{B}$ such that $\mathcal{B}\hat{\mathcal{A}}$ is close enough to the local minimizer of $\tilde{\mathcal{A}}_B(x)$.

Theorem 4.2.5. *For all $C_A > 0$ there exists $\hat{\lambda}$, $\hat{\epsilon} > 0$ such that for $\lambda > \hat{\lambda}$ the following holds. If $y(s) : [0,1] \to \Omega$ is differentiable curve with $\hat{h}_\lambda(\chi, y(s)) \leq \hat{\epsilon}$ for all s, $\hat{\mathcal{A}} \in Gl_d(\mathbb{R}) \times \mathbb{R}^d$ is the global minimizer of $h_\lambda(\cdot,\chi,y(0))$, the reparametrisation $\mathcal{B} = (B,t) \in Gl_d(\mathbb{Z}^d) \times \mathbb{Z}^d$ fulfills $\|\hat{A}^{-1}B^{-1}| \leq C_A/2$ and the compatibility condition $\frac{1}{2}\mu_1 \geq \vartheta$ is fulfilled, then there exists a differentiable function $\tilde{\mathcal{A}}_B(y(s))$ such that $\tilde{\mathcal{A}}_B(y(s))$ is a local minimizer of $J_\lambda(\cdot,\chi,y(0))$ for every s and the energy density fulfills*

$$\hat{h}_\lambda(\chi,y) \geq F_C\left(\nabla\tilde{\tau}_B(y)\right) + \frac{1}{5}\tilde{C}_\nabla\left(\frac{\rho_{2\lambda}}{\rho_\lambda}\right)\left\|\nabla\tilde{\tau}_B^{-1}(y)\right\|^2\lambda^4\|\nabla^2\tilde{\tau}_B(y)\|^2\det\left(\nabla\tilde{\tau}_B\right) \quad , \tag{4.2.110}$$

where

$$\begin{aligned}
C_{rep} &= \left(C_0^W\right)^{-1} 4^d C_A^{2d} c_2^2 \\
\tilde{C}_\nabla^{-1}(X) :=& C_{rep}\left(C_{\nabla 2}(X)^{-1} + \frac{\alpha_\nabla 2^d \|\nabla\sqrt{\tilde{\varphi}}\|_\infty^2}{C_{con}^2 X}\right) \quad , \\
F_C(A) &:= \inf\left\{U(A, A_1, B, A_2) | A_1, A_2 \in Gl_d(\mathbb{R}), B \in Gl_d(\mathbb{Z})\right\} \quad , \\
U(A, A_1, B, A_2) :=& F(A_2) - \frac{\vartheta^2}{2C_\phi^W}\lambda^{-2}\det A_2 \quad , \\
&+ \frac{1}{5} C_{Con} C_{rep}^{-1} \|\left(BA_2\right)^{-1}\|^2 \det(A)\,\lambda^2 \|BA_2 - A_1\|^2 \\
&+ \frac{1}{3}\tilde{C}_\nabla\left(\frac{\rho_{2\lambda}}{\rho_\lambda}\right)\left\|A_1^{-1}\right\|^2 \det(A)\,\lambda^2 \|A - A_1\|^2 \quad . \qquad (4.2.111)
\end{aligned}$$

$C_{\nabla 2}(X)$ is defined in Corollary 4.2.4, C_{Con} is defined in Lemma 4.2.1 and α_∇ is defined in Lemma 4.2.2.

The function $\tilde{\mathcal{A}}_B(y(s))$ can be extended along the curve of regular atoms as long as $|\tilde{\mathcal{A}}_B(y(s))| \leq C_A$. Since we started at $\|\hat{A}^{-1}B^{-1}| \leq C_A/2$ this means, we can extend it as least for a distance scaling like λ^2

Proof. **Step 1: Following one minimizer** We know from Lemma 2.2.7 that for every $x = y(0)$ there exists a minimizer $\hat{\mathcal{A}} \in Gl_d(\mathbb{R}) \times \mathbb{R}^d$ such that $h_\lambda(\hat{\mathcal{A}}, \chi, x) = \hat{h}_\lambda(\chi, x)$. We know from Theorem 2.4.3 that for large enough λ and small enough energy density $\hat{h}_\lambda(\chi, x)$, x is $(C_A, \epsilon_\rho, \epsilon_J)$-regular with $\hat{\mathcal{A}}$ satisfying

$$\begin{aligned}
\epsilon_\rho =& O(\hat{h}_\lambda(\chi, x)) + O(\lambda^{-2}) \quad , \\
\epsilon_J =& O(\hat{h}_\lambda(\chi, x)) + O(\lambda^{-2}) \quad . \qquad (4.2.112)
\end{aligned}$$

According to Corollary 2.2.2 for every reparametrisation $\mathcal{B}(x) = (B(x), t(x)) \in Gl_d(\mathbb{Z}^d) \times \mathbb{Z}^d$ with $|(BA)^{-1}| < 2C_A$ it holds

$$J_\lambda\left(\mathcal{B}\hat{\mathcal{A}}(x), \chi, x\right) \leq C_1^W \left(C_0^W\right)^{-1} \left\|B\hat{A}(x)\right\|^2 \left\|(B\hat{A}(x))^{-1}\right\|^2 J_\lambda\left(\hat{\mathcal{A}}(x), \chi, x\right). \qquad (4.2.113)$$

We estimate the norm of the matrix with the norm of the inverse and the determinant (see Lemma B.2.2). According to Lemma 2.2.7 we can estimate $\hat{A}$ with some constant c_2

$$\begin{aligned}
J_\lambda\left(\mathcal{B}\hat{\mathcal{A}}(x), \chi, x\right) \leq& C_1^W \left(C_0^W\right)^{-1} \left(\det B\hat{A}(x)\right)^2 \left\|(B\hat{A}(x))^{-1}\right\|^{2d} J_\lambda\left(\hat{\mathcal{A}}(x), \chi, x\right) \\
\leq& C_1^W \left(C_0^W\right)^{-1} 4^d C_A^{2d} \left(\det \hat{A}\right)^2 J_\lambda\left(\hat{\mathcal{A}}, \chi, x\right) \\
\leq& C_{rep} J_\lambda\left(\hat{\mathcal{A}}, \chi, x\right) \quad , \qquad (4.2.114)
\end{aligned}$$

where $C_{rep} := \left(C_0^W\right)^{-1} 4^d C_A^{2d} c_2^2$. Since the density ρ_λ does not depend on $\mathcal{A}$ and $\det A = \det BA$, the position x is $(2C_A, \epsilon_\rho, C_{rep}\epsilon_J)$-regular with $\mathcal{B}\hat{\mathcal{A}}(x)$. For large enough λ and sufficiently small ϵ the conditions of Lemma 4.2.3 are fulfilled, and there exists a unique local minimizer $\tilde{\mathcal{A}}_B$ in a neighborhood of $\mathcal{B}\hat{\mathcal{A}}$. Furthermore, we get the estimate (4.2.40) for the distance between $\mathcal{B}\hat{\mathcal{A}}$ and $\tilde{\mathcal{A}}_B$. If we combine this with the estimates (4.2.114) and (4.2.112), we get

$$\begin{aligned}\left|\mathcal{B}\hat{\mathcal{A}}(x) - \tilde{\mathcal{A}}_B(x)\right\|_\lambda \leq & \left(\frac{1}{2} C_{Con} \|A_0^{-1}\|^2 \rho_\lambda\right)^{-1/2} \sqrt{J}(\mathcal{B}\hat{\mathcal{A}}(x), \chi, x) \\ \leq & O(\sqrt{\hat{\epsilon}} + O(\lambda^{-1}) \leq \frac{1}{8}\delta_{\mathcal{A}} \quad . \end{aligned} \tag{4.2.115}$$

Additionally we have the estimate (4.2.57) from Corollary 4.2.4 for the gradients in this branch. Hence, we get

$$\begin{aligned} J_\lambda\left(\hat{\mathcal{A}}, \chi, x_0\right) \geq & C_{rep}^{-1} J_\lambda\left(\tilde{\mathcal{A}}_B, \chi, x_0\right) \\ \geq & C_{rep}^{-1} \frac{C_{con}^2 \left\|\tilde{A}_B^{-1}\right\|^2}{\alpha_\nabla 2^d \|\nabla\sqrt{\tilde{\varphi}}\|_\infty^2} \frac{\rho_\lambda^2}{\rho_{2\lambda}} \lambda^2 \left(\lambda^2 \|\nabla \tilde{A}_B(x)\|^2 + \|\nabla\tilde{\tau}(x)_B - \tilde{A}_B\|^2\right) \quad . \end{aligned} \tag{4.2.116}$$

Considering a second point $y = y(s) \in B_{1,5\lambda}(x)$ with $\hat{\lambda}(\chi, y) \leq \hat{\epsilon}$ and $\int \frac{dy}{d\tilde{s}} d\tilde{s} \geq |x-y|$ sufficiently small we obtain

$$\begin{aligned} |\tilde{A}_B(y) - \tilde{A}_B(x)| \leq & O(\lambda^{-2}|x-y|)\sqrt{J}_\lambda\left(\hat{\mathcal{A}}, \chi, x_0\right) \\ \leq & O(\lambda^{-2}|x-y|\sqrt{\hat{\epsilon}}) + O(\lambda^{-3}|x-y|) \leq \frac{1}{8}\delta_{\mathcal{A}} \quad , \\ |\tilde{\tau}_B(y) - \tilde{\tau}_B(x) - \tilde{A}_B(x)(y-x)| \leq & O(\lambda^{-1}|x-y|)\sqrt{J}_\lambda\left(\hat{\mathcal{A}}, \chi, x_0\right) \\ \leq & O(\lambda^{-1}|x-y|\sqrt{\hat{\epsilon}}) + O(\lambda^{-2}|x-y|) \leq \frac{1}{8}\delta_{\mathcal{A}} \quad . \end{aligned} \tag{4.2.117}$$

