

Stability and Regularity of Defects in Crystalline Solids



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Abstract

This thesis is devoted to the mathematical analysis of models describing the energy of defects in crystalline solids via variational methods.

The first part of this work studies a discrete model describing the energy of a point defect in a one-dimensional chain of atoms. We derive an expansion of the ground state energy using Γ -convergence, following previous work on similar models [BDMG99, BC07, SSZ11]. The main novelty here is an explicit characterisation of the first-order limit as the solution of a variational problem in an infinite lattice. Analysing this variational problem, we prove a regularity result for the perturbation caused by the defect, and demonstrate the order of the next term in the expansion.

The second main topic is a discrete model describing screw dislocations in body-centred cubic crystals. We formulate an anti-plane lattice model which describes the energy difference between deformations and, using the framework defined in [AO05], provide a kinematic description of the Burgers vector, which is a key geometric quantity used to describe dislocations. Apart from the anti-plane restriction, this model is invariant under all the natural symmetries of the lattice and in particular allows for the creation and annihilation of dislocations. The energy difference formulation enables us to provide a clear definition of what it means to be a stable deformation.

The main results of the analysis of this model are then first, a proof that deformations with unit net Burgers vector exist as globally stable states in an infinite body, and second, that deformations containing multiple screw dislocations exist as locally stable states in both infinite bodies and finite convex bodies. To prove the former result, we establish coercivity with respect to the elastic strain, and exploit a concentration compactness principle. In the latter case, we use a form of the inverse function theorem, proving careful estimates on the residual and stability of an ansatz which combines continuum linear elasticity theory with an atomistic core correction.

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Chapter 1

Introduction

Crystalline solids are found everywhere in nature, and are characterised by the fact that the atoms which constitute them lie close to the points of a lattice. In mathematical terms, these are structures with an underlying translation symmetry group; furthermore, most of those observed in nature have further rotational and reflective symmetries beyond the simple translational ones. This high level of symmetry means that the study of crystals has been bound up with mathematics since the beginnings of modern science in the 17th century [Kep11, Hoo65].

In 1934, it was hypothesised that microscopic defects which break crystal symmetries might play a role in determining the macroscopic properties of such materials [Oro34, Pol34, Tay34]. Since this initial hypothesis, and its subsequent experimental verification in the 1950s [Bol56, HHW56], crystalline defects have been the subject of intense theoretical and experimental study.

This thesis sets out a contribution to the existing body of work on crystalline defects in the form of rigorous mathematical results for models formulated to study two particular classes of these objects: point defects and dislocations. In this introductory chapter, we begin in §1.1 by providing a brief overview of the currently accepted physical understanding of this subject, and in §1.2, we give a description of recent mathematical results on models of crystalline defects. We then outline the main results of the subsequent chapters in §1.3.

1.1 A taxonomy of defects

With the developments in electron microscopy which occurred in the 1950s [HHN⁺65], it became possible to directly observe and hence classify crystalline defects found in nature for the first time. Although they violate the translation symmetry of the full crystal, different types of defect nevertheless have their own structure, and may be

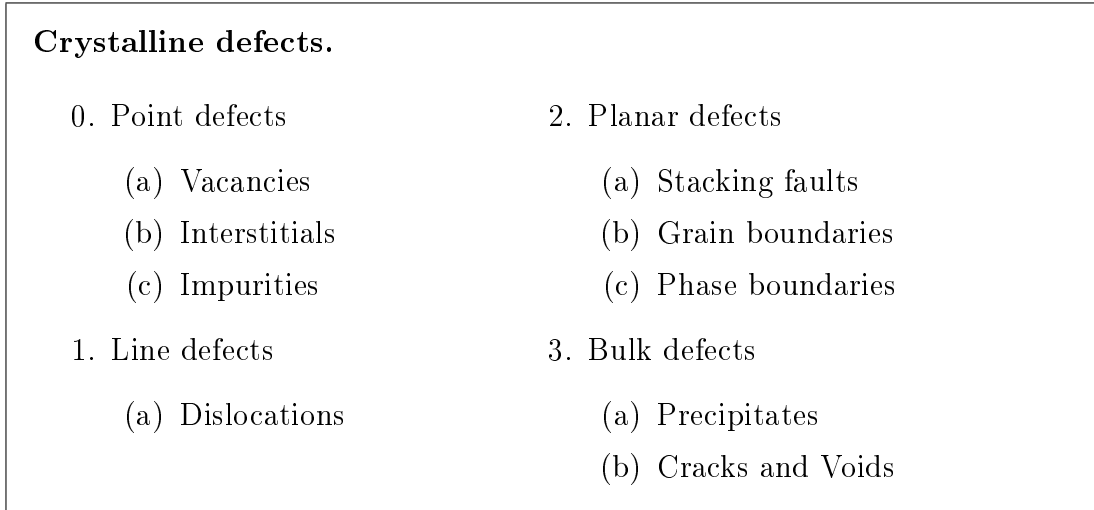


Figure 1.1: A taxonomy of crystalline defects.

broadly classified according to the ‘dimension’ of the defect within the bulk crystal, as detailed in Figure 1.1.

Since the precise classes of defects which will concern us here are impurities and dislocations, we provide a physical description of only these two here, but a fuller introduction to the physical properties of many of the classes of defects outlined in Figure 1.1 may be found in [HB11] or [AM76]. For simplicity, the descriptions provided are in the context of monatomic crystals, as this is the setting for our study here; such defects are of course also found within more complicated crystal structures.

1.1.1 Impurities

An *impurity* is an atom of a species which does not form part of the main structure of the crystal. These are most often elements such as hydrogen which have atoms that are physically smaller than those making up the rest of the crystal. Their smaller size allows them to pass between the larger atoms, and so diffuse throughout the structure. Impurities are further subclassified into *substitutional* and *interstitial* impurities. The former term describes an impurity which replaces an atom of the pure species within the structure, while the latter describes the case where the impurity sits at a point in the structure between atoms of the pure species. Examples of each of these types of point defect are shown on the left of Figure 1.2.

