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EXISTENCE AND STABILITY OF SCREW DISLOCATION CONFIGURATIONS WITH ARBITRARY NET BURGERS VECTOR

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Abstract. We consider a variational anti-plane lattice model and demonstrate that at zero temperature, there exist locally stable states containing screw dislocations, under conditions on the distance between the dislocations and on the distance between dislocations and the boundary of the crystal. In proving our results, we introduce approximate solutions which are taken from the theory of dislocations in linear elasticity, and use the inverse function theorem to show that local minimisers lie near them. This gives credence to the commonly held intuition that linear elasticity is essentially correct up to a few spacings from the dislocation core.

1. Introduction

Plasticity in crystalline materials is a highly complex phenomenon, a key aspect of which is the movement of dislocations. Dislocations are line defects within the crystal structure which were first hypothesised to act as carriers of plastic flow in [21, 23, 26], and later experimentally observed in [4, 16].

As they move through a crystal, dislocations interact with themselves and other defects via the orientation-dependent stress fields they induce [17]. This leads to complex coupled behaviour, and efforts to create accurate mathematical models to describe their motion and interaction, and so better engineer such materials are ongoing (see for example [6, 2]).

Over the last decade, a body of mathematical analysis of dislocation models has begun to develop which aims to derive models of crystal plasticity in a consistent way from models of dislocation motion and energetics. Broadly, this work starts from either atomistic models, as in [1, 8, 24, 3], or 'semidiscrete' models, where dislocations are lines or points in an elastic continuum, as in [13, 20, 25, 11, 12, 10].

In the present work we focus on the analysis of dislocations at the atomistic level: we therefore briefly recount the recent achievements in this area. In [8] the focus was on the derivation of homogenised dynamical equations for dislocations and dislocation densities starting from a generalisation of the famous Fraenkel–Kontorova model for edge dislocations. In [3], a clear mathematical framework for describing the Burgers vector of dislocations in lattices was developed, and the asymptotic form of a discrete energy is given in the regime where dislocations are far from each other relative to the lattice spacing. In [24], the emphasis was on an asymptotic description of the energy in a finite crystal undergoing anti–plane deformation with screw dislocations present, and [1] follows in this vein, broadening the class of models considered, and treating the asymptotics of a minimising movement of the dislocation energy. In a similar anti–plane setting, but in an infinite crystal, [18] demonstrated that there are globally stable states with unit Burgers vector.

In the present contribution we demonstrate the existence of *locally* stable states containing multiple dislocations with arbitrary combinations of Burgers vector. Once more, our analysis concerns crystals under anti-plane deformation, but in addition to the full lattice, we now consider finite convex domains with boundaries. Recent results contained in [1] also address the question of local stability of dislocation configurations in finite domains, but under different assumptions to those employed

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here, and using different set of techniques. Moreover, our results provide quantitative estimates on the equilibrium configurations, whereas previous results only provide estimates on the energies.

1.1. **Outline.** The setting for our results is similar to that described in [18]: our starting point is the energy difference functional

$$E^\Omega(y;\tilde{y}) := \sum_{b\in\mathcal{B}^\Omega} \big[\psi(Dy_b) - \psi(D\tilde{y}_b)\big],$$

where $\Omega \subset \Lambda$ is a subset of a Bravais lattice, $\mathcal{B}^\Omega$ is a set of pairs of interacting (lines of) atoms, Dy_b is a finite difference, and ψ is a 1-periodic potential.

We call a deformation y a *locally stable equilibrium* if $u = 0$ minimises $E^\Omega(y + u; y)$ among all perturbations u which have finite energy, and are sufficiently small in the energy norm. The key assumption upon which we base our analysis is the existence of a local equilibrium in the homogeneous lattice containing a dislocation which satisfies a condition which we term *strong stability* — this notion is made precise in §3.2.

Under this key assumption, our main result is Theorem 3.3. This states that, give a number of positive and negative screw dislocations, there exist locally stable equilibria containing these dislocations in a given domain as long as the core positions satisfy a minimum separation criterion from each other and from the boundary of the domain. Furthermore, these configurations may only be globally stable if there is one dislocation in an infinite lattice.

The proof of Theorem 3.3 is divided into two cases, that in which $\Omega = \Lambda$, and that in which Ω is a finite convex lattice polygon: these are proved in §5 and §6 respectively.

2. Preliminaries

2.1. **The lattice.** Underlying the results presented in this paper is the structure of the triangular lattice

$$\Lambda := \tfrac{a_1+a_2}{3} + [a_1, a_2]\cdot\mathbb{Z}^2, \quad \text{where } a_1 = (1,0)^T \text{ and } a_2 = \big(\tfrac{1}{2}, \tfrac{\sqrt{3}}{2}\big)^T. \tag{2.1}$$

In this section we detail some of the important geometric and topological definitions we use to conduct the analysis.

2.1.1. *The lattice complex.* For the purposes of providing a clear definition of the notion of Burgers vector in the lattice, we describe the construction of a CW complex[1] for a general lattice subset. Recall from [3] that we may define a lattice complex in 2D by first defining a set of lattice points (or 0–cells), Λ, then defining the bonds (or 1–cells), $\mathcal{B}$, and finally the cells (or 2–cells) $\mathcal{C}$, and the corresponding boundary operators, ∂. Throughout the paper, Λ, $\mathcal{B}$ and $\mathcal{C}$ will refer to the lattice complex generated by Λ as defined in (2.1) — see also [18] for further details of this construction. Here, we also consider subcomplexes generated by subsets $\Omega \subset \Lambda$.

Given $\Omega \subseteq \Lambda$, we define the corresponding sets of bonds and cells to be

$$\mathcal{B}^\Omega := \big\{(\xi,\zeta)\in\mathcal{B}\,\big|\,\xi,\zeta\in\Omega\big\} \quad\text{and}\quad \mathcal{C}^\Omega := \big\{(\xi,\zeta,\eta)\in\mathcal{C}\,\big|\,\xi,\zeta,\eta\in\Omega\big\}.$$

It is straightforward to check that this satisfies the definitions of a CW subcomplex of the full lattice complex presented in [18, §2.3], and so we may make use of the definitions of integration and p-forms as given in [3, §3] restricted to this subcomplex. To keep notation concise, we will frequently write

$$f_b := f(b) \qquad \text{when} \quad f : \mathcal{B} \to \mathbb{R} \quad \text{is a 1–form.} \tag{2.2}$$

We note that we have chosen to define Λ such that $0 \in \mathbb{R}^2$ lies at the barycentre of a cell which we will denote C_0, and more generally we will use the notation $x^C \in \mathbb{R}^2$ to refer to the barycentre of $C \in \mathcal{C}$.

[1] For further details on the definition of a CW complex and other aspects of algebraic topology, see for example [15].

2.1.2. *Lattice symmetries.* The triangular lattice is a highly symmetric structure, and all of its rotational symmetries can be described in terms of multiples of positive rotations by $\pi/3$ about various points in $\mathbb{R}^2$. We therefore fix R_6 to be the corresponding linear transformation.

We define two special classes of affine transformations on $\mathbb{R}^2$ which are automorphisms of Λ,

$$G^C(x) := \mathsf{R}_6^i(x - x^C) = 0 \quad \text{where } i \in \{0,1\} \text{ is chosen so that } G^C(\Lambda) = \Lambda,$$
$$H^C(x) := \big(G^C\big)^{-1}(x) = \mathsf{R}_6^{-i}x + x^C,$$

and note that by definition, $G^C(C) = C_0$ and $H^C(C_0) = C$. We also understand G^C, H^C as automorphisms on $\mathcal{B}$ and $\mathcal{C}$ in the following way: if $b = (\xi,\zeta) \in \mathcal{B}$ and $C' = (\xi,\zeta,\eta) \in \mathcal{C}$, then

$$G^C(b) := \big(G^C(\xi), G^C(\zeta)\big), \quad \text{and} \quad G^C(C') := \big(G^C(\xi), G^C(\zeta), G^C(\eta)\big).$$

Later, it will be important to consider the transformation of 1–forms under such automorphisms, and so we write

$$\big(f \circ G^C\big)_b := f\big(G^C(b)\big) \qquad \text{when} \quad f : \mathcal{B} \to \mathbb{R} \quad \text{is a 1–form.}$$

2.1.3. *Nearest neighbours.* We define the set of nearest neighbour directions by

$$\mathcal{R} := \{a_i \in \mathbb{R}^2 \,|\, i \in \mathbb{Z}\}, \quad \text{where} \quad a_i := \mathsf{R}_6^{i-1}a_1.$$

Given $\Omega \subseteq \Lambda$ and $\xi \in \Omega$, we define the nearest neighbour directions of ξ in Ω to be

$$\mathcal{R}_\xi^\Omega := \big\{a_i \in \mathcal{R} \,\big|\, \xi + a_i \in \Omega\big\} \subseteq \mathcal{R}.$$

2.1.4. *Distance.* To describe the distance between elements in the complex, we use the usual notion of Euclidean distance of sets,

$$\mathrm{dist}(A,B) := \inf\big\{|x-y| \,\big|\, x \in A,\, y \in B\big\}.$$

2.2. **Convex crystal domains.** In addition to studying dislocations in the infinite lattice Λ, we will also consider dislocations in a *convex lattice polygon*: We say that $\Omega \subset \Lambda$ is a *convex lattice polygon* if

$$C_0 \in \mathcal{C}^\Omega, \quad \mathrm{conv}(\Omega) \cap \Lambda = \Omega, \quad \text{and} \quad \Omega \text{ is finite.}$$

Here and throughout the paper, $\mathrm{conv}(U)$ means the closed convex hull of $U \subset \mathbb{R}^2$, and Ω will denote either a convex lattice polygon or Λ unless stated otherwise. For a convex lattice polygon, we define corresponding 'continuum' domains

$$U^\Omega := \mathrm{conv}(\Omega) \qquad \text{and} \qquad W^\Omega := \mathrm{clos}\Big(\bigcup\big\{C \in \mathcal{C}^\Omega \,\big|\, C \text{ positively–oriented}\big\}\Big).$$

We note that $\Omega \subset W^\Omega \subseteq U^\Omega$; for an illustration of an example of these definitions, see Figure 2.2.1.

2.2.1. *Boundary and boundary index.* We note that the positively–oriented boundary ∂W^Ω may be decomposed as

$$\partial W^\Omega = \big\{\xi \in \Omega \,|\, \mathcal{R}_\xi^\Omega \neq \mathcal{R}\big\} \cup \Big\{b \in \mathcal{B}^\Omega \,\Big|\, b \in \partial \sum \{C \in \mathcal{C}^\Omega \,|\, C \text{ positively–oriented}\}\Big\};$$

in other words, into the lattice points which do not have a full set of nearest neighbours, and hence lie on the 'edge' of the set Ω, and into the bonds which follow the positively–oriented boundary of the entire subcomplex within the full lattice. Since it will be necessary to sum over these sets later, we write $\xi \in \partial W^\Omega$ to mean $\xi \in \partial W^\Omega \cap \Omega$, and $b \in \partial W^\Omega$ to mean $b \in \partial C \cap \partial W^\Omega$ for some positively–oriented $C \in \mathcal{C}^\Omega$.

It is clear that since Ω is a finite set, U^Ω is a convex polygonal domain in $\mathbb{R}^2$, and ∂U^Ω is made up of finitely–many straight segments. We number the corners of such polygons according to the positive orientation of ∂U^Ω as κ_m, $m = 1,\dots,M$, and $\kappa_0 := \kappa_M$; evidently, $\kappa_m \in \Omega$ for all m. We further set $\Gamma_m := (\kappa_{m-1},\kappa_m) \subset \mathbb{R}^2$, the straight segments of the boundary.

For each m, $\kappa_m - \kappa_{m-1}$ is a lattice direction. Since any pair a_i, a_{i+1} with $i \in \mathbb{Z}$ form a basis for the lattice directions, there exists i such that

$$\kappa_m - \kappa_{m-1} = j'a_i + k'a_{i+1}, \quad \text{where} \quad j', k' \in \mathbb{N}, j' > 0.$$

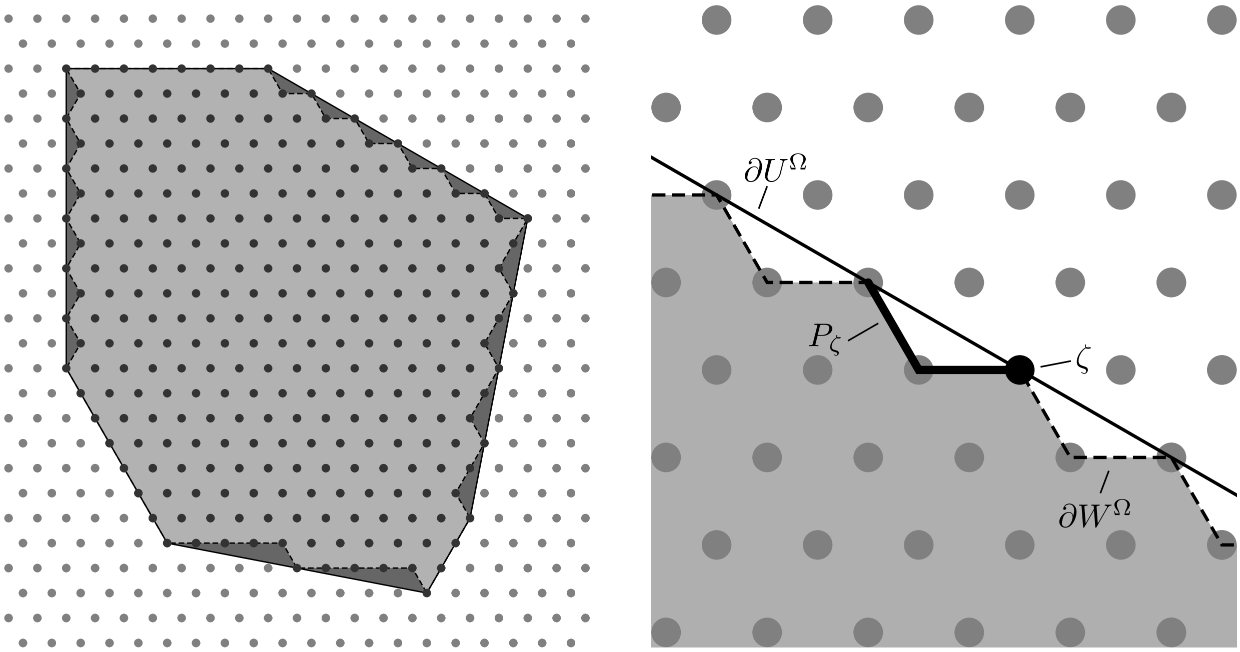

FIGURE 1. The figure on the left shows an example of a convex lattice polygon. Here, Ω is the set of dark grey points, W^Ω is the light grey region and the dark grey region corresponds to $U^\Omega \setminus W^\Omega$. The boundaries of U^Ω and W^Ω are denoted by dashed and plain lines respectively. The figure on the right illustrates the definition of P_ζ, clearly showing the periodic structure of ∂W^Ω.