For $\hat{\epsilon} \leq \epsilon_{JP}$ the points x and y will be connecting-regular according to Corollary 4.1.5, and we can use Corollary 4.1.4 to obtain $B(y,x) \in GL_d(\mathbb{Z}^d)$ and $t(x,y) \in \mathbb{Z}^d$ such that

$$\begin{aligned} \|Id - \hat{A}(x)^{-1} B(x,y) \hat{A}(y)\| < & C_J^A 2^d \lambda^{-1} \min\left\{\sqrt{J}_\lambda(\hat{\mathcal{A}}(x), \chi, x), \sqrt{J}_\lambda(\hat{\mathcal{A}}(y), \chi, y)\right\} \\ \leq & O(\lambda^{-1}\sqrt{\hat{\epsilon}} + O(\lambda^{-2}) \quad , \end{aligned} \tag{4.2.118}$$

and

$$\left|B(x,y)\hat{\tau}(y) + t(x,y) - \hat{\tau}(x) - \frac{B(x,y)\hat{A}(y) + \hat{A}(x)}{2}(y-x)\right| < C_J^\tau \|A_1\| 2^d \sqrt{J_\lambda}. \tag{4.2.119}$$

With small enough $\hat{h}_\lambda$ and large enough λ we can control the change of $\hat{\tau}$ and $\hat{A}$, because we restricted B to a compact set.

$$\begin{aligned} \lambda|B(x)\left(\hat{A}(x) - B(x,y)\hat{A}(y)\right)| &\leq \frac{1}{8}\delta_A \quad , \\ |B(x)\left(B(x,y)\hat{\tau}(y) + t(x,y) - \hat{\tau}(x) - \frac{B(x,y)\hat{A}(y) + \hat{A}(y)}{2}(y-x)\right)| &\leq \frac{1}{8}\delta_A \quad . \end{aligned} \tag{4.2.120}$$

We introduce the notation $\mathcal{B}(y) := B(x)B(x,y)$. By comparing the estimates (4.2.115), (4.2.117) and (4.2.120) we obtain

$$\begin{aligned} \lambda\left|B(y)\hat{A}(y) - \tilde{A}_B(y)\right| &\leq \lambda\left|B(y)\hat{A}(y) - B(x)\hat{A}(x)\right| \\ &\quad + \lambda\left|B(x)\hat{A}(x) - \tilde{A}_B(x)\right| + \lambda\left|\tilde{A}_B(x) - \tilde{A}_B(y)\right| \\ &\leq \frac{3}{8}\delta_{\mathcal{A}} \quad . \end{aligned} \tag{4.2.121}$$

For τ we estimate

$$\begin{aligned} &|B(x)\left(B(x,y)\hat{\tau}(y) + t(x,y) - \tilde{\tau}_B(y)\right)| \\ \leq &\left|B(x)\left(B(x,y)\hat{\tau}(y) + t(x,y) - \hat{\tau}(x) - \frac{B(x,y)\hat{A}(y) + \hat{A}(x)}{2}(y-x)\right)\right| \\ &+ |B\hat{\tau}(x) + t - \tilde{\tau}_B(x)| + \left|\tilde{\tau}_B(x) + \tilde{A}_B(x)(y-x) - \tilde{\tau}_B(y)\right| \\ &+ \left|\tilde{A}_B(x) - B(x)\frac{B(x,y)\hat{A}(y) + \hat{A}(x)}{2}(y-x)\right| \\ \leq &\frac{3}{8}\delta_{\mathcal{A}} + \frac{3}{4}\lambda|\tilde{A}_B(x) - B(y)\hat{A}(y)| + \frac{3}{4}\lambda|\tilde{A}_B(x) - B(x)\hat{A}(x)| \\ \leq &\frac{3}{8}\delta_{\mathcal{A}} + \frac{3}{4}\lambda|B(x)\hat{A}(x) - B(y)\hat{A}(y)| + \frac{3}{2}\lambda|\tilde{A}_B(x) - B(x)\hat{A}(x)| \\ \leq &\frac{21}{32}\delta_{\mathcal{A}} \quad . \end{aligned} \tag{4.2.122}$$

We summarize

$$\left|\mathcal{B}(y)\hat{\mathcal{A}}(y) - \tilde{\mathcal{A}}_B(y)\right| \leq \delta_{\mathcal{A}} \quad . \tag{4.2.123}$$

Since $\mathcal{B}(y)\hat{\mathcal{A}}(y)$ fulfills the same conditions for y as $\mathcal{B}(x)\mathcal{A}(x)$ for x we can apply Theorem 4.2.3. Hence, there is one unique local minimizer satisfying

$$\left|\mathcal{B}(y)\hat{\mathcal{A}}(y) - \tilde{\mathcal{A}}\right| \leq \delta_{\mathcal{A}} \quad . \tag{4.2.124}$$

Therefore, $\tilde{\mathcal{A}}_B(y)$ has to be this minimizer because of the estimate (4.2.123).

Step 2: The lower bound for the energy density: Due to estimate (4.2.40) we get for $\tilde{\mathcal{A}}_B(y)$

$$\begin{aligned} J_\lambda\left(\hat{\mathcal{A}}(y),\chi,y\right) \geq & C_{rep}^{-1} J_\lambda\left(\mathcal{B}(y)\hat{\mathcal{A}}(y),\chi,y\right) \\ \geq & C_{rep}^{-1} J_\lambda(\tilde{\mathcal{A}}_B,\chi,x) \\ & + \frac{1}{2} C_{Con} C_{rep}^{-1} \left\| \left(B\hat{A}\right)^{-1} \right\|^2 \rho_\lambda \left\| \mathcal{B}\hat{\mathcal{A}} - \tilde{\mathcal{A}}_B \right\|_\lambda^2 \quad . \end{aligned} \tag{4.2.125}$$

By applying corollary 4.2.4, we get

$$\begin{aligned} J_\lambda\left(\hat{\mathcal{A}}(y),\chi,y\right) \geq & \frac{1}{2} C_{Con} C_{rep}^{-1} \left| \left(B\hat{A}\right)^{-1} \right\|^2 \rho_\lambda \left\| \mathcal{B}(y)\hat{\mathcal{A}} - \tilde{\mathcal{A}}_B \right\|_\lambda^2 \\ & + \tilde{C}_\nabla\left(\frac{\rho_{2\lambda}}{\rho_\lambda}\right) \left\| \tilde{A}_B^{-1} \right\|^2 \rho_\lambda \left(\lambda^2 \|\nabla\tilde{\tau}_B - \tilde{A}_B\|^2 + \lambda^6 \|\nabla^2 \tilde{A}_B\|^2 \right) \\ & + \tilde{C}_\nabla\left(\frac{\rho_{2\lambda}}{\rho_\lambda}\right) \left\| \tilde{A}_B^{-1} \right\|^2 \rho_\lambda \left(\lambda^4 \|\nabla\tilde{A}_B\|^2 + \|\nabla^2\tilde{\tau}_B - \nabla\tilde{A}_B\|^2 \right) \quad , \end{aligned} \tag{4.2.126}$$

Now, we search a lower bound for the expression

$$\tilde{\nu} := \frac{1}{2} J_\lambda(\hat{\mathcal{A}},\chi,x) + \vartheta\left(\det\hat{A} - \rho_\lambda(\chi,x)\right) \quad . \tag{4.2.127}$$

Lemma 2.4.2 gives a lower bound for J_λ for a given ρ_λ. If we apply this estimate to $\tilde{\nu}$, we get

$$\begin{aligned} \tilde{\nu} \geq \vartheta\left(\det\hat{A} - \rho_\lambda\right) \quad & \text{for} \quad \rho_\lambda \leq \det\hat{A} \quad , \\ \tilde{\nu} \geq \frac{1}{2}\frac{C_\phi^W}{\det\hat{A}}\lambda^2(\rho_\lambda - \det\hat{A})^2 + \vartheta\left(\det\hat{A} - \rho_\lambda\right) \quad & \text{for} \quad \det\hat{A} \leq \rho_\lambda \leq \rho_1 \quad , \\ \tilde{\nu} \geq \frac{\mu_1^2 \det\hat{A}}{8C_\phi^W \lambda^2} + \frac{1}{2}\mu_1(\rho - \rho_1) + \vartheta\left(\det\hat{A} - \rho_\lambda\right) \quad & \text{for} \quad \rho_1 \leq \rho_\lambda \quad . \end{aligned} \tag{4.2.128}$$

We are searching for a uniform lower bound. For $\rho_\lambda \leq \det\hat{A}$ the lower bound is decreasing for increasing ρ_λ. For $\rho_1 \leq \rho_\lambda$ the lower bound decreases for decreasing ρ because of $\frac{1}{2}\mu_1 \geq \vartheta$. In between the estimate is just a quadratic function. Hence, we estimate for all ρ_λ

$$\tilde{\nu} \geq -\frac{\vartheta^2}{2C_\phi^W}\lambda^{-2}\det\hat{A} \quad . \tag{4.2.129}$$