Impurities are the basis for such phenomena as hydrogen and helium embrittlement, which is a major cause of failure in many metallic components exposed to

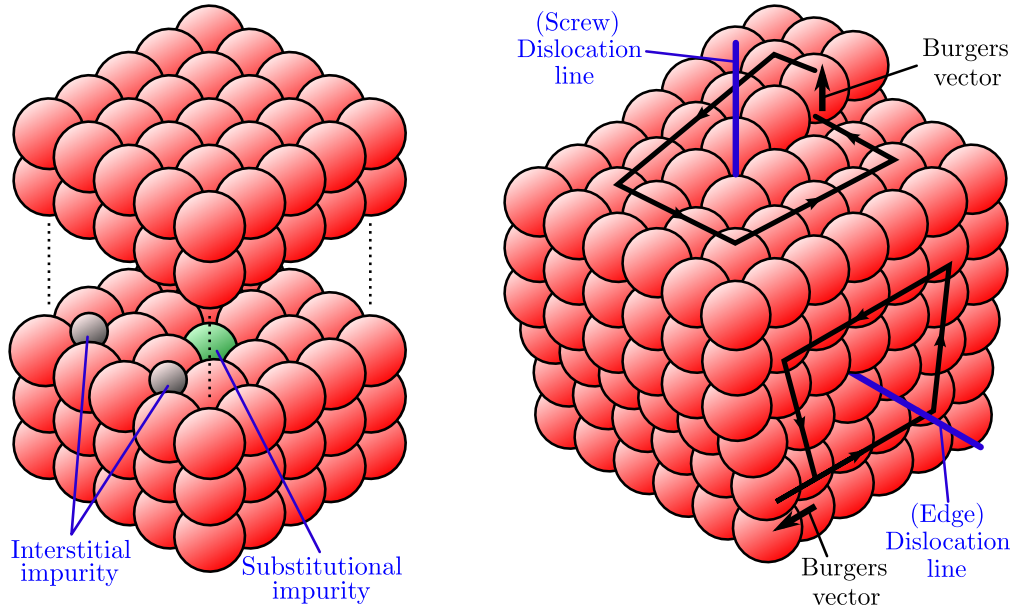


Figure 1.2: Examples of point defects and dislocations.

sources of these elements [WK00]: in particular, this is a key engineering problem for components in fusion reactors which has yet to be fully solved [GDNM⁺13].

1.1.2 Screw dislocations

In contrast to impurities, which require the introduction of other species of atom into a crystal, *dislocations* are geometric defects in the lattice structure itself. The simplest forms of dislocation are visualised via a ‘Volterra cut’, named for the class of elastic deformations studied in [Vol07]. In this procedure, the crystal is cut along a half plane, manipulated, and ‘glued up’ along the half plane once more. In the case of screw dislocations which are the particular kind of dislocation studied here, the crystal is sheared parallel to the edge of the half plane, so that lattice planes are twisted into a structure similar to a vortex; see the right hand side of Figure 1.2 for a visualisation in a simple cubic crystal. An edge dislocation, also shown in this figure, is formed by the addition of a half plane of atoms along the cut surface.

The key properties pertaining to dislocations are their *line direction* and *Burgers vector*. The dislocation line is a curve in the crystal where the distortion is most concentrated, and the line direction is then tangent to this curve. The Burgers vector describes the mismatch between lattice planes which occurs near this distortion, and is defined to be the vector difference between the beginning and end of a loop passing from atom to atom around the dislocation line which would otherwise be closed in a perfect crystal. Of necessity, Burgers vectors are therefore always lattice vectors,

and it is generally most energetically convenient for Burgers vectors to be among the shortest possible lattice vectors. Examples of such loops and the resulting Burgers vectors are shown on the right-hand side of Figure 1.2.

The Burgers vector is the key intrinsic property of a dislocation, as it is conserved along the dislocation line although the line itself may change direction and split. Dislocations may annihilate when two with opposite Burgers vector meet, so the Burgers vector may be thought of as being analogous to an electrostatic charge. For further details regarding Burgers vector conservation and a more explicit description of the Volterra cut procedure, see [HL82] and [HB11].

Probably the most important feature of dislocations is that when they are dilute within a crystal, their movement allows the material to plastically deform at much lower strains than would be expected for pure crystals. However, as strains increase, the network of dislocations may tangle up and cause the material to become stiffer, since dislocations moving on different planes may impede the motion of each other. This process is known as ‘work hardening’ (see §10.3 of [HB11]), and although it has been observed on the macroscopic scale in metalworking for thousands of years, its microscopic cause was only attributed to the movement of dislocations through the material within the last 80 years. Efforts to find an accurate and computationally-efficient predictive model which replicates this behaviour are ongoing [RLBF03, BC06].

1.2 Recent mathematical results

As remarked at the beginning of this chapter, the hypothesis that microscopic defects in crystals are responsible for macroscopic plastic behaviour was originally posed by theorists, and so the study of crystalline defects has produced a variety of mathematical models since its inception. Several of these models are now viewed as ‘classical’, chief among them being the Frenkel–Kontorova [FK38] and Peierls–Nabarro [Pei40, Nab47] models for dislocations.

In the last 20 years, there has been renewed interest in models of crystalline defects within the mathematical community: the majority of recent developments in the area have resulted from studying the energy of static defects via variational methods. A strand of work on defect dynamics has also developed, although there are significant further challenges to be met in this area. Below, we summarise some of the most important recent developments, with our main focus as before on work concerning dislocations and point defects, since these are the principal subjects of the ensuing study.

At the outset we note that in all cases, the models described here treat situations in which the dimensions have been reduced, due to the high technical barrier to performing analysis in the fully three-dimensional case. When reducing dimensions in this way, it may be seen that defects are generally best grouped by their codimension: as an example, a surface is two-dimensional in $\mathbb{R}^3$, and after dimension reduction, it is zero-dimensional in $\mathbb{R}^1$; however, the codimension in both cases is one.

1.2.1 Defect dynamics

The rigorous mathematical study of the dynamics of defects is currently only just beginning. Since obtaining accurate predictive models will allow better design of nanoscale components, it is an area of significant scientific interest for the future, and any results in this area should contribute to the ongoing debate over how best to model plasticity at this scale.

Monneau and collaborators have published a series of works concerning dislocation dynamics at various scales. In [AHLBM06] and [BCLM08], an eikonal equation describing the motion of dislocation loops in a plane is formulated, and short-time existence and uniqueness of solutions is proved. [CEHMR10] studies a transport equation describing the motion of edge dislocations whose line directions are all perpendicular to a given plane. In both cases, the equations studied govern ρ , a number density of dislocations in the material, and the dynamics considered are overdamped, i.e. where inertial effects are small.

In [EHIM09], [FIM12] and [MP12], it is demonstrated that classical models of dislocation motion (the Frenkel–Kontorova model, Peierls–Nabarro model and continuum plasticity) are linked via homogenisation limit processes.

As well as this series of papers on dislocation dynamics, the motion of grain and twin boundaries are studied in [GN00], [AV03] and [KNCV04], for example. Work has also been carried out on models of epitaxial growth (the deposition of atoms on an exterior surface of a crystal) in [Xia02] and [DMFL14], and a review of several models of this phenomenon currently under study is given in [Caf06].