Define the *lattice tangent vector* to Γ_m to be

$$\tau_m := ja_i + ka_{i+1}, \quad \text{where } \gcd(j,k) = 1 \quad \text{and} \quad \kappa_m - \kappa_{m-1} = n\tau_m \quad \text{for some } n \in \mathbb{N}.$$

This definition entails that τ_m is irreducible in the sense that no lattice direction with smaller norm is parallel to τ_m, and hence if $\zeta \in \Gamma_m \cap \partial W^\Omega$, $\zeta = \kappa_m + j\tau_m$ for some $j = \{0, \dots J_m\}$. In addition to the decomposition of ∂W^Ω into lattice points and bonds, we may also decompose into 'periods' P_ζ indexed by $\zeta \in \partial W^\Omega \cap \partial U^\Omega$, so

$$\partial W^\Omega = \bigcup_{m=1}^{M} \bigcup_{j=0}^{J_m} P_{\kappa_m + j\tau_m} \qquad \text{where} \quad P_\zeta := \big\{ x \in \partial W^\Omega \,\big|\, (x - \zeta)\cdot\tau_m \in \big[0, |\tau_m|^2\big] \big\}. \tag{2.3}$$

An illustration of the definition of P_ζ may be found on the right–hand side of Figure 2.2.1. Denoting the 1–dimensional Hausdorff measure as $\mathcal{H}^1$, we define the *index* of Γ_m, and of ∂W^Ω respectively, to be

$$\mathrm{index}(\Gamma_m) := \mathcal{H}^1(P_\zeta) \quad \text{for any } \zeta \in \Gamma_m \cap \partial W^\Omega \quad \text{and} \quad \mathrm{index}(\partial W^\Omega) := \max_{m=1,\dots,M} \mathrm{index}(\Gamma_m). \tag{2.4}$$

2.3. **Deformations and Burgers vector.** The positions of deformed atoms will be described by maps $y \in \mathscr{W}(\Omega) := \{y : \Omega \to \mathbb{R}\}$. For $y \in \mathscr{W}(\Omega)$ and $b = (\xi, \eta) \in \mathcal{B}^\Omega$, we define the finite difference

$$Dy_b = y(\eta) - y(\xi).$$

2.3.1. *Function spaces.* In addition to the space $\mathscr{W}(\Omega)$, we define

$$\mathscr{W}_0(\Omega) := \big\{ v \in \mathscr{W}(\Omega) \,\big|\, v(\xi_0) = 0 \text{ and } \mathrm{supp}(Dv) \text{ is bounded.} \big\},$$
$$\dot{\mathscr{W}}^{1,2}(\Omega) := \big\{ v \in \mathscr{W}(\Omega) \,\big|\, v(\xi_0) = 0 \text{ and } Dv \in \ell^2\big(\mathcal{B}^\Omega\big) \big\},$$

where $\xi_0 = (0, \frac{\sqrt{3}}{3})^T \in \Omega$. It is shown in [22, Prop. 9] that $\dot{\mathscr{W}}^{1,2}$ is a Hilbert space and $\mathscr{W}_0 \subset \dot{\mathscr{W}}^{1,2}$ is dense.

2.3.2. *Burgers vector.* We now slightly generalise some key definitions from [18].

Given $y : \Omega \to \mathbb{R}$, the set of associated *bond length 1-forms* is defined to be

$$[Dy] := \big\{\alpha : \mathcal{B}^\Omega \to [-\tfrac12, \tfrac12] \,\big|\, \alpha_{-b} = -\alpha_b,\ Dy_b - \alpha_b \in \mathbb{Z} \text{ for all } b \in \mathcal{B}^\Omega,\ \alpha_b \in (-\tfrac12, \tfrac12] \text{ if } b \in \partial W^\Omega\big\}.$$

A *dislocation core* of a bond length 1-form α is a positively–oriented 2-cell $C \in \mathcal{C}^\Omega$ such that $\int_{\partial C} \alpha \neq 0$.

As remarked in [18, §2.5], the Burgers vector of a single cell may only be -1, 0 or 1, so we define the set of dislocation cores to be

$$\mathcal{C}^\pm[\alpha] := \Big\{ C \in \mathcal{C}^\Omega \,\Big|\, C \text{ positively–oriented}, \int_{\partial C} \alpha = \pm 1 \Big\}.$$

We can now define the *net Burgers vector* of a deformation y with $|\mathcal{C}^\pm[\alpha]| < \infty$ (i.e., a finite number of dislocation cores) to be

$$B[y] := \sum_{C \in \mathcal{C}^\pm[\alpha]} \int_{\partial C} \alpha.$$

If Ω is a convex lattice polygon, then it is straightforward to see that $B[y] = \int_{\partial W^\Omega} \alpha$, and the requirement that $\alpha_b \in (-\frac12, \frac12]$ for $b \in \partial W^\Omega$ ensures that the net Burgers vector is independent of $\alpha \in [Dy]$.

2.4. **Dislocation configurations.** In order to prescribe the location of an array of dislocations, we define a *dislocation configuration* (or simply, a *configuration*) to be a set $\mathcal{D}$ of ordered pairs $(C, s) \in \mathcal{C}^\Omega \times \{-1, 1\}$, satisfying the condition that

$$(C, s) \in \mathcal{D} \quad \text{implies} \quad (C, -s) \notin \mathcal{D}. \tag{2.5}$$

Such sets $\mathcal{D}$ should be thought of as a set of dislocation core positions with accompanying Burgers vector ± 1. We define the minimum separation distance of a configuration to be

$$L_\mathcal{D} := \inf \big\{ \mathrm{dist}(C, C') \,\big|\, (C, s), (C', t) \in \mathcal{D}, C \neq C' \big\},$$

and in the case where Ω is a convex lattice polygon, we define the minimum separation between the dislocations and the boundary to be

$$S_\mathcal{D} := \inf \big\{ \mathrm{dist}(C, \partial W^\Omega) \,\big|\, (C, s) \in \mathcal{D} \big\}.$$

3. Main results

3.1. **Energy difference functional and equilibria.** We assume that lattice sites interact via a 1–periodic nearest–neighbour pair potential $\psi \in C^4(\mathbb{R})$, which is even about 0. We discuss possible extensions in § 3.3.2.

For a pair of displacements $y, \tilde{y} \in \mathscr{W}(\Omega)$, we define

$$E^\Omega(y; \tilde{y}) := \sum_{b \in \mathcal{B}^\Omega} \psi(Dy_b) - \psi(D\tilde{y}_b),$$

where we will drop the use of the superscript in the case where $\Omega = \Lambda$. We note immediately that this functional is well-defined whenever $y - \tilde{y} \in \mathscr{W}_0(\Omega)$. It is also clear that Gateaux derivatives in the first argument (in $\mathscr{W}_0(\Omega)$ directions) exist up to fourth order, and do not depend on the second argument. We denote these derivatives $\delta^j E^\Omega(y)$, so that for $v, w \in \mathscr{W}_0(\Omega)$, we have

$$\langle \delta E^\Omega(y), v \rangle := \sum_{b \in \mathcal{B}^\Omega} \psi'(Dy_b) \cdot Dv_b, \quad \text{and} \quad \langle \delta^2 E^\Omega(y) v, w \rangle := \sum_{b \in \mathcal{B}^\Omega} \psi''(Dy_b) \cdot Dv_b Dw_b.$$

In §4.1, we will demonstrate that under certain conditions on $\tilde{y}$, $E(y; \tilde{y})$ it may be extended by continuity in its first argument to a functional which is also well–defined for $y - \tilde{y} \in \dot{\mathscr{W}}^{1,2}(\Omega)$.

The following definition makes precise the various notions of equilibrium we will consider below.

Definition 1 (Stable Equilibrium). *(i) A displacement $y \in \mathscr{W}(\Omega)$ is a* locally stable equilibrium *if there exists $\epsilon > 0$ such that $E^\Omega(y + u; y) \geq 0$ for all $u \in \mathscr{W}_0(\Omega)$ with $\|Du\|_2 \leq \epsilon$.*

(ii) We call a locally stable equilibrium y strongly stable *if, in addition, there exists $\lambda > 0$ such that*

$$\langle \delta^2 E^\Omega(y)v, v\rangle \geq \lambda \|Dv\|^2_{\ell^2} \qquad \forall v \in \mathscr{W}_0(\Omega). \tag{3.1}$$

(iii) A displacement $y \in \mathscr{W}(\Omega)$ is a globally stable equilibrium *if $E^\Omega(y+u;y) \geq 0$ for all $u \in \mathscr{W}_0(\Omega)$.*

3.2. **Strong stability assumption.** Here, we discuss the key assumption employed in proving the main results of the paper. As motivation, we review a result from [18].

Let $\hat{y} : \mathbb{R}^2 \setminus \{0\} \to \mathbb{R}$ be the dislocation solution for anti-plane linearised elasticity [17], i.e.

$$\hat{y}(x) := \tfrac{1}{2\pi}\arg(x) = \tfrac{1}{2\pi}\arctan\left(\tfrac{x_2}{x_1}\right),$$

where we identify $x \in \mathbb{R}^2$ with the point $x_1 + ix_2 \in \mathbb{C}$, and the branch cut required to make this function single–valued is taken along the positive x_1–axis. The accepted intuition is that $\hat{y}$ provides a good description of dislocation configurations, except in a 'core' region which stores a finite amount of energy. Reasonable candidates for equilibrium configurations are therefore of the form $y = \hat{y} + u$ where $u \in \dot{\mathscr{W}}^{1,2}(\Omega)$. This intuition is made precise as follows [18, Theorem 4.5]:

Theorem 3.1 (Global stability of single dislocation Λ). *In addition to the foregoing assumptions, suppose that $\psi(r) \geq \frac{1}{2}\psi''(0)r^2$ for $r \in [-\frac{1}{2}, \frac{1}{2}]$ where $\psi''(0) > 0$, then there exists $u \in \dot{\mathscr{W}}^{1,2}(\Lambda)$ such that $\hat{y} + u$ is a globally stable equilibrium of E.*

In the present work, where we focus on multiple dislocation cores, we remove the additional technical assumptions on ψ but instead directly assume the existence of a single stable core; i.e.

(STAB): there exists $u \in \dot{\mathscr{W}}^{1,2}(\Lambda)$ such that $y = \hat{y} + u$ is a strongly stable equilibrium.

Throughout the rest of the paper, u is fixed to satisfy **(STAB)**. We denote $\lambda_d := \lambda$ to be the stability constant from (3.1) with $y = \hat{y} + u$, and fix a finite collection of cells, A, such that $\mathcal{C}^\pm[\alpha] \subset A$ for any $\alpha \in [D\hat{y} + Du]$.

Remark 3.2. To demonstrate that **(STAB)** holds for a non-trivial class of potentials ψ satisfying our assumptions, we refer to Lemma 3.3 in [18], which states that, if $\psi = \psi_{\rm lin}$, where

$$\psi_{\rm lin}(x) := \tfrac{1}{2}\lambda\,\mathrm{dist}(x, \mathbb{Z})^2,$$

then $\delta^2 E > 0$ at $y = \hat{y} + u$, a globally stable equilibrium. (Theorem 3.1 does not in fact require global smoothness of ψ.) Furthermore, it immediately follows that $\mathrm{dist}(Dy_b, \frac{1}{2} + \mathbb{Z}) \geq \epsilon_0$ for some $\epsilon_0 > 0$.

Using the inverse function theorem as stated below in Lemma 4.7, it is fairly straightforward to see that if $\psi \in \mathrm{C}^4(\mathbb{R})$ satisfies

$$\left|\psi^{(j)}(r) - \psi^{(j)}_{\rm lin}(r)\right| \leq \epsilon |r|^{p-j} \text{ for } r \in [-1/2, 1/2] \text{ and } j = 1, 2,$$

where $p > 2$ and ϵ is sufficiently small, then there exists $w \in \dot{\mathscr{W}}^{1,2}(\Lambda)$ with $\|Dw\|_{\ell^2} \leq C\epsilon$ such that $\hat{y} + u + w$ is a strongly stable equilibrium for E.

Potentials constructed in this way are by no means the only possibilities — **(STAB)** can in fact be checked for any given potential by way of a numerical calculation, using for example the methods analysed in [7].

We also remark here that in §5 of [1], a demonstration of the existence of local minimisers is given under different assumptions. Instead of **(STAB)**, structural assumptions are made on the potential, which the example we provide here also satisfies. Under these assumptions, Lemma 5.1 in [1] demonstrates that there exist energy barriers which dislocations must overcome in order to move from cell to cell. This leads to the proof of Theorem 5.5, which includes the statement that there exist local minimisers containing dislocations in finite lattices. □

3.3. **Existence Results.** We state the existence result for stable dislocation configurations in the infinite lattice and in convex lattice polygons together. To this end, we denote $S_{\mathcal{D}} := +\infty$ for the case $\Omega = \Lambda$.