We apply the estimates (4.2.126) and (4.2.129) to get a lower bound for the density

$$\begin{aligned}\hat{h}_\lambda(\chi,y) =&\frac{1}{2}J_\lambda\left(\hat{\mathcal{A}}(y),\chi,y\right)+\tilde{\nu}(\hat{A}(y),\chi,y)+F(\hat{A}(y))\\ \geq&F(\hat{A})-\frac{\vartheta^2}{2C_\phi^W}\lambda^{-2}\det\hat{A}+\frac{1}{4}C_{Con}C_{rep}^{-1}\left\|\left(B\hat{A}\right)^{-1}\right\|^2\rho_\lambda\left\|\mathcal{B}\hat{\mathcal{A}}-\tilde{\mathcal{A}}_B\right\|_\lambda^2\\ &+\frac{1}{2}\tilde{C}_\nabla\left(\frac{\rho_{2\lambda}}{\rho_\lambda}\right)\left\|\tilde{A}_B^{-1}\right\|^2\rho_\lambda\left(\lambda^2\|\nabla\tilde{\tau}_B-\tilde{A}_B\|^2+\lambda^6\|\nabla^2\tilde{A}_B\|^2\right)\\ &+\frac{1}{2}\tilde{C}_\nabla\left(\frac{\rho_{2\lambda}}{\rho_\lambda}\right)\left(\lambda^4\|\nabla\tilde{A}_B\|^2+\lambda^4\|\nabla^2\tilde{\tau}_B-\nabla\tilde{A}_B\|^2\right). \end{aligned}\tag{4.2.130}$$

Since we calculate a lower bound, we can skip the $\nabla^2\tilde{A}_B$ term. We also estimate

$$\left\|\mathcal{B}\hat{\mathcal{A}}-\tilde{\mathcal{A}}_B\right\|_\lambda^2\geq\lambda^2\left\|B\hat{A}-\tilde{A}_B\right\|^2 \quad . \tag{4.2.131}$$

Due to $2(a^2+b^2)\geq(a+b)^2$ we summarize

$$\lambda^4\|\nabla\tilde{A}_B\|^2+\lambda^4\|\nabla^2\tilde{\tau}_B-\nabla\tilde{A}_B\|^2\geq\frac{1}{2}\lambda^4\|\nabla^2\tilde{\tau}_B\|^2 \quad . \tag{4.2.132}$$

Due to the estimate 4.2.126 and matrix derivatives (see B.2.3) we get The difference between $\left\|\tilde{A}_B^{-1}\right\|^2$ and $\left\|\nabla\tilde{\tau}_B^{-2}\right\|^2$ is $O(\lambda^{-1}\sqrt{J_\lambda})$. We estimate for small energy density and large λ

$$\begin{aligned}\rho_\lambda =&\det\hat{A}+O(\sqrt{\hat{\epsilon}})+O(\lambda^{-1})\\ =&\det\tilde{A}_B+O(\sqrt{\hat{\epsilon}})+O(\lambda^{-1})\\ =&\det\nabla\tilde{\tau}_B+O(\sqrt{\hat{\epsilon}})+O(\lambda^{-1}) \quad .\end{aligned}\tag{4.2.133}$$

Hence, we get for small enough $\hat{\epsilon}$ and large enough λ.

$$\begin{aligned}\hat{h}_\lambda(\chi,y)\geq&F(\hat{A})-\frac{\vartheta^2}{2C_\phi^W}\lambda^{-2}\det\hat{A}+\frac{1}{3}\tilde{C}_\nabla\left(\frac{\rho_{2\lambda}}{\rho_\lambda}\right)\left\|\tilde{A}_B^{-1}\right\|^2\det(\nabla\tilde{\tau}_B)\lambda^2\|\nabla\tilde{\tau}_B-\tilde{A}_B\|^2\\ &+\frac{1}{5}C_{Con}C_{rep}^{-1}\left\|\left(B\hat{A}\right)^{-1}\right\|^2\left\|\mathcal{B}\hat{\mathcal{A}}-\tilde{\mathcal{A}}_B\right\|_\lambda^2\det(\nabla\tilde{\tau}_B)\\ &+\frac{1}{5}\tilde{C}_\nabla\left(\frac{\rho_{2\lambda}}{\rho_\lambda}\right)\left\|\nabla\tilde{\tau}_B^{-1}(y)\right\|^2\lambda^4\|\nabla^2\tilde{\tau}_B\|^2\det(\nabla\tilde{\tau}_B) \quad .\end{aligned}\tag{4.2.134}$$

We summarize all but the $\|\nabla^2\tilde{\tau}_B\|^2$ term to $U(\tilde{\tau}_B,\tilde{A}_B,B(y),\hat{A})$

$$\begin{aligned}\hat{h}_\lambda(\chi,y)\geq&\frac{1}{5}\tilde{C}_\nabla\left(\frac{\rho_{2\lambda}}{\rho_\lambda}\right)\left\|\nabla\tilde{\tau}_B^{-1}\right\|^2\lambda^4\|\nabla^2\tilde{\tau}_B\|^2\det(\nabla\tilde{\tau}_B)\\ &+U(\tilde{\tau}_B,\tilde{A}_B,B,\hat{A}) \quad .\end{aligned}\tag{4.2.135}$$

Finally, we use

$$U(\tilde{\tau}_B, \tilde{A}_B, B(y), \hat{A}) \geq \inf\{U(\tilde{\tau}_B, A_1, B, A_2) | A_1, A_2 \in Gl_d(\mathbb{R}), B \in Gl_d(\mathbb{Z})\} \quad . \tag{4.2.136}$$

Step 3: Range of extension

For $|\tilde{A}_B^{-1}(x)| < C$ we can estimate with the help of Lemma B.2.3

$$|(\partial_A \tilde{A}_B^{-1})(M)| = |A_B^{-1} M A^{-1}| \leq C_A^2 |M| \quad . \tag{4.2.137}$$

With this upper bound and the estimate (4.2.126) for the gradient we can bound the change of $|\tilde{A}_B^{-1}|$ along an curve $y(s)$ of length S of regular points

$$\begin{aligned} ||\tilde{A}_B^{-1}(y_2)| - |\tilde{A}_B^{-1}(y_1)|| \leq & |\tilde{A}_B^{-1}(y_2) - \tilde{A}_B^{-1}(y_1)| \\ \leq & C_A^2 |\tilde{A}_B(y_2) - \tilde{A}_B(y_1)| \\ \leq & C_A^2 |\int \nabla(\tilde{A}_B(y(s)) \frac{dy}{ds} ds| \\ \leq & C_A^2 \int \left(C_\nabla^* \rho_{2\lambda}(y)\right)^{-1/2} \lambda^{-2} J_\lambda \left(\hat{\mathcal{A}}(y), \chi, y\right) |\frac{dy}{ds}| ds \\ \leq & \left(O(\lambda^{-2}) \sqrt{O(\hat{\epsilon}) + O(\lambda^{-2})}\right) S \quad . \end{aligned} \tag{4.2.138}$$

Starting with $|\tilde{A}_B^{-1}(y_1)| \leq \frac{1}{2} C_A$, we can follow every differentiable curve for of regular points for at least a distance scaling like $O(\lambda^2)(O(\hat{\epsilon})^{-1} + O(\lambda))^{-1}$ $\square$

Remark 4.2.6. If we select $\hat{\epsilon}$ small enough, the local minimizer $\tilde{A}$ can not leave the Ericson Piterie neighborhood it started in without increasing the energy over this barrier. Therefore, in this case $\tilde{\mathcal{A}}_B$ can be extended in any connected set of regular points

Lemma 4.2.7. *There exists $\hat{\lambda} \in \mathbb{R}$ and $\hat{\epsilon}$¿0 such that for all $\lambda > \hat{\lambda}$, and all $A \in Gl_d(\mathbb{R})$ such that $F(A) \leq \hat{\epsilon}$ there exists $\hat{A}_1, \hat{A}_2 \in Gl_d(\mathbb{R})$ and $\hat{B} \in Gl_d(\mathbb{Z})$ satisfying*

$$F_C(A) = U(A, \hat{A}_1, \hat{B}, \hat{A}_2) \tag{4.2.139}$$

F_C and $U(A, A_1, B, A_2)$ are as defined in Theorem 4.2.5

Furthermore, it holds

$$F_C(A) = \min\left\{F(BA) | B \in Gl_d(\mathbb{Z}^d)\right\} + O(\lambda^{-2}) \quad . \tag{4.2.140}$$

Proof. We consider

$$\begin{aligned} U(A, A_1, B, A_2) := & F(A_2) - \frac{\vartheta^2}{2C_\phi^W} \lambda^{-2} \det A_2 \\ & + \frac{1}{5} C_{Con} C_{rep}^{-1} \| (BA_2)^{-1} \|^2 \det(A) \lambda^2 \|BA_2 - A_1\|^2 \\ & + \frac{1}{3} \tilde{C}_\nabla \left(\frac{\rho_{2\lambda}}{\rho_\lambda}\right) \left\|A_1^{-1}\right\|^2 \det(A) \lambda^2 \|A - A_1\|^2 \quad . \end{aligned}$$