1.2.2 Semidiscrete models of static defects

Motivated by the classification of defects according to their dimension, one particular approach to the modelling of defects is to treat them as singular subsets of an elastic continuum; such models are sometimes termed ‘semidiscrete’, particularly when the singular sets are explicitly tracked by the model.

In the case of dislocations, the original semidiscrete models employ the ‘core radius approach’, in which the strain field induced by a dislocation is regularised by removing the singularity concentrated on the dislocation line, along with a cylinder of material of radius ϵ around it. This procedure renders the elastic energy of the dislocation finite but dependent on the ‘core radius’ ϵ . In each of [CL05], [SZ12], [GLP10] and [DLGP12], the authors prove rigorous asymptotic limits for the energy of collections of dislocations in the parameter ϵ , assuming different forms of the elastic energy in the bulk, and the latter article additionally treats scalings in which the number of dislocations tends to infinity as ϵ tends to zero.

In [GM05], [GM06] and [CGM11], the authors study the energy asymptotics of a phase-field model for dislocations proposed in [KCO02]. Here, dislocations are described via a number density ρ , and move in a plane where there are ‘pinning sites’ of some given small radius which obstruct their motion and are intended to simulate dislocations lying parallel to another set of planes in the crystal. The papers study different energy scaling regimes, deriving asymptotics for the energy in the limit where the radius of the pinning sites tends to zero while the number of such sites increases.

[VCO07], [VCOA07], [VCMO09], [HCO10] and [GPPS13] all study the asymptotic behaviour for models of dislocation pile-ups, a term used to describe the situation where a number of dislocations become trapped behind an impermeable barrier. The first four articles contain detailed asymptotic analyses of the dislocation density induced by such pile-ups as the number of dislocations increases. The final paper deals with walls of dislocations, demonstrating a variety of scaling regimes for the energy which depend critically on the ‘aspect ratio’ between the spacing of dislocations vertically in the walls and the horizontal spacing between the walls.

Regarding models accounting for planar defects in solids, we remark that there is a huge literature on phase transitions in solids, where models have been devised in which phase boundaries appear naturally as singular sets of minimisers in variational problems: see [Bha03] and [Mül99] for wide-ranging overviews of results in this area.

1.2.3 Atomistic models of static defects

Since the results of later chapters specifically concern atomistic models of static defects, this section presents a more detailed survey of results concerning this particular class of models.

1.2.3.1 Energy asymptotics for codimension 1 defects

Beginning with [BDMG99], a series of works by Braides and collaborators have been devoted to obtaining energy asymptotics for discrete systems via the use of Γ -convergence: in particular, we note surface energies in two-dimensional discrete systems are treated in this way in [ABC06] and [BP13]. We also note the results of [The11], in which an asymptotic expansion for the ground state of a mass-spring lattice confined to some domain in $\mathbb{R}^2$ is obtained, and a clear characterisation of the surface energy contribution is given.

Here, we particularly highlight the Γ -convergence results of [BC07] and [SSZ11] concerning one-dimensional models, since the results contained in Chapter 2 are similar in flavour. In the first paper, the authors prove the following statement; in it, n corresponds to the number of atoms considered, and l corresponds to the length of the deformed configuration.

Theorem ([BC07]). *Consider the set of admissible deformations*

$$\mathcal{A}_n^l := \left\{ y : [0, 1] \rightarrow \mathbb{R} \mid y(0) = 0, y(1) = l, y \text{ affine on } \left(\frac{i}{n}, \frac{i+1}{n}\right), i = 0, \dots, n-1 \right\},$$

and define $H_n^l : \mathcal{A}_n^l \rightarrow \mathbb{R} \cup \{+\infty\}$ to be a second nearest neighbour energy

$$H_n^l(u) := \frac{1}{n} \sum_{i=0}^{n-1} J_1 \left(\frac{u\left(\frac{i+1}{n}\right) - u\left(\frac{i}{n}\right)}{1/n} \right) + \frac{1}{n} \sum_{i=0}^{n-2} J_2 \left(\frac{u\left(\frac{i+2}{n}\right) - u\left(\frac{i}{n}\right)}{2/n} \right),$$

where J_1 and J_2 satisfy certain structural hypotheses. Then H_n^l may be asymptotically expanded in terms of Γ -convergence as

$$H_n^l(u) \stackrel{\Gamma}{=} H_0^l(u) + \frac{1}{n} H_1^l(u) + o\left(\frac{1}{n}\right),$$

where $H_0^l(u)$ is an integral functional representing a continuum elastic energy, and $H_1^l(u)$ is a boundary layer energy which represents a modification to the energy arising due to fracture and boundary points.

A similar result is proved in [SSZ11], but with the additional constraint on $\mathcal{A}_n^l$ that $u\left(\frac{1}{n}\right)$ and $u\left(\frac{n-1}{n}\right)$ are also prescribed. We remark that a definition of the notion of an asymptotic expansion in terms of Γ -convergence will be given in §2.3. The interpretation of the two results is that the mean energy per atom at the ground state is approximately computed via H_0^l , i.e. continuum elasticity, with a smaller perturbation computed through H_1^l which arises due to relaxation close to the boundary of a bulk piece of crystal.

1.2.3.2 Discrete models of dislocation configurations

In [AO05], the authors describe a mathematically consistent framework for defining the Burgers vectors of dislocations in atomistic settings using the language of algebraic topology. This framework forms an important basis for the analysis in [Pon07] and [ADGP13], as well as the work contained in Chapters 3–5 of this thesis.

Theorem 3.4 of [Pon07] provides the first discrete-to-continuum limit for an atomistic model describing the energy of dislocation configurations. Building upon this work, Theorems 3.1 and 4.2 in [ADGP13] provide two terms in an asymptotic expansion via Γ -convergence for the energy of screw dislocations in an atomistic model. These results may be summarised as saying that F_ϵ , the energy functional considered, behaves like

$$F_\epsilon(u) \simeq \frac{\log(1/\epsilon)}{2\pi} |\mu(u)|(\Omega) + \gamma |\mu(u)|(\Omega) + \mathbb{W}(\mu(u)) + o(1), \quad (1.1)$$

as $\epsilon \rightarrow 0$. Here, $\mu(u)$ is a sum of signed Dirac masses which corresponds to the Burgers vector of the deformation u , $|\mu|(\Omega)$ is the total variation of the measure μ on Ω , and $\mathbb{W}(\mu)$ is the renormalised energy of μ from the theory of Ginzburg–Landau vortices.

The first term in (1.1) corresponds to the elastic energy stored in creating the dislocations represented by $\mu(u)$ in the perfect crystal. This blows up as ϵ tends to zero, since the number of atoms between the dislocation and the boundary is approximately ϵ^{-1} , and so larger and larger numbers of bonds must be broken to introduce the same dislocations. It should be noted that the discreteness of the model removes the problem of the core singularity discussed in §1.2.2, so this energy comes only from the long range strain field due to the dislocations. The second and third terms respectively represent a core energy arising due to the discreteness of the lattice, and the energy of interaction between dislocations and the boundary.