We remark here that the main achievement of this analysis is to show the constants L_0 and S_0 depend only on the number of dislocations, the potential ψ and $\mathrm{index}(\partial W^\Omega)$, and not on the specific domain Ω or its diameter.

Theorem 3.3. *Suppose that* **(STAB)** *holds and either $\Omega = \Lambda$ or Ω is a convex lattice polygon.*

(1) For each $N \in \mathbb{N}$, there exist constants $L_0 = L_0(N)$ and $S_0 = S_0\big(\mathrm{index}(\partial W^\Omega), N\big)$ such that for any core configuration $\mathcal{D}$ satisfying $|\mathcal{D}| = N$, $L_{\mathcal{D}} \geq L_0$ and $S_{\mathcal{D}} \geq S_0$, there exists a strongly stable equilibrium $z \in \mathscr{W}(\Omega)$, and for any $\alpha \in [Dz]$,

$$\mathcal{C}^{\pm}[\alpha] \subset \bigcup_{(C,s)\in\mathcal{D}} H^C(A) \qquad \textit{and} \qquad \int_{\partial H^C(A)} \alpha = s, \;\; \textit{for all } (C,s) \in \mathcal{D}.$$

In particular, $B[z] = \sum_{(C,s)\in\mathcal{D}} s$, and the conditions $L_{\mathcal{D}} \geq L_0$ and $S_{\mathcal{D}} \geq S_0$ entail that core regions $x^C + A$ do not overlap each other, or with the boundary.

(2) The equilibrium z can be written as

$$z = \sum_{(C,s)\in\mathcal{D}} s(\hat{y} + u) \circ G^C + w,$$

where $w \in \dot{\mathscr{W}}^{1,2}(\Omega)$ and $\|Dw\|_{\ell^2} \leq c(L_{\mathcal{D}}^{-1} + S_{\mathcal{D}}^{-1/2})$, where c is a constant depending only on N and $\mathrm{index}(\partial W^\Omega)$.

(3) Unless $N = 1$ and $\Omega = \Lambda$, z cannot be a globally stable equilibrium.

3.3.1. *Strategy of the proof.* In both cases, the overall strategy of proof is similar:

- We construct an approximate equilibrium z, using the linear elasticity solution for the dislocation configuration and a truncated version of the core corrector whose existence we assumed in **(STAB)**.
- For given $\mathcal{D}$, we obtain bounds which demonstrate that $\delta E^\Omega(z)$ decays to zero as $L_{\mathcal{D}}, S_{\mathcal{D}} \to \infty$, where z are the approximate equilibria corresponding to $\mathcal{D}$.
- We show that $\delta^2 E^\Omega(z) \geq \lambda_d - \epsilon$ as $L_{\mathcal{D}}$, $S_{\mathcal{D}} \to \infty$.
- We apply the Inverse Function Theorem to demonstrate the existence of a corrector $w \in \dot{\mathscr{W}}^{1,2}(\Omega)$ such that $z+w$ is a strongly stable equilibrium. Since $\|Dw\|_{\ell^2}$ can be made arbitrarily small by making more stringent requirements on $\mathcal{D}$, we can demonstrate that the condition on the core position holds, which completes the proof of parts (1) and (2) of the statement.
- Part (3) of the statement is proved by construction of explicit counterexamples.

Remark 3.4. The reduced rate $S_{\mathcal{D}}^{-1/2}$ (as opposed to $L_{\mathcal{D}}^{-1}$) with respect to separation from the boundary is due to surface stresses which are not captured by the standard linear elasticity theory that we use to construct the predicture z.

We believe that without including these effects in the predictor, it is not possible to improve the results. Constructing an improved predictor z which takes into account surface stresses may also provide a path towards approaching the problem of surface relaxation in the vectorial case, which we discuss in §3.3.2. $\square$

3.3.2. *Discussion of extensions.* We have avoided the most difficult aspect of the analysis of dislocations by imposing the strong stability assumption **(STAB)** for a single core. Once this is established (or assumed), several extensions of our analysis become possible, which we disuss in the following paragraphs.

One immediate extension is to drop the requirement that ψ is even about 0, which would be the case if the body was undergoing macroscopic shear. This extension would require us to separately assume the existence of strongly stable positive and negative dislocation cores in the full lattice, as they would no longer necessarily be symmetric. Apart from the introduction of logarithmic factors into some of the bounds we obtain, it appears that the analysis would be analogous to that contained here.

Secondly, it is straightforward to generalise the analysis carried out in §6 to 'half–plane' lattices, since the linear elastic corrector $\bar{y}$ may be explicitly constructed via a reflection principle. This suggests that in fact the analysis could be extended to hold in any convex domain with a finite number of corners $\kappa_m \in \Omega$ and tangent vectors τ_m which are lattice directions — in effect, an 'infinite' polygon. The key technical ingredient required here would be to prove decay results for the corrector problem analysed in §6.1 in such domains, which we were not able to find in the literature.

Thirdly, the assumption that interactions are governed by nearest–neighbour pair potentials only is readily lifted as well. It seems to us that a generalisation to many–body interactions with a finite range beyond nearest neighbours is conceptually straightforward (though would add some technical, and in particular notational difficulties), as long as they require suitable symmetry assumptions. Note, in particular, that the crucial decay estimates from [7] that we employ are still valid in this case.

Finally, generalisations to in–plane models seem to be relatively straightforward only in the infinite-lattice case. In the finite domain case, one would need to account for surface relaxation effects, which we have entirely avoided here by choosing an anti–plane model. The phenomenon of surface relaxation in discrete problems seems a difficult one, and to the authors' knowledge, has yet to be addressed systematically in the Applied Analysis literature, but for some results in this direction, see [27]. A possible way forward would be to impose an additional stability condition on the boundary, similar to our condition **(STAB)**, which could then be investigated separately.

4. Ancillary results

4.1. **Extension of the energy difference functional.** The following is a slight variation of [18, Lemma 4.1].

Lemma 4.1. *Let $y \in \mathscr{W}(\Omega)$, and suppose that $\delta E^\Omega(y)$ is a bounded linear functional. Then $u \mapsto E^\Omega(y+u;y)$ is continuous as a map from $\mathscr{W}_0(\Omega)$ to $\mathbb{R}$ with respect to the norm $\|D\cdot\|_2$; hence there exists a unique continuous extension of $u \mapsto E^\Omega(y+u;y)$ to a map defined on $\dot{\mathscr{W}}^{1,2}(\Omega)$. The extended functional $u \mapsto E^\Omega(y+u;y)$, $u \in \dot{\mathscr{W}}^{1,2}(\Omega)$ is three time continuously Frechet differentiable.*

Proof. The proof of this statement is almost identical to the proof of [18, Lemma 4.1] and hence we omit it. We note that in a finite domain, the condition that $\delta E^\Omega(y)$ is a bounded linear functional is always satisfied, since $\dot{\mathscr{W}}^{1,2}(\Omega)$ is a finite dimensional space. □

4.2. **Stability of the homogeneous lattice.** The following lemma demonstrates that $y = 0$ is a globally stable as well as strongly stable equilibrium. In particular, this shows that $\hat{y} + u$ cannot be a unique stable equilibrium among all $y \in \mathscr{W}(\Lambda)$.

Lemma 4.2. *Suppose that* (**STAB**) *holds, then the deformation $y \equiv 0$ is a strongly stable equilibrium for any $\Omega \subset \Lambda$. Precisely,*

$$\langle \delta^2 E^\Omega(0)v, v\rangle = \psi''(0) \sum_{b\in\mathcal{B}^\Omega} Dv_b^2 \qquad \text{and} \qquad \psi''(0) \geq \lambda_d.$$

Proof. Suppose that $v \in \mathscr{W}_0(\Omega)$ and $C^i \in \mathcal{C}$ is a sequence such that $\mathrm{dist}(C^i, 0) \to \infty$ as $i \to \infty$. Define $v^i := v \circ G^{C^i}$; if $y = \hat{y} + u$,

$$\lambda_d \|Dv\|_2^2 = \lambda_d \|Dv^i\|_2^2 \leq \langle \delta^2 E^\Lambda(y) v^i, v^i\rangle = \sum_{b\in\mathcal{B}} \psi''(Dy_b)\big(Dv^i_b\big)^2 = \sum_{b\in\mathcal{B}} \psi''\big(D(y\circ H^{C^i})_b\big) Dv_b^2,$$

and since $\mathrm{dist}(Dy_b, \mathbb{Z}) \to 0$ as $\mathrm{dist}(b, 0) \to \infty$, it follows that $0 < \lambda_d \leq \psi''(0)$.

Since ψ is even about 0 it must be that $\psi'(0) = 0$, and the statement follows trivially. □

4.3. **The linear elasticity residual.** We now prove a result estimating the residual of the pure linear elasticity predictor.

Lemma 4.3. *Let $\mathcal{D}$ be a dislocation configuration in Λ and $z := \sum_{(C,s)\in\mathcal{D}} \hat{y}\circ H^C$. For $L_{\mathcal{D}}$ sufficiently large, there exists $g : \mathcal{B} \to \mathbb{R}$ such that*

$$\langle \delta E(z), v\rangle = \sum_{b\in\mathcal{B}} g_b Dv_b \quad \textit{and} \quad |g_b| \le c \sum_{(C,s)\in\mathcal{D}} \mathrm{dist}(b, C)^{-3}. \tag{4.1}$$

Proof. The canonical form for $\delta E(z)$ is $\langle \delta E(z), v\rangle = \sum \psi'(\alpha_b)Dv_b$, where α is a bond length one-form associated with Dz. For $L_{\mathcal{D}}$ sufficiently large, arguing as in [18, Lemma 4.3] we obtain that $\alpha_b \in (-1/2, 1/2)$, which entails that $\alpha \in [Dz]$ is unique, and may be written in the form $\alpha_{(\xi,\xi+a_i)} = \int_0^1 \nabla_{a_i} z(\xi+ta_i)\,\mathrm{d}t$, where here and below ∇z will mean the extension of the gradient of z to a function in $\mathrm{C}^\infty\big(\mathbb{R}^2 \setminus \bigcup_{(C,s)\in\mathcal{D}}\{x^C\}; \mathbb{R}^2\big)$.

We note that $|\psi'(\alpha_b)| \lesssim \sum \mathrm{dist}(b, C)^{-1}$ only, so we must remove a "divergence-free component". To that end, let $\omega_b := \bigcup\{C' \in \mathcal{C} \mid \pm b \in \partial C', C' \text{ positively–oriented}\}$ and let $V := |\omega_b|$ for some arbitrary $b \in \mathcal{B}$. Further, let $\bar{C}_\epsilon := \bigcup_{(C,s)\in\mathcal{D}} B_\epsilon(x^C)$. Then, for $b = (\xi, \xi + a_i)$, we define

$$h_b := \frac{\psi''(0)}{V} \lim_{\epsilon\to 0} \int_{\omega_b\setminus\bar{C}_\epsilon} \nabla z \cdot a_i \,\mathrm{d}x \qquad \text{and} \qquad g_b := \psi'(\alpha_b) - h_b.$$

It is fairly straightforward to show that the limit exists by applying the divergence theorem, which entails that h_b and g_b are well–defined and

$$\sum_{b\in\mathcal{B}} h_b Dv_b = \lim_{\epsilon\to 0} \frac{\psi''(0)}{V} \int_{\mathbb{R}^2\setminus\bar{C}_\epsilon} \nabla z \cdot \nabla Iv \,\mathrm{d}x = 0$$

for all $v \in \mathscr{W}_0(\Lambda)$, where Iv denotes the continuous and piecewise affine interpolant of v. Thus, we obtain that $\langle \delta E(z), v\rangle = \sum_{b\in\mathcal{B}} g_b Dv_b$ as desired.

It remains to prove the estimate on g_b. Taylor expanding, we obtain

$$\psi'(\alpha_b) - h_b = \psi'(0) + \psi''(0)\bigg(\alpha_b - \frac{1}{V}\lim_{\epsilon\to 0}\int_{\omega_b\setminus\bar{C}_\epsilon} \nabla z\cdot a_i\,\mathrm{d}x\bigg) + \tfrac{1}{2}\psi'''(0)|\alpha_b|^2 + O\big(|\alpha_b|^3\big).$$

The first and third terms vanish since ψ is even. Note that $\alpha_b = \frac{1}{V}\int_{\omega_b} \nabla z \cdot a_i \,\mathrm{d}x$, where a_i is the direction of the bond b, so Taylor expanding about the midpoint of b and using the symmetry of b and ω_b to eliminate the term involving $\nabla^2 z$, we obtain

$$\int_b \nabla z \cdot a_i \,\mathrm{d}x - \frac{1}{V}\lim_{\epsilon\to 0}\int_{\omega_b\setminus\bar{C}_\epsilon} \nabla z\cdot a_i\,\mathrm{d}x = O\big(|\nabla^3 z|\big).$$

Finally, as $|\alpha_b| \lesssim \mathrm{dist}(b, C)^{-1}$ and $|\nabla^3 z| \lesssim \mathrm{dist}(b, C)^{-3}$ for all $(C, s) \in \mathcal{D}$, the stated estimate follows. □

4.4. **Regularity of the corrector.** We now slightly refine the general regularity result of Theorem 3.1 in [7], exploiting the evenness of the potential ψ.