Due to the coercivity condition on F we get

$$\begin{aligned}
&F(A_2) - \frac{\vartheta^2}{2C_\phi^W}\lambda^{-2}\det A_2\\
\geq &+ C_1^{El}\left(\det(E) - \det(A_2)\right)^2 + C_2^{El}\mathrm{dist}^2\left(A_2, E\,SO_d\right)\\
\geq &C_1^{El}\left(\det(E) - \det(A_2) - \frac{3\vartheta^2}{8C_1^{El}C_\phi^W}\lambda^{-2}\right)^2 - \frac{9\vartheta^4}{16C_1^{El}\left(C_\phi^W\right)^2}\lambda^{-4}\\
&+ C_2^{El}\mathrm{dist}^2\left(A_2, E\,SO_d\right)
\end{aligned} \tag{4.2.141}$$

Since all other terms of $U(A, A_1, B, A_2)$ are positive, this implies:

$$U(A, A_1, B, A_2) \geq -\frac{9\vartheta^4}{16C_1^{El}\left(C_\phi^W\right)^2}\lambda^{-4} \tag{4.2.142}$$

Furthermore, it holds

$$U(A, A, Id, A) = F(A) - \frac{\vartheta^2}{2C_\phi^W}\lambda^{-2}\det A_2 \leq \hat{\epsilon} \tag{4.2.143}$$

Therefore, we can conclude for all $A_1, A_2 \in Gl_d(\mathbb{R})$ and $B \in Gl_d(\mathbb{Z})$ satisfying $U(A, A_1, B, A_2) \leq U(A, A, Id, A)$

$$C_2^{El}(|A_2| - |E|)^2 \leq \hat{\epsilon} + O(\lambda^{-4}) \quad , \tag{4.2.144}$$

$$C_1^{El}\left(\det(E) - \det(A_2) - \frac{3\vartheta^2}{8C_1^{El}C_\phi^W}\lambda^{-2}\right)^2 \leq \hat{\epsilon} + O(\lambda^{-4}) \quad , \tag{4.2.145}$$

$$\frac{1}{5}C_{Con}C_{rep}^{-1}\|\left(BA_2\right)^{-1}\|^2\det\left(A\right)\lambda^2\left\|BA_2 - A_1\right\|^2 \leq \hat{\epsilon} + O(\lambda^{-4}) \quad , \tag{4.2.146}$$

$$\frac{1}{3}\tilde{C}_\nabla\left(\frac{\rho_{2\lambda}}{\rho_\lambda}\right)\left\|A_1^{-1}\right\|^2\det\left(A\right)\lambda^2\|A - A_1\|^2 \leq \hat{\epsilon} + O(\lambda^{-4}) \quad . \tag{4.2.147}$$

Due to the estimates (4.2.144) and (4.2.145) $|A_2|$ and $\det A_2$ are uniformly bounded from below and above for sufficiently large λ and sufficiently small $\hat{\epsilon}$. Due to B.2.1 also $|A_2^{-1}|$ is uniformly bounded from below and above. With $F(A) \leq \hat{\epsilon}$ and the coercivity condition on $F(A)$ we get the same bounds for $|A|$, $|A^{-1}|$ and $\det A$. According to (4.2.147) we have

$$|Id - A_1^{-1}A|^2 \leq \left\|A_1^{-1}\right\|^2\|A - A_1\|^2 \leq O(\hat{\epsilon}) + O(\lambda^{-4}) \tag{4.2.148}$$

Therefore, $|A_1^{-1}|$ $|A_1|$ and $\det A_1$ are bounded from below and above for sufficiently large λ and small $\hat{\epsilon}$. Finally, due to the estimate (4.2.146) B is also uniformly bounded. Hence, the $A_1, A_2 \in Gl_d(\mathbb{R})$ and $B \in Gl_d(\mathbb{Z})$ with $U(A, A_1, B, A_2) \leq U(A, A, Id, A)$ are a compact subset. U is continuous. Hence, there are minimizers $\hat{A}_1, \hat{B}$ and $\hat{A}_2$ fulfilling $F_C(A) = U(A, \hat{A}_1, \hat{B}, \hat{A}_2)$. We can deduce from the estimate (4.2.147) that it holds $|A - \hat{A}_1| = O(\lambda^{-2})$ and from (4.2.146) that it holds $\left\|\hat{B}\hat{A}_2 - \hat{A}_1\right\| = O(\lambda^{-2})$. Therefore, we have $|A - \hat{B}\hat{A}_2| = O(\lambda^{-2})$ and we finally get

$$F_C\,(A) = \min\left\{F(BA)|B \in Gl_d(\mathbb{Z}^d)\right\} + O(\lambda^{-2}) \quad . \tag{4.2.149}$$

□

Chapter 5

Outlook

We have studied different aspects of the model. But there are still remaining many open questions.

Plastic Relaxations The purpose of the model is to study plastic deformation. In Theorem 3.3.2 we have calculated an upper bound for the energy barrier of plastic deformation scaling like λ^2 for dimension two. However, we do not have an lower bound for the energy barrier. In fact, we have not even proved that it exists. As an important step towards this goal we have calculated a lower energy bound for the core energy of a dislocation scaling like λ^2 in Theorem 4.1.14. To calculate the upper bound for the energy barrier, we needed an bound for the energy density in terms of the effective elastic potential. The lower bound for the energy density we obtained in Theorem 4.2.5 has basically the same structure:

$$\hat{h}_\lambda(\chi, y) \geq F_C\left(\nabla\tilde{\tau}_B(y)\right) + \frac{1}{5}\tilde{C}_\nabla\left(\frac{\rho_{2\lambda}}{\rho_\lambda}\right)\left\|\nabla\tilde{\tau}_B^{-1}(y)\right\|^2\lambda^4\|\nabla^2\tilde{\tau}_B(y)\|^2\det\left(\nabla\tilde{\tau}_B\right) \quad .$$

However it uses F_C and not the effective elastic potential. The difference between F_λ and F_C is $O(\lambda^{-2})$. Hence, there holds no equality in the estimate in case of a Bravais lattice. If we integrate up this error over a sufficiently large domain, the contribution of this term will get larger than the energy barrier itself. Hence, a better lower bound for the energy density is needed, at least, if we want to calculate an energy barrier that holds for fixed λ and $L \to \infty$. Furthermore, we would need to prove that, if we have some $\psi \in C_2^\infty$ satisfying for all connected $\tilde{\Omega}$

- $\psi(z) = A_R^{-1}z$ for all $z \in \partial\tilde{\Omega}$,
- $F_\lambda\left(\nabla\psi(z)\right) \leq \hat{\epsilon}$ for all $z \in \tilde{\Omega}$,

then it holds

$$F_\lambda(A_R^{-1})|\tilde{\Omega}|dz \leq \int_{\tilde{\Omega}} F_\lambda(\nabla\psi(z))dz \quad . \tag{5.0.1}$$

This property is related to quasi convexity (compare [5]), but is adapted to study local minima instead of global minima. If this property is not fulfilled, then for sufficiently large L the lattice $\chi_{\mathcal{A}_R}$ is not a local minimum, because one can elastically deform the configuration to lower the energy without an energy barrier. If we could get a strict estimate of the form

$$F_\lambda(A_R^{-1})|\tilde{\Omega}|dz + \int_{\tilde{\Omega}} C(A_R)(\nabla\psi(z) - A_R^{-1})^2 dz \leq \int_{\tilde{\Omega}} F_\lambda(\nabla\psi(z))dz \quad , \tag{5.0.2}$$

one can use this estimate and the $\lambda^4(\|\nabla^2\tau\|^2$ term to get a lower bound for an energy barrier for elastic deformations. The change of reparametrisations is a major technical problem here, because the minimum of functions, that have some kind of convexity property, does not need to have this property itself. We expect that one can prove this, if A restricted to one map of $Gl_d(\mathbb{R})/Gl_d(\mathbb{Z})$ or in the version of the model used in [7], where reparametrisations do not change the energy density. Once these two steps are done, one should be able to conclude that a reduction of energy needs special kind of topological structure of the set of regular points. This would imply the existence of irregular areas. If one calculates an energy cost of the irregular areas as in 4.1.14, one could conclude a lower bound for the energy barrier of plastic deformation.

Combination of the approaches for the construction of Lagrangian coordinates We used two approaches to construct Lagrangian coordinates. In section 4.1 we used an estimate for the discrete gradient of $\mathcal{A}$ in finite sequences of regular points for this purpose. In section 4.2 we used an estimate for the gradient of the local minimizers along differentiable curves. On the one hand the discrete approach has the advantage that we can connect the Lagrange through small areas of irregular points. On the other hand, if the distance of the jumps are small, the estimate of the discrete gradient is much worse than the estimate for the continuous gradient. Therefore, one might want to combine both approaches. Using the continuous coordinates in regular areas and the discrete near irregular areas. The definition of the generalized burgers vector would not change at all since in the regular area we just follow one local minimizer without doing any reparametrisations.