In addition to the Γ -convergence result described above, [ADGP13] also contains a detailed study of dislocation dynamics which is based upon a minimising movement for the energy F_ϵ : this may be thought of as analogous to a time-stepped gradient flow of the energy. As part of Theorem 5.5, the main result of this analysis, the authors prove that given some choice of dislocation positions relative to Ω , and a small enough lattice spacing, there exist local minimisers of the discrete energy which contain dislocations close to the chosen positions.

1.2.3.3 Other directions

[EOS13] and [OS13] analyse the Quasicontinuum Method, a numerical method first proposed in [OPT96] to accurately calculate the properties of crystalline defects. The particular interest of these articles is that they appear to be the first to develop an error analysis for the method applied to defects which induce long-range stress fields. Such situations require special treatment to obtain good convergence and accuracy.

We remark finally that although in what follows we deal exclusively with models which ignore the electronic structure of solids, recent work concerning charged defects in crystals, for example [CDL08] and [CE11], uses an energy difference viewpoint similar to that taken in Chapter 3.

1.3 Outline of the main results

We now provide a brief overview of the results contained in the ensuing chapters.

1.3.1 Energy of a point defect in a 1D chain of atoms

In Chapter 2 we consider a model for the energy of a one-dimensional chain of atoms containing a point defect, similar to those described in §1.2.3.1. We assume that the atoms are interacting via pair potentials, and that the interactions decay sufficiently rapidly that we need to consider only interactions of nearest and next-nearest neighbours. In order to restrict attention to the energetic contribution of the point defect alone, rather than those arising due to surface relaxation effects, we assume that the chain is periodic and that the potentials grow sufficiently rapidly to prevent fracture of the chain. Assuming the chain is undergoing an externally induced dead load, f , the mean energy per atom is then

$$\mathcal{F}^\epsilon(y) = \epsilon \sum_{i=-N}^{N-1} \left(\phi_1(D_1 y_i) + \phi_2(D_2 y_i) + f_i y_i \right) + \epsilon E_d(y),$$

where $D_j y_i = \frac{y_{i+j} - y_i}{j\epsilon}$ is the relative displacement between atoms, the potentials ϕ_1 and ϕ_2 govern the interaction of nearest and next-nearest neighbours respectively, and adding E_d replaces the potentials governing the interactions between atoms of the pure species with those governing the interactions between pure and defect species. Considering ϵ as a small parameter, the main result of this chapter is Theorem 2.3.3, which states that the asymptotic expansion of the energy in terms of Γ -convergence is

$$\mathcal{F}^\epsilon(y) \stackrel{\Gamma}{=} \mathcal{F}_0(y) + \epsilon \mathcal{F}_1(y) + O(\epsilon^2),$$

where $\mathcal{F}_0(y)$ is the continuum energy associated with the pure chain of atoms and $\mathcal{F}_1(y)$ is given in terms of a minimisation problem for an infinite chain of atoms. The key advance in this result as compared to those of [BC07] and [SSZ11] is the identification of the first-order limit with an explicit variational problem. This enables us to prove Lemma 2.6.8, which states that the perturbation to the elastic field introduced by the defect decays exponentially away from the defect, and then Lemma 2.7.1, which demonstrates the next term must be at worst $O(\epsilon^2)$ and, in the particular case where $f = 0$ and the defect does not introduce a local volume change, the next term is $O(\lambda^{2/\epsilon})$ for some $\lambda \in (0, 1)$.

1.3.2 Screw dislocations as globally stable equilibria

In Chapter 3, we introduce an anti-plane lattice model for screw dislocations which bears similarities to those analysed in the articles outlined in §1.2.3.2, but rather than study the asymptotics of the ground state energy, we study equilibria containing dislocations directly. We define the energy difference functional

$$E(y; \tilde{y}) = \sum_{b \in \mathcal{B}} \psi(Dy_b) - \psi(D\tilde{y}_b), \quad (1.2)$$

where $\mathcal{B}$ denotes a set of pairs of interacting columns of atoms in an infinite crystal, Dy_b denotes a finite difference, and ψ is one-periodic potential governing the interaction between columns. Specifically, this functional models the energy of a body-centered-cubic crystal undergoing anti-plane shear parallel to the $[111]$ direction. We call a deformation y a globally stable equilibrium in this model if

$$E(y + u; y) \geq 0 \quad \text{for any deformation } u \text{ with } \|Du\|_{\ell^2(\mathcal{B})} < +\infty.$$

Here, the $\ell^2(\mathcal{B})$ norm arises since, as we show in Chapter 3, it is the weakest norm with respect to which the function $u \mapsto E(y + u; y)$ is continuous, and hence the space of functions for which $Du \in \ell^2(\mathcal{B})$ is the largest space over which this function may be continuously extended.

The main result of Chapter 4 is then Theorem 4.1.1, which states that there exist globally stable equilibria with net Burgers vector $\pm \frac{1}{2}[111]$. To prove this result we use variational techniques, exploiting the symmetries of the model to obtain an *a priori* bound on the elastic strain. This then allows us to use concentration compactness to demonstrate that minimisers exist, and have the desired net Burgers vector.

1.3.3 Screw dislocations as locally stable equilibria

Chapter 5 continues the analysis of the energy difference functional defined in (1.2), but the context is broadened to include finite convex crystals as well as infinite crystals. We call a deformation y a locally stable equilibrium of the energy if there exists $\epsilon > 0$ such that

$$E^\Omega(y + u; y) \geq 0 \quad \text{for any deformation } u \text{ with } \|Du\|_{\ell^2(\mathcal{B}^\Omega)} < \epsilon.$$

Here, E^Ω is the energy defined to include only the contributions from bonds in $\mathcal{B}^\Omega$, which is the set of bonds in the finite or infinite crystal and, as explained in §1.3.2, the $\ell^2(\mathcal{B}^\Omega)$ norm arises as the natural energy norm for this problem.

The main result of Chapter 5 is Theorem 5.1.1, which states that, under a stability assumption on an equilibrium containing a single dislocation in the full lattice, configurations containing multiple dislocations exist as locally stable equilibria, as long as the dislocations are suitably far apart and, in the case of a finite convex crystal, are sufficiently far from the boundary. To carry out this proof, we use a quantitative form of the Inverse Function Theorem, and obtain a qualitatively sharp asymptotic description of these equilibria in terms of the linear elasticity predictor and the dislocation core corrector in the full lattice. Apart from this explicit asymptotic description of the equilibria, the main achievement of this result is a demonstration that the minimal separation distances sufficient to guarantee existence are uniform in the geometry of the boundary.