Lemma 4.4. *Let u be the core corrector whose existence postulated in* **(STAB)***: then there exists a constant C_{reg} such that*

$$|Du_b| \le C_{\mathrm{reg}}\,\mathrm{dist}(b, C)^{-2} \qquad \textit{for all } b \in \mathcal{B} \textit{ and } (C, s) \in \mathcal{D}.$$

Proof. Our setting satisfies all assumptions of the $d = 2, m = 1$ (anti-plane) case described in Section 2.1 of [7] with $\mathcal{N}_\xi = \{a_i \,|\, i = 1, \dots, 6\}$ for all $\xi \in \Lambda$, and the complete set of assumptions summarized in **(pD)** in Section 2.4.5 of [7]. Using Lemma 4.3, we may apply Lemma 3.4 [7] with $p = 3$, implying $|Du_b| \lesssim \mathrm{dist}(b, C)^{-2}$. □

4.5. **Approximation by truncation.** Following [7] we define a family of truncation operators Π_R^C, which we will apply to $u \in \dot{\mathscr{W}}^{1,2}(\Omega)$. Let $\eta \in \mathrm{C}^1(\mathbb{R}^2)$ be a cut off function which satisfies

$$\eta(x) := \begin{cases} 1, & |x| \leq \frac{3}{4}, \\ 0, & |x| \geq 1. \end{cases}$$

Let Iu be the piecewise affine interpolant of u over the triangulation given by $\mathcal{T}_\Lambda = \mathcal{C}$. For $R > 2$ let $A_R := B_R \setminus B_{R/2+1}$, an annulus over which $\eta(x/R)$ is not constant. Define $\Pi_R^C : \dot{\mathscr{W}}^{1,2} \to \mathscr{W}_0$ by

$$\Pi_R^C u(\xi) := \eta\Big(\tfrac{\xi - x^C}{R}\Big)\big(u(\xi) - a_R^C\big), \qquad \text{where} \qquad a_R^C := \fint_{x^C + A_R} Iu(x)\,\mathrm{d}x.$$

In addition, we define $\Pi_R := \Pi_R^{C_0}$.

We now state the following result concerning the approximation property of the family of truncation operators Π_R^C, which follows from results in [7].

Lemma 4.5. *Let $v \in \dot{\mathscr{W}}^{1,2}(\Lambda)$ and $C \in \mathcal{C}$, then*

$$\big\|D\Pi_R^C v - Dv\big\|_{\ell^2(\mathcal{B})} \leq \gamma_1 \|Dv\|_{\ell^2(\mathcal{B}\setminus B_{R/2}(x^C))}. \tag{4.2}$$

where γ_1 is independent of R, v and C.

In particular, if $u \in \dot{\mathscr{W}}^{1,2}(\Lambda)$ is the core corrector from (**STAB**)*, then*

$$\big\|D\Pi_R^C(u \circ G^C) - D(u \circ G^C)\big\|_{\ell^2(\mathcal{B})} \leq \gamma_2 R^{-1}, \tag{4.3}$$

where γ_2 is independent of R and C.

Proof. Since $\|\cdot\|_{\ell^2(\mathcal{B})}$ is invariant under composition of functions with lattice automorphisms we can assume, without loss of generality, that $C = C_0$. The estimate (4.2) then is simply a restatement of [7, Lemma 4.3]. The second estimate (4.3) then follows immediately from Lemma 4.4. $\square$

Next, we show that the assumption **(STAB)** implies that that $\delta^2 E^\Lambda(\hat{y} + \Pi_R u)$ is positive for sufficiently large R.

Lemma 4.6. *There exist constants $\lambda_{d,R}$ such that*

$$\langle \delta^2 E^\Lambda\big(\hat{y} + \Pi_R u\big)v, v\rangle \geq \lambda_{d,R}\|Dv\|_2^2 \qquad \text{for all} \quad v \in \mathscr{W}_0, \tag{4.4}$$

and $\lambda_{d,R} \to \lambda_d > 0$ as $R \to \infty$.

Proof. Noting that $\|Dv\|_\infty \leq \|Dv\|_2$ for any $v \in \dot{\mathscr{W}}^{1,2}(\Lambda)$,

$$\begin{aligned}\langle \delta^2 E^\Lambda(\hat{y} + \Pi_R u)v, v\rangle &= \big\langle[\delta^2 E^\Lambda(\hat{y} + \Pi_R u) - \delta^2 E^\Lambda(\hat{y} + u)]v, v\big\rangle + \big\langle \delta^2 E^\Lambda(\hat{y} + u)v, v\big\rangle, \\ &\geq \big(\lambda_d - \|\psi'''\|_\infty \big\|D\Pi_R u - Du\big\|_\infty\big)\|Dv\|_2^2, \\ &\geq \big(\lambda_d - \epsilon_R\big)\|Dv\|_2^2,\end{aligned}$$

where $\epsilon_R \lesssim R^{-1}$ as $R \to \infty$ by Lemma 4.5. $\square$

4.6. **Inverse Function Theorem.** We review a quantitative version of the inverse function theorem, adapted from [19, Lemma B.1].

Lemma 4.7. *Let X, Y be Hilbert spaces, $w \in X$, $F \in C^2(B_R^X(w); Y)$ with Lipschitz continuous Hessian, $\|\delta^2 F(x) - \delta^2 F(y)\|_{L(X,Y)} \leq M\|x - y\|_X$ for any $x, y \in B_R^X(w)$. Furthermore, suppose that there exist constants $\mu, r > 0$ such that*

$$\langle \delta^2 F(w)v, v\rangle \geq \mu\|v\|_X^2, \quad \|\delta F(w)\|_Y \leq r, \quad \text{and} \quad \tfrac{2Mr}{\mu^2} < 1,$$

then there exists a locally unique $\bar{w} \in B_R^X(w)$ such that $\delta F(\bar{w}) = 0$, $\|w - \bar{w}\|_X \leq \frac{2r}{\mu}$ and

$$\langle \delta^2 F(\bar{w})v, v\rangle \geq \big(1 - \tfrac{2Mr}{\mu^2}\big)\mu\|v\|_X^2.$$

5. Proof for the Infinite Lattice

Before considering the case of finite lattice domains, we first set out to prove Theorem 3.3 in the case when $\Omega = \Lambda$. In this case we are able to give a substantially simplified argument that concerns only the interaction between dislocations rather than the additional difficulty of the interaction of dislocations with the boundary which is present in the finite domain case.

5.1. **Analysis of the predictor.** Suppose that $\mathcal{D}$ is a dislocation configuration in Λ: we define an approximate solution (predictor) with truncation radius R to be

$$z := \sum_{(C,s)\in\mathcal{D}} s\left(\hat{y} + \Pi_R u\right) \circ G^C. \tag{5.1}$$

The following lemma provides an estimate on the residual of such approximate solutions in terms of $L_{\mathcal{D}}$.

Lemma 5.1. *Suppose z is the approximate solution for a dislocation configuration $\mathcal{D}$ in Λ as defined in (5.1) with truncation radius $R = L_{\mathcal{D}}/5$. Then there exists $L_0 = L_0(N)$ and a constant $c = c(N)$, such that, whenever $L_{\mathcal{D}} > L_0$,*

$$\left\|\delta E(z)\right\|_{\dot{\mathscr{W}}^{1,2}(\Lambda)^*} \leq c L_{\mathcal{D}}^{-1}.$$

Proof. Enumerate the elements of $\mathcal{D}$ as (C^i, s^i) where $i = 1, \dots, N$. Setting $G^i := G^{C^i}$, let $y^i := (\hat{y} + \Pi_R u) \circ G^i$ and $\hat{y}^i := \hat{y} \circ G^i$. Let $r := 2(R+1) = 2(L_{\mathcal{D}}/5 + 1)$ and v be any test function in $\dot{\mathscr{W}}^{1,2}(\Lambda)$ and define

$$v^i := \Pi_r^{C^i} v \quad \text{for } i = 1, \dots, N, \qquad \text{and} \qquad v^0 := v - \sum_{i=1}^N v^i.$$

Lemma 4.5 implies that $\|Dv^i\|_2 \lesssim \|Dv\|_2$ for $i = 0, \dots, N$.

By assumption **(STAB)**, $\delta E(\hat{y} + u) = 0$, so we may decompose the residual into

$$\begin{aligned}
\langle \delta E(z), v\rangle &= \sum_{i=0}^N \langle \delta E(z), v^i\rangle, \\
&= \left\langle \delta E(z), v^0\right\rangle + \sum_{i\neq 0} \left\langle \delta E(z) - \delta E(y^i), v^i\right\rangle \\
&\qquad + \sum_{i\neq 0} \left\langle \delta E(y^i) - \delta E\big(\hat{y}^i + u\circ G^i\big), v^i\right\rangle \\
&=: \mathrm{T}_1 + \mathrm{T}_2 + \mathrm{T}_3.
\end{aligned} \tag{5.2}$$

The term T_1*:* Employing Lemma 4.3, and using the fact that $z = \sum_{i=1}^N \hat{y} \circ G^i$ in $\operatorname{supp}(v^0)$ we obtain that

$$\begin{aligned}
\left|\mathrm{T}_1\right| = \left|\langle \delta E(z), v^0\rangle\right| &\leq \sum_{b\in\mathcal{B}} |g_b||Dv_b^0| \lesssim \sum_{b\in\mathcal{B}} \sum_{i=1}^N \operatorname{dist}(b, C^i)^{-3} |Dv_b^0| \\
&\lesssim \sum_{i=1}^N \Bigg(\sum_{\substack{b\in\mathcal{B} \\ \operatorname{dist}(b,C^i)\geq r/2-1}} \operatorname{dist}(b, C^i)^{-6} \Bigg)^{1/2} \|Dv^0\|_2 \lesssim r^{-2} \|Dv\|_2.
\end{aligned} \tag{5.3}$$

The term T_2*:* Here, we have $z - y^i = \sum_{j\neq i} \hat{y}^j$ in the support of v^i. We expand

$$\begin{aligned}\big\langle \delta E(z) - \delta E\big(y^i\big), v^i\big\rangle &= \sum_{b\in\mathcal{B}} \psi''(s_b) \sum_{j\neq i} D\hat{y}^j_b Dv^i_b \\ &= \psi''(0) \sum_{j\neq i}\sum_{b\in\mathcal{B}} D\hat{y}^j_b Dv^i_b + \sum_{b\in\mathcal{B}} h_b Dv^i_b, \end{aligned} \tag{5.4}$$

where $|s_b| \lesssim (1+\mathrm{dist}(b,C^i))^{-1}$ and

$$|h_b| = \Big|\big(\psi''(s_b) - \psi''(0)\big)\sum_{j\neq i} D\hat{y}^j_b\Big| \lesssim (1+\mathrm{dist}(b,C^i))^{-2}L_{\mathcal{D}}^{-1}.$$

We have Taylor expanded and used the evenness of ψ to arrive at the estimate on the right. The first group of terms in (5.4) can be estimated as in (5.3) to obtain $|\sum_{b\in\mathcal{B}} D\hat{y}^j_b Dv^i_b| \lesssim L_{\mathcal{D}}^{-2}\|Dv\|_2$ for all $j\neq i$. For the second group in (5.4), we have

$$\Big|\sum_{b\in\mathcal{B}} h_b Dv^i_b\Big| \lesssim L_{\mathcal{D}}^{-1}\bigg(\sum_{\substack{b\in\mathcal{B}\\ \mathrm{dist}(b,C^i)\le r+1}} (1+\mathrm{dist}(b,C^i))^{-4}\bigg)^{1/2}\|Dv^i\|_2 \lesssim L_{\mathcal{D}}^{-2}\|Dv\|_2.$$

The term T_3*:* The final group in (5.2) is straightforward to estimate using the truncation result of Lemma 4.5, giving

$$\big|\big\langle \delta E(y^i) - \delta E(\hat{y}^i + u\circ G^i), v^i\big\rangle\big| \le \|\psi''\|_\infty \|D\Pi_R u - Du\|_2\|Dv^i\|_2 \lesssim R^{-1}\|Dv\|_2.$$

Conclusion: Inserting the estimates for $\mathrm{T}_1, \mathrm{T}_2, \mathrm{T}_3$ into (5.2) we obtain

$$\big|\langle \delta E(z), v\rangle\big| \lesssim \Big(r^{-2} + L_{\mathcal{D}}^{-2} + R^{-1}\Big)\|Dv\|_2 \lesssim L_{\mathcal{D}}^{-1}\|Dv\|_2. \qquad \square$$

5.2. **Stability of the predictor.** We proceed to prove that $\delta^2 E(y)$ is positive, where y is the predictor constructed in (5.1). This result employs ideas similar to those used in the proof of [7, Theorem 4.8], modified here to an aperiodic setting and extended to cover the case of multiple defect cores.

Lemma 5.2. *Let z be a predictor for a dislocation configuration $\mathcal{D}$ in Λ, as defined in* (5.1)*, where $|\mathcal{D}| = N$. Then there exist postive constants $R_0 = R_0(N)$ and $L_0 = L_0(N)$ such that if $R \ge R_0$ and $L_{\mathcal{D}} \ge L_0$, there exists $\lambda_{L,R} \ge \lambda_d/2$ so that*

$$\langle \delta^2 E(z)v, v\rangle \ge \lambda_{L,R}\|Dv\|_2^2 \qquad \textit{for all } v \in \dot{\mathscr{W}}^{1,2}(\Lambda).$$

Proof. Lemma 4.6 implies the existence of R_0 such that $\lambda_{d,R} \ge 3\lambda_d/4 > 0$ for all $R \ge R_0$, thus we choose a truncation radius $R \ge R_0$ which will remain fixed for the rest of the proof. We now argue by contradiction. Suppose that there exists no L_0 satisfying the statement; it follows that there exists $\mathcal{D}^n$, a sequence of dislocation configurations such that

(1) $N := |\mathcal{D}^n|$, $\big|\big\{(C,+1)\in\mathcal{D}^n\big\}\big|$ and $\big|\big\{(C,-1)\in\mathcal{D}^n\big\}\big|$ are constant,
(2) $L^n := L_{\mathcal{D}^n} \to \infty$ as $n\to\infty$ and
(3) $\delta^2 E(z^n) < \lambda_d/2$ for all n, where z^n is the approximate solution corresponding to the configuration $\mathcal{D}^n$ in Λ with truncation radius R, as defined in (5.1).