Modification of the model: As we have seen in Theorem 3.3.2 and Theorem 4.2.5 the energy cost for a dislocation is $O(\lambda^2)$ in our model. Furthermore we noticed in the Perspective 3.3.3 there are reasons to believe that for dimension three the lowest energy path will have nothing to do with dislocations. Finally in many real materials a rank one connection between two crystal structures is observed. However in our model these kind of connections have not extraordinary low energy. Hence, in general our model is not very good for estimating the energy of irregular areas. And all points in λ distance of a defect will be irregular. A possible way to deal with this would be to introduce a variable λ. One could add an term

$$C\lambda^{-k}\rho_\lambda \tag{5.0.3}$$

where $C > 0$ and $k \in \mathbb{Z}$ and minimize over λ for every point as we minimize over $\mathcal{A}$. In regular areas this would lead to relatively large λ values and the behavior of the model would not change much. For points x close to irregularities $\lambda(x)$ would shrink down such that the irregularity will be not inside the ball $B_{2\lambda}(x)$. This would be a similar strategy to the adaptive grit method in numerics. On first sight this might look like a completely arbitrary modification. However if one would derives our model from a particle- particle interaction model or from Schrdinger equation. One basically would derive the potential W in our model by putting all but one atoms in $B_{2\lambda}(x)$ on a lattice position calculate the energy of this one atom depending on its position. However, this procedure neglects the long range interaction of this atom with atoms outside $B_{2\lambda}(x)$. The effect of these atoms would be estimated with $C\lambda^{-k}\rho_\lambda$ in the modified version. Of course for this we would need to pay the price to make a technical complicated model even more complicated.

Appendix A

Notation

This section is supposed to help maintaining an overview about the notation, the different kind of constants, parameters and variables.

General notations

- $Gl_d(\mathbb{R}) := \left\{M \in \mathbb{R}^{d\times d} | \det M > 0\right\}$.
- $Gl_d(\mathbb{Z}) := \left\{M \in \mathbb{Z}^{d\times d} | \det M = 1\right\}$.
- $< X, Y >:= \sum_{i=1}^{n} X_i Y_i$ is the scalar product of two vectors. $X, Y \in \mathbb{R}^n$
- $|X| :=< X, X >^{1/2}$ the Euclidean norm of a vector $X \in R^n$.
- $\mathrm{dist}(x, U) = \inf\{|x - y| | y \in U\}$ is the distance between a set U and vector x.
- $SO_d := \left\{M \in \mathbb{R}^{d\times d} | \forall x, y \in \mathbb{R}^d : |Mx| = |x|, \det A = 1\right\}$ is the set of rotations of $\mathbb{R}^d$.
- $B_r(x) := \left\{y \in \mathbb{R}^d | |x - y| \leq\right\}$ the ball of radius r around x.
- w_d is the Lebesgue measure of $B_1(0)$.
- $B_r(U) := \{x | \exists y \in U \text{ such that } |x - y| < r\}$ where $U \subseteq \mathbb{R}^d$ is the r neighborhood of U.
- $Q_a(x) := [-\frac{a}{2}, \frac{a}{2})^d + x$ is the semi-open cube with length a and midpoint x.
- $\mathrm{diam}(U) := 2 \inf\{r | \exists x \in R \text{ such that } U \subseteq B_r(x)\}$ the diameter of the set $U \subseteq \mathbb{R}^d$.
- $|M| := \sup\{|Mx|/|x| \; |x \in R^d/0\}$ the matrix norm induced by the euclidean vector norm.

- $Tr(M) := \sum_{i=1}^{d} M_{ii}$ is the trace of a matrix $A \in \mathbb{R}^{d\times d}$.
- M^T is the transposed matrix to A.
- $\|M\| := Tr(M^T M)$ is the Frobenius norm of a matrix.
- $\|\mathcal{M}\|_\lambda = \left(\lambda^2\|M\| + |\mu|^2\right)^{1/2}$ is a norm of $\mathcal{M} = (M, \mu) \in \mathbb{R}^{d\times d} \times \mathbb{R}^d$ adapted to this model.
- $Q[X] = Q(X, ..., X)$ where $Q : (\mathbb{R}^d)^n \to \mathbb{R}$ and $X \in R^d$
  Example: Taylor expansion
  $f(x) = f(x_0) + \nabla f(x_0)[x - x_0] + 1/2\nabla^2 f(x_0)[x - x_0] + ...$
- $\mathbf{j} = (j_1, ..., j_d) \in \mathbb{N}^d$ is a multi index.
- $\mathbf{j}! = \prod_{k=1}^{d} j_d!$
- $X^{\mathbf{j}} = \prod_{k=1}^{d} X_k^{j_k}$ for all $X \in R^d$
- $|U|$ where $U \subseteq \mathbb{R}^d$ is the Lebesgue measure of U

Definition of the Model

These definitions are introduced in Section 1.3:

N	the number of atoms.
d	the dimension.
χ	our atom configuration.
x_i	the position of the atom i.
Ω	our domain in which the atoms are moving.
L	the length-scale of Ω
x	a position in $B_{2\lambda}(\Omega)$.
χ_I	the set of inner atoms that can move in Ω.
N_I	the number of the inner atoms.
χ_S	the set of atoms, that are fixed in $B_{4\lambda}(\Omega)/\Omega$.
N_S	the number of the outer atoms.
$\mathcal{A}$	the lattice parameters fitted to the configuration.
$\chi_{\mathcal{A}}$	$:= A^{-1}(\mathbb{Z} - \tau)$ the Bravais lattice determined by $\mathcal{A} = (A, \tau)$
$\mathcal{B}$	called a reparametrisation
$H_\lambda(\chi)$	the many particle energy function.
$\hat{h}_\lambda(\chi, x)$	the energy density.
$h_\lambda(\mathcal{A}, \chi x)$	the pre-energy density.
$F(A)$	the elastic energy function
E	a minimizer of F.
C_1^{El}	a constant in the coercivity condition on F.

C_2^{El}	a constant in the coercivity condition on F.
$J_\lambda(\mathcal{A}, \chi, x)$	measuring the mean square distance between the configuration χ and the lattice $\chi_{\mathcal{A}} + x$.
φ	a C_c^∞ cut-off function.
$\tilde{\varphi}(x)$	$:= \varphi(\lvert x\rvert)$.
C_φ	$:= \int_{\mathbb{R}^d} \varphi(\lvert x\rvert)dx$ the normalization constant for C_φ.
$C_{\varphi 2}$	$:= \int_{\mathbb{R}^d} x^2\varphi(\lvert x\rvert)dx$
λ	the mesoscopic scale.
W	the periodic potential used to construct J_λ.
c_Θ^0	the lower bound for $\lvert\nabla^2 W\rvert$ in the convex region.
c_Θ^1	the upper bound for $\lvert\nabla^2 W\rvert$ in the convex region.
Θ_W	a lower bound for the area of convexity of W.
C_0^W	a constant in the coercivity condition on W
C_1^W	a constant in the coercivity condition on W
$\rho_\lambda(\chi, x)$	the particle density.
ϑ	the energy cost of a vacancy.
$\nu_\lambda(\chi, A, x)$	the part of the energy function that penalizes the vacancies
V	the hard core potential.
s_0	the radius of the hard core repulsion.
ρ_d^{max}	an upper bound for particle density due to the hard core repulsion

Further notation

C_m	a constant (see 2.1.2).
β	maximal distance of regular atoms to the lattice
$\chi_{\mathcal{A},\beta,x}^{reg}$	the set of irregular atoms (see 2.2.4).
$\chi_{\mathcal{A},\beta,x}^{irr}$	the set of irregular atoms(see 2.2.4).
$\rho_{\mathcal{A},\beta}^{reg}(x)$	the density of regular atoms (see 2.2.4).
$\rho_{\mathcal{A},\beta}^{irr}(x)$	the density of irregular atoms (see 2.2.4).
$C_{\lvert A\rvert}$	a constant bounding $\lvert A\rvert$ (see2.3.2)
$\hat{\mathcal{A}}(x)$	the minimizer of $h_\lambda(\cdot, \chi, x)$
c_k	for $k = 1...6$ are constants determining a compact subset of $Gl_d(\mathbb{R})$ (see 2.2.6).
$V_{\mathcal{A}(\chi)}(y)$	parameter for the effective particle potential (see 2.2.8).
ϵ_ρ	parameter for the regularity of the density (see 2.2.8).
ϵ_J	constant for the regularity of J_λ (see 2.2.8).
C_A	is a parameter that controls $\lvert A^{-1}\rvert$(see 2.2.8).
C_ϕ^W	is a constant (see 2.4.1).
ρ_1	is some (see 2.4.2) .
μ_1	(see 2.4.2).
$\mathcal{A}_R$	$= (A_R, \tau_R)$ the parameters of a Bravais lattice,

	if the atom configuration is a lattice.
$\delta\mathcal{A}$	$= (\delta A, \delta\tau)$ the difference between the prescribed and the fitted lattice (see 3.1.2)
$F_\lambda(G, z)$	the local effective elastic potential (see 3.1.1).
$F_\lambda(G)$	the average effective elastic potential (see 3.1.1).
$\psi \in C^3$	describes a elastically deformed configuration by $\chi = \psi(\mathbb{Z}^d)$.
u	For a deformed Bravais lattice $\psi(z) = A_R^{-1}z + u(z)$.
$(\nabla F)_{loc}$	coefficient of a Taylor series like estimate see 3.2.2.
$(\nabla^2 F)_{loc}$	coefficient of a Taylor series like estimate see 3.2.2.
C_Q	a constant (see Theorem 3.2.3).
c_J^A	a constant (see 4.1.2).
c_J^τ	a constant (see 4.1.2)
$\hat{\epsilon}_J$	the maximal ϵ_J for jumping regular points (see 4.1.3).
C_J^A	a constant (see 4.1.4).
C_J^τ	a constant (see 4.1.4).
C_{con}	a constant (see 4.2.1).
α_∇	a constant (see 4.2.2)
$C_{\nabla^2}(X)$	a constant only denpenden on the ration of $\rho_2\lambda$ and ρ_λ (see 4.2.4)
$F_C(A)$	is a modified elastic potential (see 4.2.5)

Asymtotics In most lemmata we consider λ that are larger that some $\hat{\lambda}$. Additionally, in some lemmata energy density or regularity constants that are below some threshold. We use the symbol $Y = O(X)$ in the sense that there exists a constant C such that $|Y| \leq CX$, if the conditions are satisfied.