1.3.4 Other sources for these results

The vast majority of results contained in this thesis are also available in the following articles.

- T. Hudson. Gamma-expansion for a 1D Confined Lennard-Jones model with point defect. *Networks & Heterogeneous Media*, 8(2), 2013.
- T. Hudson and C. Ortner. Existence and stability of a screw dislocation under anti-plane deformation. *Arch. Ration. Mech. Anal.*, April 2014. Available online.
- T. Hudson and C. Ortner. Analysis of stable screw dislocation configurations in an anti-plane lattice model. *ArXiv e-prints*, March 2014.

Chapter 2

Asymptotics for the ground state energy of a chain of atoms containing a point defect

2.1 Outline

We begin our analysis of crystalline defects by presenting a rigorous asymptotic expansion describing the ground state of a point defect in a one-dimensional chain of atoms. In §2.2, we describe the model analysed here in detail, and carry out a formal asymptotic analysis in order to motivate the assumptions used in the subsequent rigorous results. §2.3 then briefly introduces Γ -convergence, the analytical tool we use to prove these results, and defines the topology in which the results are proven. §2.4 is devoted to proving the Γ -convergence result for the first term in the expansion, after which §2.5 presents some results deriving properties of this term. These properties are used in §2.6 to develop a proof of the Γ -convergence result for the second term in the expansion, and §2.7 then studies the order of subsequent terms in the expansion.

The results proved in this chapter form the basis of [Hud13].

2.2 Modelling a point defect in a one-dimensional chain of atoms

2.2.1 Physical model

For now, fix $N \in \mathbb{N}$ and consider $2N$ atoms indexed by

$$i \in \{-N, \dots, N-1\},$$

which have a spatial density of $2N/L$ where L is the total length of the deformed configuration. As remarked in §1.3, we choose to avoid boundary effects by making the domain periodic. We therefore identify an atom indexed by $i = N$ with the atom $i = -N$, and by defining $\epsilon = 1/2N$, we choose to take reference positions for these atoms to be

$$x_i := i\epsilon \in \Omega_\epsilon := \left\{ -\frac{1}{2}, -\frac{1}{2} + \epsilon, \dots, \frac{1}{2} \right\}.$$

Let $\Omega := [-\frac{1}{2}, \frac{1}{2}]$, so that $\Omega_\epsilon = \Omega \cap \epsilon\mathbb{Z}$. It should be noted at the outset that the choice to use $2N$ atoms appears to be a restriction; in fact, the results obtained below hold when this assumption is lifted, but making this choice avoids certain notational issues which would otherwise obscure the exposition here. Furthermore, we note here that throughout this chapter, we will frequently write $\epsilon \rightarrow 0$ to mean $N \rightarrow \infty$.

Fixing the coordinate system in the deformed configuration so that atom $-N$ lies at 0, any configuration can be described by a map

$$y : \Omega_\epsilon \rightarrow [0, L] \quad \text{such that} \quad y(-\tfrac{1}{2}) = 0, y(\tfrac{1}{2}) = L.$$

We will use the shorthand $y_i := y(x_i)$, and extend y to a map on the whole of $\epsilon\mathbb{Z}$ by periodicity in the relative displacement, i.e. by defining

$$y_{2Nk+i+1} - y_{2Nk+i} := y_{i+1} - y_i \quad \text{for any } k \in \mathbb{Z} \quad \text{and} \quad i \in \{-N, \dots, N-1\}.$$

The atoms in the chain are assumed to interact through pair potentials which decay rapidly so that it suffices to consider only the interactions between atoms and their 2 immediate neighbours on either side. We assume that all atoms per period except one are of the same type, the former being regarded as the ‘pure’ species. As in [BDMG99], the potential energy of a bond between atoms is assumed to be expressed as a function of the relative displacement

$$D_j y_i := \frac{y_{i+j} - y_i}{x_{i+j} - x_i} = \frac{y_{i+j} - y_i}{j\epsilon}. \quad (2.1)$$

This scaling corresponds to a situation in which the distance between atoms in the deformed configuration is small compared with the macroscopic lengthscale, and where a reference configuration has been chosen such that the distance between atoms in the reference and deformed configurations are of the same order; this is a natural physical setting when the material is behaving elastically.

In the case where all atoms are of the pure species, a bond connecting nearest neighbours with relative length s has energy $\phi_1(s)$, and the energy of a bond connecting second neighbours with relative length s has energy $\phi_2(s)$. The internal energy

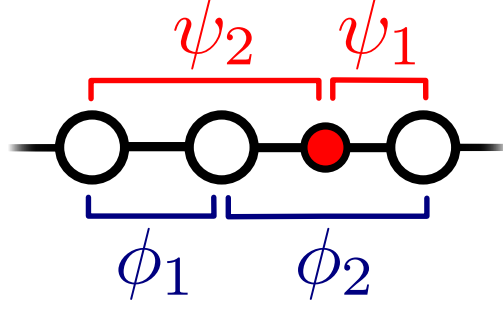


Figure 2.1: Pair potentials for 1D chain: here the impurity is shown in red, and the pure atoms in white.

of the configuration arising from the interatomic forces when all atoms are pure is therefore

$$E_p^\epsilon(y) := \sum_{i=-N}^{N-1} \phi_1(D_1 y_i) + \phi_2(D_2 y_i).$$

By reindexing, it is always possible to ensure that the impurity has index $i = 0$, and we will assume this throughout the chapter. The energy of bonds of relative length s between the impurity and its neighbours is $\psi_1(s)$ for the nearest neighbours and $\psi_2(s)$ for second neighbours (see Figure 2.1). The presence of the defect therefore causes a modification of the internal energy which is included by adding

$$\begin{aligned} E_d(y) := & \psi_2(D_2 y_{-2}) - \phi_2(D_2 y_{-2}) + \psi_1(D_1 y_{-1}) - \phi_1(D_1 y_{-1}) \\ & + \psi_1(D_1 y_0) - \phi_1(D_1 y_0) + \psi_2(D_2 y_0) - \phi_2(D_2 y_0) \end{aligned}$$

to $E_p^\epsilon(y)$. Finally, we also consider dead loads f_i acting on each atom. Assuming that atoms initially lie at the equilibrium positions for the pure internal energy, $L(x_i + \frac{1}{2})$, the work done by these forces is

$$E_f^\epsilon(y) := \sum_{i=-N}^{N-1} f_i(y_i - L(x_i + \frac{1}{2})).$$

This energetic contribution may be thought of as the work done by the linearisation of some external force field near the homogeneous linear state $y_i = L(x_i + \frac{1}{2})$. To keep notation concise, we will frequently write u_i to mean the displacement away from the homogeneous linear state, i.e.