The first condition may be assumed without loss of generality by taking subsequences. We enumerate the elements $(C^{n,i}, s^{n,i})$ of $\mathcal{D}^n$, and write $G^{n,i} := G^{C^{n,i}}$ and $H^{n,i} := H^{C^{n,i}}$. By translation invariance and the fact that ψ is even, we may assume without further loss of generality that $(C^{n,1}, s^{n,1}) = (C_0, +1)$. For each n,

$$\lambda_n := \inf_{\substack{v\in\dot{\mathscr{W}}^{1,2}(\Lambda)\\ \|Dv\|_2 = 1}} \langle \delta^2 E(z^n)v, v\rangle < \lambda_d/2$$

exists since $\delta^2 E(z)$ is a bounded bilinear form on $\dot{\mathscr{W}}^{1,2}(\Lambda)$ for any $z \in \mathscr{W}(\Lambda)$. Let $v^n \in \mathscr{W}_0(\Lambda)$ be a sequence of test functions such that $\|Dv^n\|_2 = 1$ and

$$\lambda_n \leq \langle \delta^2 E(z^n) v^n, v^n \rangle \leq \lambda_n + n^{-1}.$$

Since v^n is bounded in $\dot{\mathscr{W}}^{1,2}(\Lambda)$, it has a weakly convergent subsequence. By the translation invariance of the norm and taking further subsequences without relabelling, we further assume that $\bar{v}^{n,i} := v^n \circ H^{n,i}$ weakly converges for each i. We now employ the result of [7, Lemma 4.9]. This states that there exists a sequence of radii, $r^n \to \infty$, for which we may also assume $r^n \leq L^n/3$, so that for each $i = 1, \dots, N$,

$$w^{n,i} := \Pi_{r^n}^{C^{n,i}} v^n \quad \text{satisfies} \quad w^{n,i} \circ H^{n,i} \to \bar{w}^i \quad \text{and} \quad (v^n - w^{n,i}) \circ H^{n,i} \rightharpoonup 0 \quad \text{in } \dot{\mathscr{W}}^{1,2}(\Lambda).$$

Writing $\bar{w}^{n,i} := w^{n,i} \circ H^{n,i}$, and defining $w^{n,0} := v^n - \sum_{i=1}^N w^{n,i}$, it follows that

$$\langle \delta^2 E(z^n) v^n, v^n \rangle = \sum_{i,j=0}^{N} \langle \delta^2 E(z^n) w^{n,i}, w^{n,j} \rangle = \sum_{i=0}^{N} \langle \delta^2 E(z^n) w^{n,i}, w^{n,i} \rangle + 2 \sum_{i=1}^{N} \langle \delta^2 E(z^n) w^{n,0}, w^{n,i} \rangle,$$

where, by choosing $r^n \leq L^n/3$, we have ensured that $\mathrm{supp}\{w^{n,i}\}$ for $i = 1, \dots, N$ only overlaps with $\mathrm{supp}\{w^{n,0}\}$, and hence all other 'cross–terms' vanish. For $i = 1, \dots, N$,

$$\begin{aligned} \langle \delta^2 E(z^n) w^{n,i}, w^{n,i} \rangle &= \langle [\delta^2 E(z^n \circ H^{n,i}) - \delta^2 E(\hat{y} + \Pi_R u)] \bar{w}^{n,i}, \bar{w}^{n,i} \rangle + \langle \delta^2 E(\hat{y} + \Pi_R u) \bar{w}^{n,i}, \bar{w}^{n,i} \rangle, \\ &\geq \Big(\lambda_{d,R} - \tfrac{N \|\psi'''\|_\infty}{2L^n/3} \Big) \|D w^{n,i}\|_2^2. \end{aligned} \tag{5.5}$$

For the $i = 0$ term, we have

$$\begin{aligned} \langle \delta^2 E(z^n) w^{n,0}, w^{n,0} \rangle &= \langle [\delta^2 E(z^n) - \delta^2 E(0)] w^{n,0}, w^{n,0} \rangle + \langle \delta^2 E(0) w^{n,0}, w^{n,0} \rangle, \\ &\geq \Big(\psi''(0) - \tfrac{N \|\psi'''\|_\infty}{r^n} \Big) \|D w^{n,0}\|_2^2. \end{aligned} \tag{5.6}$$

For the cross–terms, Since we assumed that $r^n \leq L^n/3$, we deduce that

$$\langle \delta^2 E(z^n) w^{n,0}, w^{n,i} \rangle = \langle \delta^2 E(z^n)(v^n - w^{n,i}), w^{n,i} \rangle.$$

Using the translation invariance of E, and adding and subtracting terms, we therefore write

$$\begin{aligned} \big\langle \delta^2 E(z^n) w^{n,0}, w^{n,i} \big\rangle &= \big\langle \big[\delta^2 E(z^n \circ H^{n,i}) - \delta^2 E(\hat{y} + \Pi_R u) \big] (\bar{v}^{n,i} - \bar{w}^{n,i}), \bar{w}^{n,i} \big\rangle \\ &\quad + \big\langle \delta^2 E(\hat{y} + \Pi_R u)(\bar{v}^{n,i} - \bar{w}^{n,i}), \bar{w}^{n,i} - \bar{w}^i \big\rangle \\ &\quad + \big\langle \delta^2 E(\hat{y} + \Pi_R u)(\bar{v}^{n,i} - \bar{w}^{n,i}), \bar{w}^i \big\rangle, \\ &=: \mathrm{T}_1 + \mathrm{T}_2 + \mathrm{T}_3. \end{aligned}$$

Estimating the first two terms on the right hand side, we obtain:

$$\mathrm{T}_1 \leq \tfrac{N \|\psi'''\|_\infty}{2L^n/3} \Big(\|Dv^{n,i}\|_2 + \|Dw^{n,i}\|_2 \Big) \|Dw^{n,i}\|_2 \leq \tfrac{N \|\psi'''\|_\infty}{L^n/3} \qquad \text{and}$$

$$\mathrm{T}_2 \leq \|\psi''\|_\infty \Big(\|Dv^{n,i}\|_2 + \|Dw^{n,i}\|_2 \Big) \|D\bar{w}^{n,i} - D\bar{w}^i\|_2,$$

both of which converge to 0 as $n \to \infty$. Since $\bar{v}^{n,i} - \bar{w}^{n,i} \rightharpoonup 0$ as $n \to \infty$, it follows that $\mathrm{T}_3 \to 0$ as well, and hence

$$\langle \delta^2 E(z^n) w^{n,0}, w^{n,i} \rangle \to 0 \tag{5.7}$$

as $n \to \infty$ for each i. Putting (5.7) and the result of Lemma 4.2 together with (5.5) and (5.6),

$$\langle \delta^2 E(z^n) v^n, v^n \rangle \geq (\lambda_{d,R} - \epsilon^n) \sum_i \|Dw^{n,i}\|_2^2 + \epsilon^n, \tag{5.8}$$

where $\epsilon^n \to 0$ as $n \to \infty$. All that remains is to verify that

$$\liminf_{n \to \infty} \Big(\sum_i \|Dw^{n,i}\|_2^2 - \|Dv^n\|_2^2 \Big) \geq 0. \tag{5.9}$$

By definition, $\sum_i |Dw_b^{n,i}|^2 \neq |Dv_b^n|^2$ only when $b \in \mathrm{supp}\{Dw^{n,i}\} \cap \mathrm{supp}\{Dw^{n,0}\}$ for some $i = 1, \dots, N$. In such cases,

$$|Dw_b^{n,0}|^2 + |Dw_b^{n,i}|^2 - |Dv_b^n|^2 = -2\, Dw_b^{n,0} Dw_b^{n,i}.$$

Therefore, consider

$$\delta^{n,i} := \sum_{b\in\mathcal{B}} Dw_b^{n,0} Dw_b^{n,i} = \sum_{b\in\mathcal{B}} \big(Dw^{n,0}\circ H^{n,i}\big)_b \big(D\bar{w}_b^{n,i} - D\bar{w}_b^i\big) + \sum_{b\in\mathcal{B}} \big(Dw^{n,0}\circ H^{n,i}\big)_b D\bar{w}_b^i.$$

Since $w^{n,0}\circ H^{n,i} \rightharpoonup 0$ and $\bar{w}^{n,i} \to \bar{w}^i$, it follows that $\delta^{n,i} \to 0$, and thus (5.9) holds. Further,

$$\lambda_n + n^{-1} \geq \langle \delta^2 E(z^n) v^n, v^n\rangle \geq (\lambda_{d,R} - \epsilon^n)\Big(1 - \sum_i \delta^{n,i}\Big) + \epsilon^n,$$

and so for n sufficiently large, it is clear that $\lambda_n \geq 2\lambda_{d,R}/3 \geq \lambda_d/2 > 0$, which contradicts the assumption that $\lambda_n < \lambda_d/2$ for all n. □

5.3. **Conclusion of the proof of Theorem 3.3, Case $\Omega = \Lambda$.**

5.3.1. *Proof of (2).* Lemma 5.1 and Lemma 5.2 now enable us to state that there exist L_0 and R_0 depending only on $N = |\mathcal{D}|$ such that whenever $\mathcal{D}$ satisfies $L_{\mathcal{D}} \geq L_0$, $R \geq R_0$, and z is an approximate solution corresponding to $\mathcal{D}$ with truncation radius R,

$$\lambda_{L,R} \geq \mu := \frac{\lambda_d}{2} > 0, \qquad \text{and} \qquad \|\delta E(z)\| < r := \min\Big\{\frac{c\lambda_d}{4L_{\mathcal{D}}}, \frac{\lambda_d^2}{16\,\|\psi'''\|_\infty}\Big\}.$$

We note that

$$\|\delta^2 E(z+u) - \delta^2 E(z+v)\| \leq \|\psi'''\|_\infty \|Du - Dv\|_2,$$

so setting $M := \|\psi'''\|_\infty$, we may apply Lemma 4.7, since $\frac{2Mr}{\mu^2} \leq \frac{1}{2} < 1$. It follows that there exists $w \in \dot{\mathscr{W}}^{1,2}(\Lambda)$ with $\|Dw\|_2 \leq c' L_{\mathcal{D}}^{-1}$ such that

$$\delta E(z+w) = 0, \qquad \langle \delta^2 E(z+w)v, v\rangle \geq \frac{\lambda_d}{4}\|Dv\|_2^2,$$

and so $z + w$ is a strongly stable equilibrium. The constant c' depends only on N, the number of dislocation cores, establishing item (2) of Theorem 3.3.

5.3.2. *Proof of (1).* We now complete the proof of item (1) of Theorem 3.3 by showing that any $\alpha' \in [Dz + Dw]$ satisfies the other conditions of the statement. We begin by increasing R_0 if necessary to ensure that $\frac{N}{2\pi R_0} \leq \frac{1}{4}$. Suppose that z is a predictor for a configuration $\mathcal{D}$ in Λ satisfying $L_{\mathcal{D}} \geq L_0$ and $R \geq R_0$. If $\alpha \in [Dz]$, by increasing R_0, we have ensured that

$$\alpha_b \in [-\tfrac{1}{4}, \tfrac{1}{4}] \qquad \text{for any } b \notin \bigcup_{(C,s)\in\mathcal{D}} \mathrm{supp}\{D\Pi_R^C u\},$$

and furthermore

$$\alpha_b = \sum_{(C,s)\in\mathcal{D}} s(\hat{\alpha}\circ G^C)_b \qquad \text{for any } b \notin \bigcup_{(C,s)\in\mathcal{D}} \mathrm{supp}\{D\Pi_R^C u\}.$$

Let $\alpha' \in [Dz + Dw]$, and so if $L_{\mathcal{D}} > 4c'$, where c' is the constant arising in the proof of (2), $z + w$ is a strongly stable local equilibrium such that $\|Dw\|_\infty \leq \|Dw\|_2 < \frac{1}{4}$. When $b \notin \mathrm{supp}\{D\Pi_R^C u\}$ for any $(C, s) \in \mathcal{D}$, this choice entails that $\alpha'_b = \alpha_b + Dw_b$.

Taking A to be a collection of positively-oriented cells such that $B_R(0) \subset \mathrm{clos}(A) \subset B_{L_{\mathcal{D}}/2}(0)$ and setting $A^C := H^C(A)$,

$$\int_{\partial A^{C'}} \alpha' = \int_{\partial A^{C'}} \sum_{(C,s)\in\mathcal{D}} s\,(\hat{\alpha}\circ G^C) + Dw = s' \qquad \text{for any } (C', s') \in \mathcal{D}, \qquad \text{and}$$

$$\int_{\partial C} \alpha' = 0 \qquad \text{for any} \quad C \notin \bigcup_{(C,s)\in\mathcal{D}} A^C, \quad \text{implying} \quad \mathcal{C}^\pm[\alpha'] \subset \bigcup_{(C,s)\in\mathcal{D}} H^C(A).$$

5.3.3. *Proof of (3).* We divide the proof of (3) when $\Omega = \Lambda$ into two cases: $B[z+w] = 0$, and $|B[z+w]| > 1$.