Appendix B

Basic calculations

B.1 Convexity and minimization

Most of our results are based on the convexity of the function W near to its minima that leads to local convexity of J_λ and h_λ near their local minima. In this part of the appendix we state general estimates for the local minima of locally convex functions.

The second derivative of J_λ and h_λ for given x and χ has different scaling in λ for the A direction and the τ direction Lemma B.1.1 is specifically adapted for convex functions $g(\mathcal{A}, X)$ with this property and that additionally depended on the a variable $X \in R^n$ If we have a suitable upper bound on the first derivative at one $\mathcal{A}_0$, we get the existence of a local minimizer in the neighborhood of $\mathcal{A}_0$ Additionally we get an upper bound for the distance between the local minimizer $\mathcal{A}_0$. Furthermore we use implicit functions theorem to prove that the local minimizer is a differentiable function of X.

Lemma B.1.1. *If* $g \in \left(\mathbb{R}^{d\times d} \times \mathbb{R}^d\right) \times \mathbb{R}^n \to \mathbb{R}$ *fulfills*

1) g is 2-times continuously differentiable.

2) There exists $C > 0$, $\mathcal{A}_0 \in \mathbb{R}^{d\times d} \times \mathbb{R}^d$ *and* $X_0 \in \mathbb{R}^n$ *such that for all* $\mathcal{A} \in \mathbb{R}^{d\times d} \times \mathbb{R}^d$ *satisfying* $\|\mathcal{A} - \mathcal{A}_0\|_\lambda \leq R$ *and all* $\mathcal{M} \in \mathbb{R}^{d\times d} \times \mathbb{R}^d$ *it holds*

$$\partial^2_{\mathcal{A}} g(\mathcal{A}, X_0)[\mathcal{M}] \geq C\|\mathcal{M}\|^2_\lambda \quad . \tag{B.1.1}$$

3) There exists $D \leq CR$ *such that for all* $\mathcal{M} \in \mathbb{R}^{d\times d} \times \mathbb{R}^d$*:*

$$|\partial_{\mathcal{A}} g_\lambda(\mathcal{A}_0, X_0)[\mathcal{M}]| \leq D\|\mathcal{M}\|_\lambda \quad , \tag{B.1.2}$$

Then it holds

1) There exists a unique local minimizer

$$\tilde{\mathcal{A}}(X_0) := \arg\min\{g_\lambda(\mathcal{A}, X_0) | \mathcal{A} \in \mathbb{R}^{d\times d} \times R^d \textit{with } \|\mathcal{A} - \mathcal{A}_0\|_\lambda < R\} \quad . \tag{B.1.3}$$

2) Furthermore, the local minimizer fulfills

$$\frac{2D}{C} \geq \|\tilde{\mathcal{A}}(X_0) - \mathcal{A}_0\|_\lambda \quad . \tag{B.1.4}$$

If additionally there exists for any $j = 1..n$ a $C_j^D > 0$ such that for all $\mathcal{A} \in \mathbb{R}^{d\times d} \times \mathbb{R}^d$ satisfying $\|\mathcal{A} - \mathcal{A}_0\|_\lambda \leq R$ it holds

$$|\partial_{X_j}\partial_{\mathcal{A}} g(\mathcal{A}, X_0)| \leq C_j^D \|\mathcal{M}\|_\lambda \quad , \tag{B.1.5}$$

then additionally there exists a differentiable functions $\tilde{\mathcal{A}}(X)$ in a neighborhood of X_0 such that

$$\tilde{\mathcal{A}}(X) := \arg\min\{g_\lambda(\mathcal{A}, X) | \mathcal{A} \in \mathbb{R}^{d\times d} \times R^d with \ \ \|\mathcal{A} - \mathcal{A}_0\|_\lambda < R\} \quad , \tag{B.1.6}$$

and

$$\|\nabla_{X_j}\tilde{\mathcal{A}}(X)[\mathcal{M}]\|_\lambda \leq \frac{C_j^D}{C} \quad . \tag{B.1.7}$$

Proof. We take some $\mathcal{A}$ with $\|\mathcal{A} - \mathcal{A}_0\|_\lambda \leq C$ and obtain

$$\begin{aligned} g(\mathcal{A}, \chi, x) =& g(\mathcal{A}_0, \chi_0, x) + \partial_{\mathcal{A}} g(\mathcal{A}_0, \chi_0, x)[\mathcal{A} - \mathcal{A}_0] + \frac{1}{2}\partial^2_{\mathcal{A}} g(\bar{\mathcal{A}}, \chi_0, x)[\mathcal{A} - \mathcal{A}_0] \\ \geq& g(\mathcal{A}_0, \chi, x) - D\|\mathcal{A} - \mathcal{A}_0\|_\lambda + \frac{C}{2}\|\mathcal{A} - \mathcal{A}_0\|^2_\lambda \quad . \end{aligned} \tag{B.1.8}$$

The local minimizer fulfills and $g(\mathcal{A}, \chi, x) \leq (\mathcal{A}_0, \chi, x)$. Therefore, we have the estimate

$$\begin{aligned} 0 \geq& - D\|\mathcal{A} - \mathcal{A}_0\|_\lambda + C/2\|\mathcal{A} - \mathcal{A}_0\|^2_\lambda \\ \frac{2D}{C} \geq& \|\mathcal{A} - \mathcal{A}_0\|_\lambda \quad . \end{aligned} \tag{B.1.9}$$

At the local minimizer the derivative $\partial_{\mathcal{A}} g(\tilde{\mathcal{A}}, \chi, x)$ is zero. Hence, we get for all $\mathcal{A} \in B^\lambda_R(\mathcal{A}_0)$ the estimate

$$\begin{aligned} g(\mathcal{A}, \chi_0, x) \geq& g(\tilde{\mathcal{A}}, \chi_0, x) + \frac{1}{2}\partial^2_{\mathcal{A}} g(\bar{\mathcal{A}}, \chi, x)[\mathcal{A} - \tilde{\mathcal{A}}] \\ \geq& g(\tilde{\mathcal{A}}, \chi_0, x) + \frac{C}{2}\|\mathcal{A} - \tilde{\mathcal{A}}\|^2_\lambda \quad . \end{aligned} \tag{B.1.10}$$

In particular the minimizer is unique. For a local minimizer of g holds

$$0 = \partial_{\mathcal{A}} g(\tilde{\mathcal{A}}, X)(\mathcal{M}) \quad . \tag{B.1.11}$$

According to implicit function theorem there is a differentiable solution $\tilde{\mathcal{A}}(X)$ satisfying the equation (B.1.11), if $\det \partial^2_{\mathcal{A}} h(\tilde{\mathcal{A}}, X) \neq 0$. This is implied by the strict convexity given by condition (B.1.1). Because g is two times continuous differentiable, it is strictly convex in a neighborhood of X_0. Therefore, there exists a solution of the equation in this neighborhood and the solution is a local minimizers of g. Since $0 = \partial_{\mathcal{A}} g(\tilde{\mathcal{A}}, X)$, it is also zero for tested with any $\mathcal{M} = (M, \mu) \in \mathbb{R}^{d\times d} \times \mathbb{R}$

$$0 = \partial_{\mathcal{A}} g(\tilde{\mathcal{A}}, X)[\mathcal{M}] \quad . \tag{B.1.12}$$

Since this holds for all X in a neighborhood of X_0, the derivative in direction X_j is zero for all j, and we get

$$\begin{aligned} 0 =& \frac{d}{dX_j} \partial_{\mathcal{A}} g(\tilde{\mathcal{A}}(X), X)\,[\mathcal{M}] \\ =& \partial_{\mathcal{A}} \left(\partial_{\mathcal{A}} g \left(\tilde{\mathcal{A}}(X), X \right) [\mathcal{M}] \right) \left[\nabla_{Xj} \tilde{\mathcal{A}}(X) \right] + \partial_{Xj} \left(\partial_{\mathcal{A}} g(\tilde{\mathcal{A}}(X), X)[\mathcal{M}] \right) \quad . \end{aligned} \tag{B.1.13}$$

We test the equation with $\mathcal{M} = \nabla_{Xj} \tilde{\mathcal{A}}(X)$

$$\partial^2_{\mathcal{A}} g(\tilde{\mathcal{A}}(X), X) \left[\nabla_{Xj} \tilde{\mathcal{A}}(X) \right] = -\partial_{Xj} \left(\partial_{\mathcal{A}} g(\tilde{\mathcal{A}}(X), X)[\nabla_{Xj} \tilde{\mathcal{A}}(X)] \right) \quad . \tag{B.1.14}$$

We estimate the left side of (B.1.14) with the condition (B.1.1) from above and the right side with the condition (B.1.5) from below, and obtain

$$\begin{aligned} C_j^D \|\mathcal{M}\|_\lambda \leq& C \|\nabla_{Xj} \tilde{\mathcal{A}}(X)\|_\lambda^2 \\ \|\nabla_{Xj} \tilde{\mathcal{A}}(X)\|_\lambda \leq& \frac{C_j^D}{C} \quad . \end{aligned} \tag{B.1.15}$$

Hence, we get

$$\sum_{j=1}^n \|\nabla_{Xj} \tilde{\mathcal{A}}(X)\|_\lambda^2 \leq \sum_{j=1}^n \frac{\left(C_j^D\right)^2}{C^2} \quad . \tag{B.1.16}$$

□

In the next lemma we calculate estimates for the minimizer and the minimum of a function strictly convex function, for which we can bound the second derivative from below and above with positive definite matrices, and additionally know the derivative in on point x. The lemma is similar to Lemma B.1.1 Since we do not imply a special scaling between the different variables, this lemmata is a little bit more general. Additionally we also calculate a lower bound for the distance between x and the minimizer.