$$u_i := y_i - L(x_i + \frac{1}{2}),$$

and we extend f by periodicity to a map over $\epsilon\mathbb{Z}$ by defining

$$f_{2kN+i} = f_i \quad \text{for any } k \in \mathbb{Z}.$$

Adding together the internal energy and the work done by the imposed external force field, the total energy for the atomistic system is therefore

$$E^\epsilon(y) := E_p^\epsilon(y) + E_d(y) + E_f^\epsilon(y). \quad (2.2)$$

2.2.2 Formal analysis

At low temperatures, we expect that atoms in the system should approximately minimise the energy E^ϵ . We therefore seek to characterise the minimal energy and the states which attain this minimum. We will consider the situation when N is large and the material is behaving elastically. In this case, interatomic displacements should vary slowly over the domain, and so we assume, for the purposes of this formal analysis only, that the Cauchy–Born hypothesis holds (for more information, see [Zan96]). This states that interatomic displacements follow linear deformations of small volumes of the solid, and so we assume that

$$D_1 y_i, D_2 y_i \simeq Dy(x_i),$$

where $y : \Omega \rightarrow [0, L]$ is some suitably smooth function describing the displacement, and so approximately,

$$\phi_1(D_1 y_i) + \phi_2(D_2 y_i) \simeq \phi_1(Dy(x_i)) + \phi_2(Dy(x_i)).$$

This motivates the definition of W , the continuum elastic energy density,

$$W(s) := \phi_1(s) + \phi_2(s). \quad (2.3)$$

The total energy is approximately

$$E^\epsilon(y) \simeq \sum_{i=-N}^{N-1} W(Dy(x_i)) + E_d(y) + E_f^\epsilon(y).$$

Since the energy is given in terms of a sum of potentials which grows linearly in the number of atoms, one would expect that the the ground state energy also grows linearly in the number of atoms, and so it makes sense to look at the mean energy per atom, ϵE^ϵ , as N becomes large. Since the impurity is of fixed small size relative to the total number of atoms, one would also expect that $\epsilon E_d(y)$ vanishes as $\epsilon \rightarrow 0$, and hence

$$\epsilon E^\epsilon(y) \simeq \epsilon \sum_{i=-N}^{N-1} W(Dy(x_i)) + f_i u_i \simeq \mathcal{F}_0(y) := \int_{\Omega} W(Dy) + f u \, dx,$$

where $u(x) = y(x) - L(x + \frac{1}{2})$. Assuming that minimisers of $\mathcal{F}_0$ satisfy the Euler–Lagrange equation for this functional,

$$\frac{d}{dx}(W'(Dy)) = f,$$

this equation may be integrated once to give

$$W'(Dy) = \sigma + \Sigma, \quad \text{where} \quad \sigma(x) = \int_{-1/2}^x f(t) dt. \quad (2.4)$$

The defect should then contribute a further term proportional to its size, $O(\epsilon)$, to the mean energy per atom. Physically, we expect that any perturbation to the minimiser caused by the impurity would also occur close to the defect, induced by internal stresses arising due to the mismatch between ϕ_i and ψ_i near the defect. Earlier, the impurity was chosen to be indexed by $i = 0$, so when N is large, we make the ansatz that close to the defect $D_1 y_i \simeq F_0 + r_i$, where $F_0 := Dy(0)$, and r_i is a small perturbation. Defining

$$\sigma_{-N}^\epsilon := -\frac{1}{2}\epsilon f_{-N} \quad \text{and} \quad \sigma_i^\epsilon := \sigma_{i-1}^\epsilon + \epsilon f_{i-1},$$

then summing by parts, the work done by external forces may be rewritten as

$$\sum_{i=-N}^{N-1} f_i u_i = - \sum_{i=-N}^{N-1} \sigma_i^\epsilon D_1 u_i \quad \text{and} \quad \int_{\Omega} f u \, dx = - \int_{\Omega} \sigma \, Du \, dx.$$

We remark that the definition of σ_{-N}^ϵ given here has been chosen for technical reasons that will become clear during the course of §2.6.1; summing by parts at this point does not require any particular choice.

The additional energy arising due to the defect is then approximately

$$E^\epsilon(y) - \epsilon^{-1} \mathcal{F}_0(y) \simeq \tilde{E}_\infty(r),$$

where $\tilde{E}_\infty$ is defined to be

$$\begin{aligned} \tilde{E}_\infty(r) &:= \tilde{E}_d(r) + \sum_{i=-\infty}^{\infty} \left(\phi_1(F_0 + r_i) + \phi_2\left(F_0 + \frac{r_i + r_{i+1}}{2}\right) - W(F_0) + \sigma(0) r_i \right), \\ \tilde{E}_d(r) &:= \psi_2\left(F_0 + \frac{r_{-2} + r_{-1}}{2}\right) - \phi_2\left(F_0 + \frac{r_{-2} + r_{-1}}{2}\right) + \psi_1(F_0 + r_{-1}) - \phi_1(F_0 + r_{-1}) \\ &\quad + \phi_1(F_0 + r_0) - \psi_1(F_0 + r_0) + \psi_2\left(F_0 + \frac{r_0 + r_1}{2}\right) - \phi_2\left(F_0 + \frac{r_0 + r_1}{2}\right). \end{aligned}$$

Applying the Euler–Lagrange equation (2.4) for $\mathcal{F}_0$ to evaluate $\sigma(0)$ gives

$$\tilde{E}_\infty(r) \simeq \tilde{E}_d(r) + \sum_{i=-\infty}^{\infty} \phi_1(F_0 + r_i) + \phi_2\left(F_0 + \frac{r_i + r_{i+1}}{2}\right) - W(F_0) - (W'(F_0) - \Sigma) r_i,$$

and the periodic boundary conditions imply that $\sum_i r_i = 0$. Since we expect decaying solutions, assigning the ‘core’ of the defect an energy $C(r)$, and Taylor expanding the potentials outside some radius R , gives

$$\tilde{E}_\infty(r) \simeq C(r) + \frac{1}{2} \sum_{|i| \geq R} \phi_1''(F_0) r_i^2 + \phi_2''(F_0) \left(\frac{r_i + r_{i+1}}{2} \right)^2.$$

To minimise this energy, r_i should approximately satisfy

$$\frac{1}{2} \phi_2''(F_0) (r_{i-1} + r_i) + \phi_1''(F_0) r_i + \frac{1}{2} \phi_2''(F_0) (r_i + r_{i+1}) = 0.$$

Making the usual ansatz for such equations, $r_i = a\lambda^i$, a solution of this form requires that

$$\frac{1}{2} \phi_2''(F_0) + W''(F_0) \lambda + \frac{1}{2} \phi_2''(F_0) \lambda^2 = 0.$$

If ϕ_1 and W are convex and ϕ_2 is concave at F_0 , as might be expected in the case of Lennard-Jones pair potentials, then a straightforward analysis of the roots of this equation implies that there are two positive real roots which multiply to give 1. These two roots correspond to an exponentially decaying solution and an exponentially growing solution: the latter may be excluded on physical grounds.