Suppose $z+w$ is a strongly stable equilibrium such that $B[z+w] = 0$, arising from statement (2) of Theorem 3.3. It follows that $|\{(C,1) \in \mathcal{D}\}| = |\{(C,-1) \in \mathcal{D}\}|$, so enumerating pairs $(C^i_+, 1), (C^i_-, -1) \in \mathcal{D}$, we define

$$v^i(x) := \tfrac{1}{2\pi}\big[\arg\big(x - x^{C^i_+}\big) - \arg\big(x - x^{C^i_-}\big)\big], \quad \text{and} \quad v(x) := \sum_i v^i(x), \tag{5.10}$$

where v^i is a function with a branch cut of finite length. As for approximate solutions z, we may extend ∇v^i to a function which is $\mathrm{C}^\infty(\mathbb{R}^2 \setminus \{x^{C^i_+}, x^{C^i_-}\}; \mathbb{R}^2)$. It may then be directly verified that $|\nabla v^i(x)| \lesssim |x|^{-2}$ for $|x|$ suitably large, and hence when v^i is understood as a function in $\mathscr{W}(\Lambda)$, it follows that $v^i \in \dot{\mathscr{W}}^{1,2}(\Omega)$.

It may now be checked that $Dz_b - Dv_b \in \mathbb{Z}$ for all $b \in \mathcal{B}$, and hence

$$E(z-v; z+w) = E(0; z+w) = -E(z+w; 0) < 0, \quad \text{as} \quad 0 = \operatorname*{argmin}_{u \in \dot{\mathscr{W}}^{1,2}(\Omega)} E(u; 0)$$

by Lemma 4.2, in contradiction to the assumption that $z+w$ was a globally stable equilibrium.

If $|B[z+w]| > 1$, then without loss of generality, we suppose $B[z+w] > 1$. We will only consider the case where $B[z+w] = 2$ here, leaving the general case for the interested reader. Suppose for contradiction that $z+w$ is a strongly stable equilibrium given by (2) in Theorem 3.3 with $B[z+w] = 2$, and that $z+w$ is additionally globally stable. If true, then any configuration of the form

$$y = \hat{y} + \hat{y} \circ G^C \tag{5.11}$$

must satisfy $E(y; z+w) \geq 0$, since by a similar argument to that used in the previous case, we may define y such that $y - z \in \dot{\mathscr{W}}^{1,2}(\Lambda)$. Our strategy is to construct a sequence y^n of the form (5.11) such that $E(y^{n+1}; y^n) \leq -C < 0$, and hence prove a contradiction. To that end, define a sequence of cells C^n such that x^{C^n} lies on the positive x-axis for all n, with

$$\operatorname{dist}(C^n, C^{n+1}) < \operatorname{dist}(0, C^n), \quad \operatorname{dist}(0, C^0) \geq K \quad \text{and} \quad \operatorname{dist}(C^{n-1}, C^n) \geq K,$$

where K is a parameter we will choose later. Our choice of y^n is then

$$y^n := \hat{y} + \hat{y} \circ G^{C^n}.$$

If K is sufficiently large, we note that $\alpha^n \in [Dy^n]$ is unique. Letting $v^n := y^n - y^{n-1}$, decompose $Dv^n = \beta^n + Z^n_b$, where $\beta^n = \alpha^n_b - \alpha^{n-1}_b$, and $Z^n_b = Dv^n_b - \beta^n_b$ has support only on bonds crossing the x-axis between $x^{C^{n-1}}$ and x^{C^n}.

We consider $E(y^{n-1}; y^n) = -E(y^n; y^{n-1})$: arguing as in Lemma 5.2 of [18],

$$\begin{aligned}
E(y^{n-1}; y^n) &= \sum_{b \in \mathcal{B}} \psi(\alpha^{n-1}_b) - \psi(\alpha^n_b) \\
&= \sum_{b \in \mathcal{B}} \psi(\alpha^n_b - \beta^n_b) - \psi(\alpha^n_b) - \psi'(\alpha^n_b)(-\beta^n_b) + \langle \delta E(y^n), -Dv^n \rangle - \sum_{b \in \mathcal{B}} \psi'(\alpha^n_b)(-Z^n_b), \\
&\geq \tfrac{1}{2}(\psi''(0) - \epsilon)\|\beta^n\|_2^2 - C - \langle \delta E(y^n), Dv^n \rangle + \sum_{b \in \mathcal{B}} \psi'(\alpha^n_b) Z^n_b.
\end{aligned}$$

Employing the result of Lemma 4.3, we find that we may write

$$-\langle \delta E(y^n), Dv^n \rangle + \sum_{b \in \mathcal{B}} \psi'(\alpha^n_b) Z^n_b = \sum_{b \in \mathcal{B}} -g^n_b \beta^n_b + h^n_b Z^n_b \geq -\|g^n\|_2 \|\beta^n\|_2 + \sum_{b \in \mathcal{B}} h^n_b Z^n_b.$$

It may be verified that $\|g^n\|_2$ is uniformly bounded in n, using the properties demonstrated in Lemma 4.3, and that Z^n_b is negative on bonds of the form $(\xi, \xi + a_2)$ or $(\xi, \xi + a_3)$ crossing the x-axis. Since by assumption $\operatorname{dist}(C^{n-1}, C^n) < \operatorname{dist}(0, C^{n-1})$, h^n_b is negative for all bonds in $\operatorname{supp}\{Z^n\}$ — in particular, these assertions imply that

$$\sum_{b \in \mathcal{B}} h^n_b Z^n_b \geq 0, \quad \text{and so} \quad E(y^{n-1}; y^n) \geq c_0 \|\beta^n\|_2^2 - c_1$$

for some constants $c_0, c_1 > 0$ which depend only on ψ. Applying Jensen's inequality to β^n on a series of closed curves around C^n, we find that

$$\|\beta^n\|_2^2 \geq c \log(\mathrm{dist}(C^{n-1}, C^n)) \geq c' \log(K),$$

where c, c' are constants depending only on the lattice, and hence as long as K is suitably large, we have that $E(y^{n-1}; y^n) \geq C \geq 0$. Thus

$$E(y^k; z+w) = \sum_{n=1}^{k} E(y^n; y^{n-1}) + E(y^0; z+w) \leq -Ck + E(y^0; z+w),$$

and letting $k \to \infty$, we have a contradiction to the fact that $z+w$ is a globally stable equilibrium.

6. Proof for Finite Lattice Polygons

As in §5, we construct approximate solutions and prove estimates on the derivative and hessian of the energy evaluated at these points so that we may apply Lemma 4.7. The two main differences between this and the preceding analysis are (i) z defined in 5.1 does *not* satisfy the natural boundary conditions of Laplace's equation in a finite domain, and (ii) we must estimate residual force contributions at the boundary, which cannot be achieved by a simple truncation argument as used in §4.5 — at this stage the fact that Ω has a boundary plays a crucial role.

To obtain a predictor satisfying the natural boundary conditions we introduce a *boundary corrector*, $\bar{y} \in C^1(U^\Omega) \cap C^2(\mathrm{int}(U^\Omega))$, corresponding to a configuration $\mathcal{D}$ in Ω which satisfies

$$-\Delta \bar{y} = 0 \quad \text{in } U^\Omega, \qquad \nabla \bar{y} \cdot \nu = -\sum_{(C,s)\in\mathcal{D}} s\nabla(\hat{y} \circ G^C) \cdot \nu \quad \text{on } \partial U^\Omega, \tag{6.1}$$

where ν is the outward unit normal on ∂U^Ω. §6.1 is devoted to a study of this problem and its solution.

We then define an approximate solution (predictor) corresponding to $\mathcal{D}$ in Ω with truncation radius R as

$$z := \sum_{(C,s)\in\mathcal{D}} s\left(\hat{y} + \Pi_R u\right) \circ G^C + \bar{y}. \tag{6.2}$$

6.1. **Analysis of boundary corrector.**

Here, as remarked above, we give proofs of several important facts about the boundary corrector. Since we are considering a boundary value problem in a polygonal domain, we use the theory developed in [14] to obtain regularity of solutions to (6.1).

Noting that the boundary corrector problem is linear, it suffices to analyse the problem when only one positive dislocation is present at a point $x' \in U^\Omega$. We therefore consider the problem

$$-\Delta \bar{y} = 0 \quad \text{in } U^\Omega, \qquad \nabla \bar{y} \cdot \nu = g_m \quad \text{on } \Gamma_m, \tag{6.3}$$

where as in §2.2, Γ_m are the straight segments of ∂U^Ω between corners (κ_{m-1}, κ_m), ν is the outward unit normal, and

$$g_m(s) := -\nabla \hat{y}(s - x') \cdot \nu \qquad \text{for } s \in \Gamma_m.$$

As before, by $\nabla \hat{y}(x - x')$ we mean the extension of the gradient of $\hat{y}(x - x')$ to a function in $\mathrm{C}^\infty(\mathbb{R}^2 \setminus \{x'\})$. Since ν is constant along Γ_m, it follows that $g_m \in \mathrm{C}^\infty(\Gamma_m)$, and so applying Corollary 4.4.3.8 in [14], it may be seen that this problem has a solution in $\mathrm{H}^2(U^\Omega)$ which is unique up to an additive constant, as long as $\int_{\partial U^\Omega} g = 0$. This condition may be verified by standard contour integration techniques, for example. Furthermore, $\bar{y}$ is harmonic in the interior of U^Ω, and hence analytic on the same set.

We now obtain several bounds for solutions of the problem (6.3) in terms of $\mathrm{dist}(x', \partial U^\Omega)$, taking note of the domain dependence of any constants. The key fact used to construct these estimates is that $\hat{y} + \bar{y}$ is a harmonic conjugate of the Green's function for the Laplacian with Dirichlet boundary conditions on U^Ω.

Lemma 6.1. *Suppose U^Ω is a convex lattice polygon, and $\bar{y}$ solves* (6.3)*. Then there exist constants c_1 and c_2 which are independent of the domain such that*

$$|\nabla\bar{y}(x)| \leq c_1 \operatorname{dist}(x,x')^{-1} \quad \textit{for any } x \in U^\Omega, \qquad \|\nabla\bar{y}\|_\infty \leq c_1 \operatorname{dist}(x',\partial U^\Omega)^{-1}, \tag{6.4}$$

$$\textit{and} \quad \|\nabla^2\bar{y}\|_{\mathrm{L}^2(U^\Omega)} \leq c_3 \frac{\log(\operatorname{dist}(x',\partial U^\Omega))}{\operatorname{dist}(x',\partial U^\Omega)}. \tag{6.5}$$

Proof. We begin by noting that $\hat{y}(x-x') = \frac{1}{2\pi}\arg(x-x')$ is a harmonic conjugate of $\frac{1}{2\pi}\log(|x-x'|)$, and we will further demonstrate that $\bar{y}$ is a harmonic conjugate of Ψ, the solution of the Dirichlet boundary value problem

$$-\Delta\Psi(x) = 0 \quad \text{in } U^\Omega, \qquad \Psi(s) = -\tfrac{1}{2\pi}\log(|x-x'|) \quad \text{on } \partial U^\Omega.$$

By virtue of Corollary 4.4.3.8 in [14], there exists a unique $\Psi \in \mathrm{H}^2(U^\Omega)$ solving this problem, and since Ψ is harmonic in U^Ω, a simply connected region, a harmonic conjugate Ψ^* exists. By definition, Ψ^* satisfies the Cauchy–Riemann equations

$$\nabla\Psi^*(x) = \mathsf{R}_4^T\nabla\Psi(x) \quad \text{for all } x \in U^\Omega, \tag{6.6}$$

where R_4 is the matrix corresponding a positive rotation through $\frac{\pi}{2}$ about the origin. In particular,

$$\frac{\partial\Psi^*}{\partial\nu} = \frac{\partial\Psi}{\partial\tau} = \frac{(x-x')}{2\pi|x-x'|^2}\cdot\mathsf{R}_4\nu = -\nabla\hat{y}(x-x')\cdot\nu \quad \text{on } \partial U^\Omega, \quad \text{and} \quad -\Delta\Psi^* = 0 \text{ in } U^\Omega,$$

where τ is the unit tangent vector to ∂U^Ω with the positive orientation. By uniqueness of solutions for (6.3), it follows that $\Psi^* = \bar{y}$ up to an additive constant, and hence $\bar{y}$ is a harmonic conjugate of Ψ. Furthermore, by differentiating (6.6),

$$\|\nabla^2\Psi\|_{\mathrm{L}^2(U^\Omega)} = \|\nabla^2\bar{y}\|_{\mathrm{L}^2(\Omega)}. \tag{6.7}$$

The identities (6.6) and (6.7) will allow us to use estimates on the derivatives of Ψ to directly deduce (6.4) and (6.5).

To prove (6.4), we rely upon Proposition 1 in [9], which states that there exists a constant c_1 depending only on $\operatorname{diam}(U^\Omega)$ such that

$$|\nabla\Psi(x)| \leq c_1 \operatorname{dist}(x',x)^{-1}.$$

However, as $U^\Omega \subset \mathbb{R}^2$, it is straightforward to see by a change of variables and a scaling argument that the constant c_1 cannot depend on $\operatorname{diam}(U^\Omega)$, and is therefore independent of the domain (as long as it remains convex). Taking the Euclidean norm of both sides in (6.6) now implies the pointwise bound in (6.4), and the L^∞ bound follows immediately as the partial derivatives of $\bar{y}$ satisfy the strong maximum principle.