Lemma B.1.2. *If $F : \mathbb{R}^d \to \mathbb{R}$ is a two times differentiable strictly convex function with*

$$c_1[z] \leq \nabla^2 F[z] \leq c_2[z] \quad , \tag{B.1.17}$$

where $0 < c_1 < c_2$ *are positive definite, symmetric real matrix, then the minimizing* $\hat{y}$ *of* F *fulfills for all* x

$$F(x) - \frac{1}{2}c_2^{-1}[\nabla F(x)] \leq F(\hat{y}) \leq F(x) - \frac{1}{2}c_2^{-1}[\nabla F(x)] \quad , \tag{B.1.18}$$

$$c_1\left[\hat{y} - x + c_1^{-1}\nabla F\right] \leq \left(c_1^{-1} - c_2^{-1}\right)[\nabla F(x)] \quad . \tag{B.1.19}$$

Proof. We use the Taylor expansion of $F((1-t)x + ty)$ in t up to second order, and get

$$F(y) = F(x) + \nabla F(x)[y-x] + \int_0^1 (1-t)\nabla^2 F((1-t)x + ty)[y-x]dt \quad . \tag{B.1.20}$$

We apply condition (B.1.17) and get

$$F(x) + \langle \nabla F(x), y - x\rangle + \frac{1}{2}c_1[y-x] \leq F(y) \leq F(x) + \nabla F(x)[y-x] + \frac{1}{2}c_2[y-x] \quad . \tag{B.1.21}$$

Since c_1 and c_2 are strictly positive, we can invert them. We rewrite the inequality

$$\begin{aligned} F(y) \geq & F(x) + \nabla F(x)(y-x) + \frac{1}{2}(y-x)c_1[y-x] \\ \geq & F(x) + \left\langle \nabla F(x)c_1^{-1}, c_1(y-x)\right\rangle + \frac{1}{2}c_1^{-1}\left[c_1(y-x)\right] \\ \geq & F(x) - \frac{1}{2}c_1^{-1}[\nabla F(x)] + \frac{1}{2}c_1^{-1}\left[c_1(y-x) + \nabla F\right] \quad . \end{aligned} \tag{B.1.22}$$

For y with $F(y) \leq F(x)$ it holds

$$|c_1|\frac{1}{2}c_1^{-1}[\nabla F(x)] \geq \left(c_1(y-x) + \nabla F\right)^2 \quad . \tag{B.1.23}$$

Therefore, the set of y with $F(y) \leq F(x)$ is compact and the continuous F attains its minimum on it. We can apply the calculation (B.1.22) for c_2 to get an upper bound

$$F(y) \leq F(x) - \frac{1}{2}c_2^{-1}[\nabla F(x)] + \frac{1}{2}c_2^{-1}\left[c_2(y-x) + \nabla F(x)\right] \quad . \tag{B.1.24}$$

The minimum of $\hat{y}$ of F has to be lower than the minimum of the upper bound. Therefore, we have

$$\begin{aligned} -\frac{1}{2}c_2^{-1}[\nabla F(x)] \geq & -\frac{1}{2}c_1^{-1}[\nabla F(x)] + \frac{1}{2}c_1^{-1}\left[c_1(y-x) + \nabla F\right] \quad , \\ \frac{1}{2}\left(c_1^{-1} - c_2^{-1}\right)[\nabla F(x)] \geq & \frac{1}{2}c_1^{-1}\left[c_1(y-x) + \nabla F(x)\right] \quad . \end{aligned} \tag{B.1.25}$$

□

The next lemma is a simple application of implicit function theorem. if we have a function of the form $F(X) = \min_y \{(f(X,Y)\}$ for a convex function F we can express the derivatives of F in form of the derivatives of f

Lemma B.1.3. *If $f \in C_2(\mathbb{R}^n \times R^m)$ and there exists $r_X > 0$, $r_Y > 0$, $X_0 \in \mathbb{R}^n$ and $Y_0 \mathbb{R}^m$ such that*

1) $\partial_Y f(X_0, Y_0) = 0$,

2) $\partial_Y^2 f(X,Y) > 0$ for all $(X,Y) \in B_{r_X}(X_0) \times B_{r_Y}(Y_0)$,

then there exists some $r > 0$ and a differentiable function $Y(X)$ in $B_r(X_0)$ such that

$$\partial_Y f(X, Y(X)) = 0 \quad , \tag{B.1.26}$$

$$\frac{dY}{dX} = -\left(\partial_Y^2 f(X,Y)\right)^{-1} \partial_X \partial_Y f(X,Y) \quad . \tag{B.1.27}$$

$$\tag{B.1.28}$$

Furthermore, for $F(X) = \min\{f(X,Y) | Y \in B_{r_Y}(Y_0)\}$ it holds

$$\partial_X F(X) = = \partial_X f(X,Y) \quad , \tag{B.1.29}$$

$$\partial_X^2 F(X) = \partial_X^2 f(X,Y) - \partial_X \partial_Y f(X,Y) (\partial_Y^2 f(X,Y))^{-1} \partial_X \partial_Y f(X,Y) \quad . \tag{B.1.30}$$

Proof. Because it holds $\partial_Y^2 f(X,Y) > 0$, all eigenvalues of $\partial_Y^2 f(X,Y)$ are strictly bigger than zero. Hence, $\det \partial_Y^2 f(X,Y)$ is not zero and the conditions for implicit function theorem are satisfied. Therefore, it holds $0 = \partial_Y f(X, Y(X))$. Due to $\partial_Y^2 f(X,Y) > 0$ this stationary point has to be a local minimizer. If we calculate the derivative of $0 = \partial_Y f(X, Y(X))$, we get

$$\begin{aligned} 0 =& \frac{d}{dX} \partial_Y f(X,Y) \\ & \partial_X \partial_Y f(X,Y) + \partial_Y^2 f(X,Y) \frac{dY}{DX} \quad , \\ \frac{dY}{dX} =& -(\partial_Y^2 f(X,Y))^{-1} \partial_X \partial_Y f(X,Y) \quad . \end{aligned} \tag{B.1.31}$$

Furthermore because $\partial_Y f(X,Y) = 0$

$$\partial_X F(X) = \partial_X f(X,Y) + \partial_Y f(X,Y) \frac{dY}{DX} = \partial_X f(X,Y) \quad . \tag{B.1.32}$$

The same way we get with equation (B.1.31)

$$\begin{aligned} \partial_X^2 F(X) =& \frac{d}{dX} \partial_X f(X,Y) \\ =& \partial_X^2 f(X,Y) + \partial_X \partial_Y f(X,Y) \frac{dY}{DX} \\ =& \partial_X^2 f(X,Y) - \partial_X \partial_Y f(X,Y) (\partial_Y^2 f(X,Y))^{-1} \partial_X \partial_Y f(X,Y) \quad . \end{aligned} \tag{B.1.33}$$

□

Remark B.1.4. If we minimize the function $f(X)$ with some $g(X) = g$ constant, we have to consider the Lagrange functional: $L(X) = f(X) - \mu(g(X) - g)$ Hence, we get for the minimizer

$$\begin{aligned} 0 =& \partial_{X_i} f(X) - \mu \partial_{X_i} g(X) \quad , \\ \mu =& \frac{\partial_{X_i} f(X)}{\partial_{X_i} g(X)} \quad . \end{aligned} \tag{B.1.34}$$

We will introduce now $f(g) = \min\{f(X)|g(X) = G\}$

$$\begin{aligned} \frac{df(g)}{dg} =& \sum_i \partial_{X_i} f(X) \frac{dX_i}{dg} \\ =& \mu \sum_i \partial_{X_i} g(X) \frac{dX_i}{dg} \\ =& \mu \frac{dg}{dg} = \mu \quad . \end{aligned} \tag{B.1.35}$$

Lemma B.1.5. *Let for any $i = 1...n$ there exits $c_i > 0$ and $b_i \in \mathbb{R}^d$. If we minimize over all $x = (x_1...x_n) \in \left(\mathbb{R}^d\right)^n$ the function*

$$J(x) = \sum_i c_i x_i^2 \quad , \tag{B.1.36}$$

with the constrain

$$\rho = \sum_i d_i x_i \quad , \tag{B.1.37}$$

then the minimizer $\hat{x}$ and the minimum fulfill

$$\begin{aligned} \hat{x}_i =& \frac{d_i}{2c_i} \left(\sum_i \frac{d_i^2}{2c_i} \right)^{-1} \rho \quad , \\ min_{x\in\mathbb{R}^n} J(x) =& \left(\sum_i \frac{d_i^2}{c_i} \right)^{-1} \rho^2 \quad . \end{aligned} \tag{B.1.38}$$

Proof. We consider the Lagrange function:

$$L(x) = \sum_i c_i x_i^2 + \mu \left(\rho - \sum_i d_i x_i \right) \quad . \tag{B.1.39}$$

We obtain

$$\begin{aligned} 0 =& \frac{\partial L}{\partial x_i} \quad , \\ \hat{x}_i =& \frac{d_i}{2c_i} \quad . \end{aligned} \tag{B.1.40}$$

We apply this on equation (B.1.37) and get

$$\begin{aligned} \rho =& \mu \sum_i \frac{d_i^2}{2c_i} \quad , \\ \mu =& \left(\sum_i \frac{d_i^2}{2c_i} \right)^{-1} \rho \quad . \end{aligned} \tag{B.1.41}$$

Due to equation (B.1.40) we obtain

$$\begin{aligned} \hat{x}_i =& \frac{d_i}{2c_i} \left(\sum_i \frac{d_i^2}{2c_i} \right)^{-1} \rho \quad , \\ J =& \left(\sum_i \frac{d_i^2}{c_i} \right)^{-1} \rho^2 \quad . \end{aligned} \tag{B.1.42}$$

□

B.2 Basic properties of matrices

In this section we present different elementary properties of matrices, that we use throughout the thesis. For matrices the euclidean norm $|A|$ is bounded from below and above by the Frubenius norm $\|A\|$.