These formal results motivate the assumptions made on the potentials and external force which are detailed in §2.2.3: the rest of this chapter is then devoted to proving rigorous versions of these results using Γ -convergence.

2.2.3 Confined Lennard-Jones model

We will assume that all potentials ϕ_i and ψ_i are C^2 on the interval $(0, \infty)$. Additionally, we suppose the potentials and external forces satisfy the following conditions, which we term the ‘Confined Lennard-Jones model’.

The Confined Lennard-Jones model.

1. The nearest neighbour potentials are infinite for negative bond lengths, and blow up as bond lengths approach zero, i.e.

$$\begin{aligned} \phi_1(s), \psi_1(s) &= +\infty \quad \text{for } s \leq 0, \\ \lim_{s \rightarrow 0+} \phi_1(s) &= +\infty \quad \text{and} \quad \lim_{s \rightarrow 0+} \psi_1(s) = +\infty. \end{aligned}$$

2. The nearest neighbour potentials are l -convex with $l > 0$, i.e. for any $s > 0$,

$$\phi_1''(s), \psi_1''(s) \geq l > 0.$$

3. The second neighbour potentials ϕ_2 and ψ_2 are concave.
4. The second neighbour potentials ϕ_2 and ψ_2 are ‘dominated’ by the nearest neighbour potentials ϕ_1 and ψ_1 , i.e. there exist constants $\alpha \in (0, 1)$ and $C \in \mathbb{R}$ such that for any $s > 0$,

$$\begin{aligned} \phi_2(s) &\geq -\alpha \phi_1(s) + C, & \phi_2(s) &\geq -\alpha \psi_1(s) + C, \\ \psi_2(s) &\geq -\alpha \phi_1(s) + C, & \psi_2(s) &\geq -\alpha \psi_1(s) + C. \end{aligned}$$

5. The ‘pure’ potentials are such that the resulting continuum elastic potential is l -convex with $l > 0$, i.e. if W is defined as in (2.3), for any $s > 0$,

$$W''(s) = \phi_1''(s) + \phi_2''(s) \geq l > 0.$$

6. We assume $f_i = f(x_i)$ for some $f \in C^2(\Omega)$.

These assumptions are designed to prevent fracture of the chain which would need to be taken into account if we simply used a Lennard-Jones-like potential (see for example the analysis contained in [BC07] and [SSZ11]), and hence allows us to isolate the contribution of the point defect more easily.

Assumption 1 states that the atoms undergo a strongly repulsive interaction when they approach each other, typical of those used in Molecular Dynamics simulations for Materials Science applications (see Chapter 10 of [LR04]). The assumption that

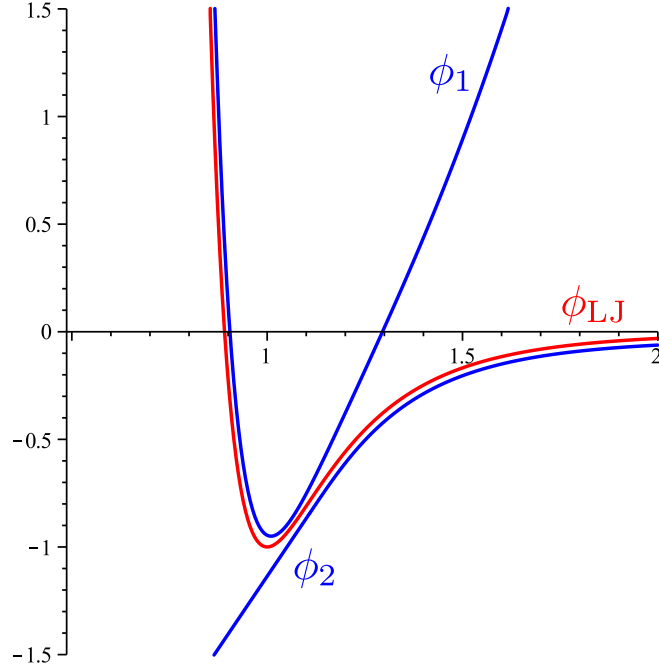


Figure 2.2: Typical potentials satisfying the assumptions of the Confined Lennard-Jones model which approximate the Lennard-Jones potential, $\phi_{\text{LJ}}(r) := r^{-12} - 2r^{-6}$.

the potentials are $+\infty$ when relative bond lengths are negative is not restrictive, since it prevents reordering of the atoms in the deformed configuration relative to the reference configuration. Such reorderings may always be dealt with by reindexing, and so to simplify the arguments below, we employ this hypothesis instead.

Assumptions 2 and 3 simulate the behaviour of a typical Lennard-Jones pair interaction, which is convex for short bond lengths, and concave for any bond longer than some critical length (the original Lennard-Jones potential is shown in Figure 2.2 as ϕ_{LJ}). Under strains of up to 10%, nearest neighbours lie in the convex part of the potential, and all other atoms lie in the concave part.

Assumption 4, when combined with Assumption 2, enforces the elastic behaviour of the material and prevents fracture from being favourable: it is this assumption which ‘confines’ the model.

Assumption 5 prevents any form of microstructure from forming. Since this is not the focus of this study, this assumption avoids significant analytical complications.

2.2.4 Immediate consequences

These assumptions lead to two estimates which we will use frequently throughout this chapter. First, the fact that ϕ_2 is concave implies that

$$\frac{1}{2}\phi_1(a) + \frac{1}{2}\phi_1(b) + \phi_2\left(\frac{a+b}{2}\right) \geq \frac{1}{2}W(a) + \frac{1}{2}W(b). \quad (2.5)$$