To prove (6.5), we use the classical *a priori* bounds for the Poisson problem. In order to do so, we must introduce an auxiliary problem with homogeneous boundary conditions. We therefore seek a solution to

$$-\Delta(\Psi-\Phi) = \Delta\Phi \quad \text{in } U^\Omega, \qquad \Psi-\Phi \in \mathrm{H}^2(U^\Omega)\cap\mathrm{H}^1_0(U^\Omega),$$

where the function $\Phi : \mathbb{R}^2 \to \mathbb{R}$ is defined to be

$$\Phi(x) := -\tfrac{1}{2\pi}\phi\big(|x-x'|/\operatorname{dist}(x',\partial U^\Omega)\big)\log(|x-x'|),$$

$$\text{where} \quad \phi \in \mathrm{C}^\infty([0,+\infty)) \quad \text{and} \quad \phi(r) = \begin{cases} 0 & r \in [0,\frac{1}{4}], \\ 1 & r \geq 1. \end{cases}$$

By construction $\Phi \in \mathrm{C}^\infty(U^\Omega)$, and $\nabla^2\Phi \in \mathrm{L}^2(\mathbb{R}^2)$. Thus $\Delta\Phi \in \mathrm{L}^2(U^\Omega)$, and the existence of a unique solution $\Psi-\Phi \in \mathrm{H}^2(U^\Omega)\cap\mathrm{H}^1_0(U^\Omega)$ follows from [14, Theorem 3.2.1.2]). Furthermore, inspecting the proof of [14, Theorem 4.3.1.4], we see that

$$\|\nabla^2(\Psi-\Phi)\|_{\mathrm{L}^2(U^\Omega)} = \|\Delta\Phi\|_{\mathrm{L}^2(U^\Omega)} \leq \|\nabla^2\Phi\|_{\mathrm{L}^2(\mathbb{R}^2)},$$

and thus a straightforward integral estimate yields

$$\|\nabla^2\Psi\|_{\mathrm{L}^2(U^\Omega)} \leq \|\nabla^2(\Psi-\Phi)\|_{\mathrm{L}^2(U^\Omega)} + \|\nabla^2\Phi\|_{\mathrm{L}^2(\mathbb{R}^2)} \leq c_2\frac{\log\big(\mathrm{dist}(x',\partial U^\Omega)\big)}{\mathrm{dist}(x',\partial U^\Omega)},$$

where c_2 is independent of the domain. □

6.2. **Analysis of the predictor.** Here, we prove that the predictor defined in (6.2) is indeed an approximate equilibrium. Our first step is to formulate the analogue of Lemma 4.3 in the polygonal case.

Lemma 6.2 (Finite domain stress lemma). *Let Ω be a convex lattice polygon, $\mathcal{D}$ a dislocation configuration in Ω and $z := \sum_{(C,s)\in\mathcal{D}}\hat{y}\circ G^C + \bar{y}$, where $\bar{y}$ solves* (6.1)*. Then there exist L_0 and S_0 which depend only on $N = |\mathcal{D}|$ such that whenever $L_{\mathcal{D}} \geq L_0$ and $S_{\mathcal{D}} \geq S_0$, there exist $g : \mathcal{B}^\Omega \to \mathbb{R}$ and $\Sigma : \{b \in \partial W^\Omega\} \to \mathbb{R}$ such that*

$$\langle \delta E^\Omega(z), v\rangle = \sum_{b\in\mathcal{B}^\Omega} g_b Dv_b + \sum_{b\in\partial W^\Omega}\Sigma_b Dv_b,$$

and furthermore

$$|g_b| \leq c_1 \sum_{(C,s)\in\mathcal{D}}\big(1+\mathrm{dist}(b,C)\big)^{-3} + c_1\|\nabla^2\bar{y}\|_{\mathrm{L}^2(\omega_b)} \qquad \textit{for all}\quad b\notin\partial W^\Omega, \tag{6.8}$$

$$\textit{and}\quad |g_b+\Sigma_b| \leq c_2 \sum_{(C,s)\in\mathcal{D}}\big(1+\mathrm{dist}(P_\zeta,C)\big)^{-1} + c_1\|\nabla^2\bar{y}\|_{\mathrm{L}^2(\omega_b)} \qquad \textit{for all}\quad b\in P_\zeta\subset\partial W^\Omega. \tag{6.9}$$

The constant c_1 is independent of the domain, and c_2 depends linearly on $\mathrm{index}(\partial W^\Omega)$.

Proof. We begin by choosing L_0 and S_0 to ensure that $\alpha \in [Dz]$ is unique: since the constant in (6.4) is independent of the domain, and $D\hat{y}$ has a fixed rate of decay, this choice depends only on N as stated. Furthermore, we have the representation $\alpha_{(\xi,\xi+a_i)} = \int_0^1 \nabla z(\xi+ta_i)\cdot a_i\,\mathrm{d}t$, where ∇z is to be understood as the extension of the gradient of z to a function in $\mathrm{C}^\infty(U^\Omega\setminus\bigcup_{(C,s)\in\mathcal{D}}\{x^C\})$.

Let $\omega_b := \bigcup\{C\in\mathcal{C}^\Omega \mid \pm b\in\partial C, C \text{ positively oriented}\}$, the union of any cells which b lies in the boundary of. For $b\notin\partial W^\Omega$, ω_b is always a pair of cells, and we set $V := |\omega_b|$ for any $b\notin\partial W^\Omega$.

Let $\bar{C}_\epsilon := \bigcup_{(C,s)\in\mathcal{D}} B_\epsilon(x^C)$. If $b = (\xi,\xi+a_i)$, define

$$h_b := \frac{\psi''(0)}{V}\lim_{\epsilon\to 0}\int_{\omega_b\setminus\bar{C}_\epsilon}\nabla z\cdot a_i\,\mathrm{d}x \qquad\text{and}\qquad g_b := \psi'(\alpha_b) - h_b.$$

As in the proof of Lemma 4.3, an application of the divergence theorem demonstrates that the former (and hence the latter) definition makes sense. Let $v\in\mathscr{W}(\Omega)$, and denote its piecewise linear interpolant Iv; applying the divergence theorem once more,

$$\sum_{b\in\mathcal{B}^\Omega} h_b Dv_b = \lim_{\epsilon\to0}\frac{\psi''(0)}{V}\int_{W^\Omega\setminus\bar{C}_\epsilon}\nabla z\cdot\nabla Iv\,\mathrm{d}x = \frac{\psi''(0)}{V}\int_{\partial W^\Omega} Iv\,\nabla z\cdot\nu\,\mathrm{d}s.$$

Recalling the definition of P_ζ from (2.3), we find that

$$\sum_{b\in\mathcal{B}^\Omega} h_b Dv_b = \sum_{\zeta\in\partial W^\Omega\cap\partial U^\Omega}\frac{\psi''(0)}{V}\int_{P_\zeta} Iv\,\nabla z\cdot\nu\,\mathrm{d}s.$$

By considering the integral over a single period, we may integrate by parts

$$\int_{P_\zeta} Iv\,\nabla z\cdot\nu\,\mathrm{d}s = Iv(\zeta+\tau)\int_{P_\zeta}\nabla z\cdot\nu\,\mathrm{d}s - \int_{P_\zeta} Iv'\bigg(\int_{\gamma_\zeta^s}\nabla z\cdot\nu\,\mathrm{d}t\bigg)\,\mathrm{d}s,$$

where γ_ζ^s is the arc–length parametrisation of the Lipschitz curve following P_ζ between ζ and s, τ is the relevant lattice tangent vector, and Iv' is the derivative along the curve following P_ζ. Applying the divergence theorem to the region bounded by P_ζ and ∂U^Ω (as seen on the right of Figure 2.2.1) and using the boundary conditions $\nabla z \cdot \nu = 0$ on ∂U^Ω, it follows that $\int_{P_\zeta} \nabla z \cdot \nu = 0$. Splitting the domain of integration P_ζ into individual bonds and noting that $\nabla I v$ is constant along each bond,

$$\int_{P_\zeta} Iv\, \nabla z \cdot \nu \,\mathrm{d}s = -\sum_{b\in P_\zeta} \int_{b=(\xi,\xi+a_i)} \nabla I v \cdot a_i \Big(\int_{\gamma^s_\zeta} \nabla z \cdot \nu \,\mathrm{d}t \Big) \,\mathrm{d}s,$$

$$= \sum_{b\in P_\zeta} \Sigma_b D v_b, \quad \text{where} \quad \Sigma_b := -\int_b \int_{\gamma^x_\zeta} \nabla z \cdot \nu \,\mathrm{d}t \,\mathrm{d}s.$$

This concludes the proof of the first part of the statement.

To obtain (6.8), we Taylor expand the potential to obtain

$$g_b = \psi''(0) \Big(\int_b \nabla z \cdot a_i \,\mathrm{d}x - \lim_{\epsilon\to 0} \frac{1}{V} \int_{\omega_b \setminus \bar{C}_\epsilon} \nabla z \cdot a_i \,\mathrm{d}x \Big) + O\big(|Dz_b|^3\big).$$

Since $\nabla z = \sum_{(C,s)\in\mathcal{D}} \nabla \hat{y} \circ G^C + \nabla \bar{y}$, the only change to the analysis carried out in the proof of Lemma 4.3 is to estimate the terms involving $\nabla\bar{y}$. As $\int_b \nabla \bar{y} \cdot a_i \,\mathrm{d}x = \frac{1}{|\omega_b|} \int_{\omega_b} \nabla I \bar{y} \cdot a_i \,\mathrm{d}x$, applying Jensen's inequality and standard interpolation error estimates (see for example §4.4 of [5]) gives

$$\int_b \nabla \bar{y} \cdot a_i \,\mathrm{d}x - \frac{1}{V} \int_{\omega_b} \nabla \bar{y} \cdot a_i \,\mathrm{d}x = \frac{1}{V} \int_{\omega_b} \big(\nabla I \bar{y} - \nabla \bar{y} \big) \cdot a_i \,\mathrm{d}x \le \frac{1}{\sqrt{V}} \big\| \nabla I \bar{y} - \nabla \bar{y} \big\|_{\mathrm{L}^2(\omega_b)} \le c \big\| \nabla^2 \bar{y} \big\|_{\mathrm{L}^2(\omega_b)}$$

where $c > 0$ is a fixed constant. Applying Young's inequality and (6.4) to estimate $|Dz_b|^3$ now leads immediately to (6.8).

Estimate (6.9) follows in a similar way: Taylor expanding g_b, but noting that $|\omega_b| = V/2$ and ω_b is no longer symmetric, the same argument used above gives

$$|g_b + \Sigma_b| \le \int_b \Big| \tfrac{1}{2} \nabla z \cdot a_i - \int_{\gamma^s_\zeta} \nabla z \cdot \nu \,\mathrm{d}t \Big| \,\mathrm{d}s + c \|\nabla^2 \bar{y}\|_{\mathrm{L}^2(\omega_b)} + \sum_{(C,s)\in\mathcal{D}} \big\| \nabla^2 \hat{y} \circ G^C \big\|_{\mathrm{L}^\infty(\omega_b)} + O(|Dz_b|^3).$$

Applying (6.4) to the first and last terms and and using the decay of $\nabla\hat{y}$ now yields

$$|g_b + \Sigma_b| \le c\big(1 + |P_\zeta|\big) \sum_{(C,s)\in\mathcal{D}} \big(1 + \mathrm{dist}(P_\zeta, C)\big)^{-1} + c \|\nabla^2 \bar{y}\|_{\mathrm{L}^2(\omega_b)}.$$

Upon recalling the definition of $\mathrm{index}(\partial W^\Omega)$ from (2.4), the proof is complete. □

We can now deduce a residual estimate for the predictor in the finite domain case.

Lemma 6.3. *Suppose Ω is a convex lattice polygon, and z is the approximate solution corresponding to a dislocation configuration $\mathcal{D}$ in Ω defined in* (6.2) *with truncation radius $R = \min\big\{L_\mathcal{D}/5, S_\mathcal{D}^{1/2}\big\}$. Then there exist constants L_0, S_0 and c depending only on $N = |\mathcal{D}|$ and* $\mathrm{index}(\partial W^\Omega)$ *such that whenever $L_\mathcal{D} \ge L_0$ and $S_\mathcal{D} \ge S_0$,*

$$\big\| \delta E^\Omega(z) \big\|_{(\dot{\mathscr{W}}^{1,2}(\Omega))^*} \le c\Big(L_\mathcal{D}^{-1} + S_\mathcal{D}^{-1/2} \Big).$$

Proof. We begin by enumerating the elements $(C^i, s^i) \in \mathcal{D}$, and set $G^i := G^{C^i}$. For $i = 1, \dots, N$, we let $\hat{y}^i = \hat{y} \circ G^i$, let $y^i = (\hat{y} + \Pi_R u) \circ G^i$, and let $\bar{y}^i$ be the corrector solving (6.3) with $x' = x^{C^i}$.

Define $r := 2(R+1) = 2\big(\min\big\{L_\mathcal{D}/5, S_\mathcal{D}^{1/2}\big\} + 1\big)$. Taking a test function $v \in \dot{\mathscr{W}}^{1,2}(\Omega)$, let

$$v^i(\xi) := \Pi_r^{C^i} v(\xi) \qquad \text{and} \qquad v^0(\xi) := v(\xi) - \sum_i v^i(\xi).$$

Lemma 4.5 implies there is a universal constant independent of Ω such that $\|Dv^i\|_2 \le C\|Dv\|_2$ for any $i = 0, \dots, N$. Adding and subtracting terms, we write

$$\begin{aligned}\langle \delta E^\Omega(z), v\rangle &= \langle \delta E^\Omega(z), v^0\rangle + \sum_i \big\langle \big[\delta E^\Omega(z) - \delta E^\Lambda(y^i)\big], v^i\big\rangle \\ &\qquad + \sum_i \big\langle \big[\delta E^\Lambda(y^i) - \delta E^\Lambda\big(\hat y^i + u\circ G^i\big)\big], v^i\big\rangle, \\ &=: \mathrm{T}_1 + \mathrm{T}_2 + \mathrm{T}_3. \end{aligned} \tag{6.10}$$

We estimate each of these terms in turn.