Lemma B.2.1. *For all $A \in \mathbb{R}^{d \times d}$ we have*

$$|A| \leq \|A\| \leq \sqrt{d}|A| \quad . \tag{B.2.1}$$

Proof. Per definition of $|A|$ there exist e_1 with $|e_1| = 1$ and $|Ae_1| = |A|$

$$Ae_1 = |A|\tilde{e}_1 \quad . \tag{B.2.2}$$

$|A|$ and $\|A\|$ independent of the basis we use for $\mathbb{R}^d$ We calculate them in a basis with e_1 as the first basis vector and get

$$|A|^2 = |Ae_1|^2 \leq \sum_{i=1}^{d} |Ae_i|^2 = \|A\|^2 \quad . \tag{B.2.3}$$

Furthermore, we get

$$d|A|^2 = d|Ae_1|^2 \geq \sum_{i=1}^{d} |Ae_i|^2 = \|A\|^2 \tag{B.2.4}$$

□

We can use $|A|$ to bound $|A^{-1}|$ and the other way around, if $\det A$ is bounden from below and above.

Lemma B.2.2. *For all $A \in Gl_d(\mathbb{R})$ it holds*

$$\begin{aligned} |A^{-1}| \leq & |A|^{d-1} \det A^{-1} \quad , \\ |A| \leq & |A^{-1}|^{d-1} \det A \quad . \end{aligned} \tag{B.2.5}$$

Proof. We set without lose of generality $d = 3$. Per definition of $|A^{-1}|$ there exist $\tilde{e}_1$, e_1 with norm 1 such that

$$\begin{aligned} A^{-1}\tilde{e}_1 = & |A^{-1}|e_1 \quad , \\ |A^{-1}|^{-1}\tilde{e}_1 = & Ae_1 \quad . \end{aligned} \tag{B.2.6}$$

We form a orthonormal basis with e_1 and obtain

$$\begin{aligned} Ae_1(Ae_2 \times Ae_3) = & \det A \quad , \\ |Ae_1||Ae_2||Ae_3| \geq & \det A \quad , \\ |A^{-1}|^{-1}|Ae_2||Ae_3| \geq & \det A \quad , \\ |Ae_2||Ae_3| \det A^{-1} \geq & |A^{-1}| \\ |A|^2 \det A^{-1} \geq & |A^{-1}| \quad . \end{aligned} \tag{B.2.7}$$

For the second estimate just exchange the roles of A and A^{-1}. □

We are using matrix derivatives in several occasions in the thesis. There are two perspectives on this derivatives. On the one hand, the matrix can be seen as a linear map and the derivative is the functional derivative of the linear map. On the other hand, the matrix can be seen as a vector. And the matrix derivative are ordinary vector derivatives determined by the components. In the next lemma we the matrix derivative of $\det A$, A^{-1} and $\|A^{-1}\|$.

Lemma B.2.3. *For all $A \in Gl_d(R^d)$ and all $M \in \mathbb{R}^{d\times d}$ it holds:*

$$\begin{aligned} \partial_A \det A[M] = & Tr\left(A^{-1}M\right) \det A \quad , \\ \partial_A A^{-1}[M] = & - A^{-1}MA^{-1} \quad , \\ \partial_{A_{\alpha\beta}} \|A^{-1}\|^2[M] = & - 2Tr\left(\left(A^{-1}\right)^{+} A^{-1}MA^{-1}\right) \quad . \end{aligned} \tag{B.2.8}$$

In coordinates we can write the derivatives:

$$\begin{aligned} \partial_{A_{\alpha,\beta}}(\det A) = & adj(A)_{\beta,\alpha} = A^{-1}_{\beta\alpha} \det A \\ \partial_{A_{\alpha\beta}} A^{-1}_{hk} = & - A^{-1}_{h\alpha} A^{-1}_{\beta k} \end{aligned} \tag{B.2.9}$$

Furthermore, we have for all $M_1, M_2 \in \mathbb{R}^{d\times d}$

$$\partial^2_A \det A\left(M_1, M_2\right) = Tr\left(A^{-1}M_1\right) Tr\left(A^{-1}M_2\right) \det A - Tr\left(A^{-1}M_2A^{-1}M_1\right) \det A \tag{B.2.10}$$

Proof. **Derivative of the determinant:**

If one uses Laplace expansion, one can immediately see that the partial derivative of the determinant in direction of one of the components is the corresponding minor. Hence, it is the entry of the cofactor matrix. For the functional derivative we obtain

$$\begin{aligned}\partial_A \det A[M] =& \lim_{t\to 0} \frac{\det(A+tM) - \det A}{t} \\ =& \lim_{t\to 0} \frac{(\det(Id + tA^{-1}M) - 1)\det A}{t} \quad .\end{aligned} \tag{B.2.11}$$

If we apply Leipnitz formula on $\det(Id + tA^{-1}M)$, we get products of the components of $Id + tA^{-1}M$. For each of this factors we have one term from the identity and one from $tA^{-1}M$. The summands that are linear in t are those with the contribution of $tA^{-1}M$ in on factor and the contribution of Id in all other. Since all non vanishing components of Id are belong to the diagonal The one contribution $tA^{-1}M$ has to belong to the diagonal too. We get:

$$\begin{aligned}\det A \partial_A \det A[M] =& \lim_{t\to 0} \frac{1 + tTr(A^{-1}M) + O(t^2) - 1)}{t} \\ =& Tr\left(A^{-1}M\right)\det A \quad .\end{aligned} \tag{B.2.12}$$

The derivative of the inverse: In coordinates:

$$\begin{aligned} A_{ij}A^{-1}_{jk} =& \delta_{ik} \quad , \\ \partial_{\alpha\beta}(A_{ij}A^{-1}_{jk}) =& 0 \quad , \\ \partial_{\alpha\beta}A_{ij}A^{-1}_{jk} + A_{ij}\partial_{\alpha\beta}A^{-1}_{jk} =& 0 \quad , \\ A_{ij}\partial_{\alpha\beta}A^{-1}_{jk} =& -\delta_{i\alpha}\delta_{j\beta}A^{-1}_{jk} \quad , \\ A^{-1}_{hi}A_{ij}\partial_{\alpha\beta}A^{-1}_{jk} =& -\delta_{i\alpha}\delta_{j\beta}A^{-1}_{hi}A^{-1}_{jk} \quad , \\ \delta_{hj}\partial_{\alpha\beta}A^{-1}_{jk} =& -\delta_{i\alpha}\delta_{j\beta}A^{-1}_{hi}A^{-1}_{jk} \quad , \\ \partial_{\alpha\beta}A^{-1}_{hk} =& -A^{-1}_{h\alpha}A^{-1}_{\beta k} \quad .\end{aligned} \tag{B.2.13}$$

We calculate the functional derivative:

$$\begin{aligned}\partial_A A^{-1}[M] =& \lim_{t\to 0} \frac{(A+tM)^{-1} - A^{-1}}{t} \\ =& \lim_{t\to 0} \frac{A^{-1}\sum_{i=0}^{\infty}\left(-tMA^{-1}\right)^n - A^{-1}}{t} \\ =& \lim_{t\to 0} \frac{A^{-1} - tA^{-1}MA^{-1} + O(t^2) - A^{-1}}{t} \\ =& -A^{-1}MA^{-1}\end{aligned} \tag{B.2.14}$$

The Second derivative of the determinant We the obtain for first derivative tested with $M \in \mathbb{R}^{d\times d}(\mathbb{R})$

$$\partial_A \det A[M_1] = Tr\left(A^{-1}M_1\right)\det A \quad . \tag{B.2.15}$$

The second derivative is

$$\begin{aligned}\partial_A^2 \det A\left(M_1, M_2\right) =&\partial_A\left(Tr\left(A^{-1}M_1\right)\det A\right)\left(M_2\right)\\ =&Tr\left(\partial_A A^{-1}\left(M_2\right)M_1\right)\det A + Tr\left(A^{-1}M_1\right)\partial_A \det A(M_2)\\ =&-Tr\left(A^{-1}M_2A^{-1}M_1\right)\det A + Tr\left(A^{-1}M_1\right)Tr\left(A^{-1}M_2\right)\det A\end{aligned} \tag{B.2.16}$$

□

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