The term T_1*:* Applying Lemma 6.2 and the fact that $z = \sum_{i=1}^N \hat y^i + \bar y^i$ in $\mathrm{supp}(v^0)$, we make a similar estimate to that in Lemma 5.1:

$$\begin{aligned}\big|\mathrm{T}_1\big| &= \Bigg|\sum_{b\in\mathcal{B}^\Omega} g_b Dv^0_b + \sum_{b\in\partial W^\Omega}\Sigma_b Dv^0_b\Bigg| \\ &\le c_1\Bigg(\Bigg(\sum_{\substack{(C,s)\in\mathcal{D},\, b\in\mathcal{B}^\Omega\\ \mathrm{dist}(b,C)\ge r/2-1}} \big(1+\mathrm{dist}(b,C)\big)^{-6}\Bigg)^{1/2} + \|\nabla^2\bar y\|_{\mathrm{L}^2(W^\Omega)}\Bigg)\|Dv^0\|_2 \\ &\qquad + c_2\Bigg(\sum_{\zeta\in\partial W^\Omega\cap\partial U^\Omega}\big(1+\mathrm{dist}(P_\zeta, C^i)\big)^{-2}\Bigg)^{1/2}\|Dv^0\|_2, \\ &\le c\Big(r^{-2} + S_{\mathcal{D}}^{-1}\log(S_{\mathcal{D}}) + \mathrm{index}\big(\partial W^\Omega\big)^{1/2} S_{\mathcal{D}}^{-1/2}\Big)\|Dv^0\|_2. \end{aligned} \tag{6.11}$$

To arrive at the final line we have used (6.5), and the constant c here is independent of the domain and the index.

The term T_2*:* For the second set of terms, we have $z - y^i = \sum_{j\ne i}\hat y^j + \sum_j \bar y^j$ in the support of v^i. We expand as in Lemma 5.1 to obtain

$$\begin{aligned}\big\langle \delta E^\Omega(z) - \delta E\big(y^i\big), v^i\big\rangle &= \sum_{b\in\mathcal{B}^\Omega}\psi''(s_b)\Bigg(\sum_{j\ne i} D\hat y^j_b + \sum_{j=0}^N D\bar y^j_b\Bigg)Dv^i_b, \\ &= \psi''(0)\sum_{b\in\mathcal{B}^\Omega}\Bigg(\sum_{j\ne i} D\hat y^j_b + D\bar y^j_b\Bigg)Dv^i_b + \psi''(0)\sum_{b\in\mathcal{B}^\Omega} D\bar y^i_b Dv^i_b + \sum_{b\in\mathcal{B}^\Omega} h_b Dv^i_b, \end{aligned} \tag{6.12}$$

where $|s_b| \lesssim \sum_{j\ne i}(1+\mathrm{dist}(b, C^j))^{-1} + S_{\mathcal{D}}^{-1}$ and a Taylor expansion yields

$$|h_b| = \Bigg|\big(\psi''(s_b) - \psi''(0)\big)\Bigg(\sum_{j\ne i} D\hat y^j_b + \sum_{j=0}^N D\bar y^j_b\Bigg)\Bigg| \lesssim |s_b|^2\, r^{-1}.$$

Applying Lemma 6.2 to the first term in (6.12), a similar argument to that used to arrive at (6.11) gives

$$\sum_{b\in\mathcal{B}^\Omega}\Bigg(\sum_{j\ne i} D\hat y^j_b + D\bar y^j_b\Bigg)Dv^i_b \le c\Big(r^{-2} + S_{\mathcal{D}}^{-1}\log(S_{\mathcal{D}})\Big)\|Dv^i\|_2.$$

Applying the global form of (6.4) to the second term in (6.12),

$$\sum_{b\in\mathcal{B}^\Omega} D\bar y^i_b Dv^i_b \le c_1\, r S_{\mathcal{D}}^{-1}\|Dv^i\|_2,$$

and finally,

$$\sum_{b\in\mathcal{B}^\Omega} h_b Dv^i_b \le r^{-1}\Bigg(\Bigg(\sum_{\substack{b\in\mathcal{B}^\Omega,\,(C,s)\in\mathcal{D}\\ \mathrm{dist}(b,C)\ge r-1}}\big(1+\mathrm{dist}(b,C)\big)^{-4}\Bigg)^{1/2} + rS_{\mathcal{D}}^{-2}\Bigg)\|Dv^i\|_2 \le c\Big(r^{-2} + S_{\mathcal{D}}^{-2}\Big)\|Dv^i\|_2.$$

Combining these estimates gives

$$\langle \delta E^{\Omega}(z) - \delta E(y^i), v^i\rangle \leq c\big(r^{-2} + S_{\mathcal{D}}^{-1}\log(S_{\mathcal{D}}) + rS_{\mathcal{D}}^{-1}\big)\|Dv^i\|_2. \tag{6.13}$$

The term T_3*:* The final group may be once more estimated using the truncation result of Lemma 4.5, giving

$$\big|\big\langle \delta E(y^i) - \delta E(\hat{y}^i + u\circ G^i), v^i\big\rangle\big| \lesssim R^{-1}\|Dv^i\|_2. \tag{6.14}$$

Conclusion: Inserting the estimates (6.11), (6.13) and (6.14) into (6.10), and using the fact that $\|Dv^i\|_2 \lesssim \|Dv\|_2$, we obtain the bound

$$\big|\langle \delta E^{\Omega}(z), v\rangle\big| \lesssim \Big(L_{\mathcal{D}}^{-1} + S_{\mathcal{D}}^{-1/2}\Big)\|Dv\|_2. \qquad \square$$

6.3. **Stability of the predictor.** Next we prove the stability of the predictor configuration defined in (6.2).

Lemma 6.4. *Given I_0 and $N \in \mathbb{N}$, there exist $R_0 = R_0(N)$, $L_0 = L_0(N)$ and $S_0 = S_0(N, I_0)$ such that whenever z is the approximate solution corresponding to a dislocation configuration $\mathcal{D}$ in a convex lattice polygon Ω with truncation radius R given in* (6.2)*, and furthermore:*

1. $\mathrm{index}(\partial W^{\Omega}) \leq I_0$*,*
2. $S_{\mathcal{D}} \geq S_0$*,* $L_{\mathcal{D}} \geq L_0$ *and* $R \geq R_0$*,*

then there exists $\lambda \geq \lambda_d/2$ such that

$$\langle \delta^2 E^{\Omega}(z)v, v\rangle \geq \lambda\|Dv\|_2^2 \qquad \text{for all} \quad v \in \dot{\mathscr{W}}^{1,2}(\Omega).$$

Proof. Fixing I_0 and N, we choose R_0 and L_0 such that the conclusion of Lemma 5.2 holds for any dislocation configuration $\mathcal{D}$ in Λ with $|\mathcal{D}| = N$. Throughout the proof, we fix R to be any number with $R \geq R_0$, and we will consider only configurations such that $L_{\mathcal{D}} \geq L_0$.

Suppose for contradiction that there exists a sequence of domains Ω^n with accompanying dislocation configurations $\mathcal{D}^n$ which together satisfy

1. $\mathrm{index}(\partial W^{\Omega^n}) = I_0$,
2. $N := |\mathcal{D}^n|$, $|\{(C,+1)\in\mathcal{D}^n\}|$ and $|\{(C,-1)\in\mathcal{D}^n\}|$ are constant,
3. $(C_0,+1)\in\mathcal{D}^n$,
4. $S^n := S_{\mathcal{D}^n} \to \infty$ as $n\to\infty$ and
5. $\delta^2 E^{\Omega^n}(z^n) < \lambda_d/2$ for all n, where
$$z^n := \sum_{(C,s)\in\mathcal{D}^n} s(\hat{y} + \Pi_R u)\circ G^C + \bar{y}^n,$$
and $\bar{y}^n$ solves (6.1) with $\Omega = \Omega^n$.

We note that condition (3) may be assumed without loss of generality by applying lattice symmetries. Condition (5) implies that there exists $v^n \in \dot{\mathscr{W}}^{1,2}(\Omega^n)$ such that $\|Dv^n\|_2 = 1$ and

$$\lambda^n := \inf_{\substack{v\in\dot{\mathscr{W}}^{1,2}(\Omega^n)\\ \|Dv\|_2 = 1}} \langle \delta^2 E^{\Omega^n}(z^n)v, v\rangle = \langle \delta^2 E^{\Omega^n}(z^n)v^n, v^n\rangle < \lambda_d/2,$$

since this is a minimisation problem for a continuous function over a compact set.

For each n, enumerate $(C^{n,i}, s^{n,i}) \in \mathcal{D}^n$, and let $G^{n,i} := G^{C^{n,i}}$ and $H^{n,i} := H^{C^{n,i}}$. Considering Dv^n as an element of $\ell^2(\mathcal{B})$ by extending

$$Dv_b^n := \begin{cases} Dv_b^n & b\in\mathcal{B}^{\Omega}, \\ 0 & b\in\mathcal{B}\setminus\mathcal{B}^{\Omega}, \end{cases}$$

there exists a subsequence such that $Dv^n\circ H^{n,i}$ is weakly convergent for each i. For given i and j, $\mathrm{dist}(C^{n,i}, C^{n,j})$ either remains bounded or tends to infinity, and so define an equivalence relation $i\sim j$ if and only if $\mathrm{dist}(C^{n,i}, C^{n,j})$ is uniformly bounded as $n\to\infty$.

By possibly taking further subsequences, we may assume that if $i \sim j$ then $Q^{ji} := G^{n,j} \circ H^{n,i}$ is constant along the sequence, and hence if $Dv^n \circ H^{n,i} \rightharpoonup D\bar{v}^i$ for each i,

$$D\bar{v}^j \circ Q^{ji} = D\bar{v}^i \qquad \text{when} \quad i \sim j.$$

For each equivalence class, $[i]$, define

$$y^{n,[i]} := \sum_{j\in[i]} s^j(\hat{y} + \Pi_R u) \circ G^{n,j}.$$

Using the result of [7, Lemma 4.9], there exists a sequence $r^n \to \infty$ which we may also assume satisfies

$$r^n \leq \min_{i\nsim j} \big\{\mathrm{dist}(C^{n,i}, C^{n,j})\big\}/5 \quad \text{and} \quad r^n \leq S^n/5,$$

so that, defining $w^{n,[i]} := \Pi_{r^n}^{C^{n,i}} v^n$,

$$w^{n,[i]} \circ H^{n,i} \to \bar{w}^{[i]} \text{ in } \dot{\mathscr{W}}^{1,2}(\Lambda) \qquad \text{and} \qquad (Dv^n - Dw^{n,[i]}) \circ H^{n,i} \rightharpoonup 0 \text{ in } \ell^2(\mathcal{B}),$$

where i is a fixed representative of $[i]$. Further defining $Dw^{n,0} := Dv^n - \sum_{[i]} Dw^{n,[i]}$, we have

$$\langle \delta^2 E^{\Omega^n}(z^n)v^n, v^n\rangle = \langle \delta^2 E^{\Omega^n}(z^n)w^{n,0}, w^{n,0}\rangle + \sum_{[i]} \Big(2\langle \delta^2 E^{\Omega^n}(z^n)w^{n,[i]}, w^{n,0}\rangle + \langle \delta^2 E^{\Omega^n}(z^n)w^{n,[i]}, w^{n,[i]}\rangle\Big).$$

The definition of r^n and (6.4) imply that $\|\nabla \bar{y}^n\|_{\mathrm{L}^\infty(U^{\Omega^n})} \leq c_1/r^n$, where c_1 is independent of n, so in a similar fashion to the proof of Lemma 5.2, we obtain:

$$\begin{aligned}
\big\langle \delta^2 E^{\Omega^n}(z^n)w^{n,0}, w^{n,0}\big\rangle &= \big\langle [\delta^2 E^{\Omega^n}(z^n) - \delta^2 E^{\Omega^n}(0)]w^{n,0}, w^{n,0}\big\rangle + \big\langle \delta^2 E^{\Omega^n}(0)w^{n,0}, w^{n,0}\big\rangle \\
&\geq \big(\psi''(0) - c/r^n\big)\big\|Dw^{n,0}\big\|_2^2, \\
\big\langle \delta^2 E^{\Omega^n}(z^n)w^{n,[i]}, w^{n,[i]}\big\rangle &= \big\langle [\delta^2 E^{\Omega^n}(z^n) - \delta^2 E^{\Lambda}(y^{n,[i]})]w^{n,[i]}, w^{n,[i]}\big\rangle + \big\langle \delta^2 E^{\Lambda}(y^{n,[i]})w^{n,[i]}, w^{n,[i]}\big\rangle, \\
&\geq \big(\lambda_{L,R} - c/r^n\big)\big\|Dw^{n,[i]}\big\|_2^2, \qquad \text{and} \\
\big\langle \delta^2 E^{\Omega^n}(z^n)w^{n,0}, w^{n,[i]}\big\rangle &\to 0 \qquad \text{as} \quad n \to \infty,
\end{aligned}$$

where c represents a constant independent of n. Furthermore, the arguments of the proof of Lemma 5.2 imply that

$$\liminf_{n\to\infty} \Big(\sum_i \|Dw^{n,[i]}\|_2^2 - \|Dv^n\|_2^2\Big) \geq 0,$$

and so we deduce that

$$\lambda_n = \big\langle \delta^2 E^{\Omega^n}(z^n)v^n, v^n\big\rangle \geq \lambda_d/2 > 0$$

for n sufficiently large, providing the required contradiction. □

6.4. **Conclusion of the proof of Theorem 3.3, Convex Lattice Polygon Case.** To conclude the proof of conclusions (1) and (2) of Theorem 3.3, we may apply small modifications of the arguments used in §5.3.2 and §5.3.2, and hence we omit these.

To prove conclusion (3), recall the result of Lemma 4.2, which states that $y \equiv 0$ is a globally stable equilibrium in any lattice domain. When Ω is a convex lattice polygon, $\mathscr{W}(\Omega) \subset \dot{\mathscr{W}}^{1,2}(\Omega)$, so if $z+w$ is the local equilibrium for E^Ω constructed in (1), then $-z-w \in \dot{\mathscr{W}}^{1,2}(\Omega)$, and furthermore

$$E(z+w-z-w; z+w) = E(0; z+w) = -E(z+w; 0) < 0, \qquad \text{as} \qquad 0 = \operatorname*{argmin}_{u\in\dot{\mathscr{W}}^{1,2}(\Omega)} E(u; 0).$$

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