Second, by using the concavity of the second neighbour potentials once more, we have

$$\begin{aligned} & \frac{1}{2}\phi_1(a) + \psi_2\left(\frac{a+b}{2}\right) + \psi_1(b) + \phi_2\left(\frac{b+c}{2}\right) + \psi_1(c) + \psi_2\left(\frac{c+d}{2}\right) + \frac{1}{2}\phi_1(d) \\ & \geq \frac{1}{2}(\phi_1(a) + \psi_2(a)) + (\psi_1(b) + \frac{1}{2}\phi_2(b) + \frac{1}{2}\psi_2(b)) \\ & \quad + (\psi_1(c) + \frac{1}{2}\psi_2(c) + \frac{1}{2}\phi_2(c)) + \frac{1}{2}(\phi_1(d) + \psi_2(d)), \end{aligned}$$

and Assumption 4 now implies

$$\begin{aligned} & \frac{1}{2}\phi_1(a) + \psi_2\left(\frac{a+b}{2}\right) + \psi_1(b) + \phi_2\left(\frac{b+c}{2}\right) + \psi_1(c) + \psi_2\left(\frac{c+d}{2}\right) + \frac{1}{2}\phi_1(d) \\ & \geq (1-\alpha)\left(\frac{1}{2}\phi_1(a) + \psi_1(b) + \psi_1(c) + \frac{1}{2}\phi_1(d)\right) + 3C, \\ & \geq \frac{1}{2}l\left(\frac{1}{2}a^2 + b^2 + c^2 + \frac{1}{2}d^2\right) + 3C. \quad (2.6) \end{aligned}$$

2.3 Γ -convergence as a tool for asymptotic analysis

Γ -convergence is a form of convergence specifically tailored to be suited to variational problems, and may be defined as follows.

Definition 2.3.1 (Γ -convergence). Let (X, d) be a metric space, and $F_j : X \rightarrow \mathbb{R} \cup \{+\infty\}$ be a sequence of functions. (F_j) is said to Γ -converge to $F : X \rightarrow \mathbb{R} \cup \{+\infty\}$, written $\Gamma\text{-}\lim_{j \rightarrow \infty} F_j = F$, if the following two conditions hold.

1. (liminf inequality) For any sequence (x_j) such that $x_j \rightarrow x$,

$$\liminf_{j \rightarrow \infty} F_j(x_j) \geq F(x).$$

2. (limsup inequality) There exists a sequence (x_j) such that $x_j \rightarrow x$ and

$$\limsup_{j \rightarrow \infty} F_j(x_j) \leq F(x).$$

As an illustration of the utility of this form of convergence in the study of variational problems, the following lemma is a particular case of Theorem 1.21 in [Bra02]: we state it here without proof.

Lemma 2.3.1 ([Bra02]). *Suppose (X, d) is a metric space and $F_j : X \rightarrow \mathbb{R} \cup \{+\infty\}$ is a sequence of functions for which there exists a compact set $K \subseteq X$ such that $\min_K F_j = \min_X F_j$. Then if $\Gamma\text{-}\lim_{j \rightarrow \infty} F_j = F$, it follows that*

$$\min_{x \in X} F(x) = \lim_{j \rightarrow \infty} \min_{x \in X} F_j(x),$$

and furthermore if $x_j \in \operatorname{argmin}_X F_j$, then every convergent subsequence of (x_j) converges to a minimum point of F .

This result may be interpreted as saying that the minimum of F provides an approximation of the minima of F_j , and that the points at which the minimum of F is attained are also approximately minimum points of F_j . It is possible to further develop this idea and state the following definition of an asymptotic expansion via Γ -convergence as proposed in [AB93] and discussed extensively in [BT08].

Definition 2.3.2 (Asymptotic expansion via Γ -convergence). Let (X, d) be a metric space, and $F_j : X \rightarrow \mathbb{R} \cup \{+\infty\}$ be a sequence of functions. We write

$$F_j(x) \stackrel{\Gamma}{=} \sum_{k=0}^N \omega_k(j) F^k(x) + o(\omega_N(j))$$

to mean that for $K = 0, \dots, N$,

$$\Gamma\text{-}\lim_{j \rightarrow \infty} \frac{F_j(x) - \sum_{k=0}^{K-1} \omega_k(j) m^k}{\omega_K(j)} = F^K(x),$$

where $m^k = \min_{x \in X} F^k(x)$, and $\lim_{i \rightarrow \infty} \frac{\omega_{k+1}(i)}{\omega_k(i)} = 0$ for $k = 0, \dots, N-1$.

If F_j satisfies the assumptions of Lemma 2.3.1, repeated application of the first conclusion of that result gives

$$\min_{x \in X} F_j(x) = \sum_{k=0}^N \omega_k(j) m^k + o(\omega_N(j)) \quad \text{as } j \rightarrow \infty,$$

and hence F^k provide a sequence of variational problems, the solutions of which provide an approximation of the minima of F_j as $j \rightarrow \infty$. The second conclusion cannot be used to say anything further in general, unless we know something more about the structure of F_j and F^k .

Inspired by the notion of ‘completeness’ of such asymptotic expansions defined in [BT08], we write

$$F_j(x) \stackrel{\Gamma}{=} \sum_{k=0}^N \omega_k(j) F^k(x) + O(\omega_{N+1}(j))$$

to mean that the expansion is *complete up to order* $\omega_{N+1}(j)$, i.e.

$$F_j(x) \stackrel{\Gamma}{=} \sum_{k=0}^N \omega_k(j) F^k(x) + o(\omega_N(j))$$

as before, but additionally

$$\Gamma\text{-}\lim_{j \rightarrow \infty} \frac{F_j(x) - \sum_{k=0}^N \omega_k(j) m^k}{\theta(j)} = \begin{cases} 0 & x \in \operatorname{argmin}_X F^N, \\ +\infty & \text{otherwise,} \end{cases}$$

for any sequence $\theta(j)$ such that $\omega_N(j) \ll \theta(j) \ll \omega_{N+1}(j)$ as $j \rightarrow \infty$. This definition is a natural extension of the previous one, as it entails directly that

$$\min_{x \in X} F_j(x) = \sum_{k=0}^N \omega_k(j) m^k + O(\omega_{N+1}(j)) \quad \text{as } j \rightarrow \infty.$$

The model described in §2.2.1 provides such a sequence of variational problems for the energy defined in (2.2) indexed by $N \in \mathbb{N}$, and hence Γ -convergence provides an ideal tool for the rigorous justification of the arguments in §2.2.2.

2.3.1 Preliminaries and main result

Since Γ -convergence is defined with respect to a metric space, we make precise the spaces in which we work here. Throughout this chapter, we use the usual notation for Lebesgue and Sobolev spaces, with $\|\cdot\|_p$ and $\|\cdot\|_{1,p}$ being the norms on $L^p(\Omega)$ and $W^{1,p}(\Omega)$. We write $y^\epsilon \rightarrow y$ in L^p or $y^\epsilon \rightarrow y$ in $W^{1,p}$ (or H^1) to mean

$$\|y^\epsilon - y\|_p \rightarrow 0 \quad \text{or} \quad \|y^\epsilon - y\|_{1,p} \rightarrow 0 \quad \text{respectively.}$$

We write $y_\epsilon \rightharpoonup y$ or ‘ y_ϵ converges weakly to y ’ in H^1 if

$$\langle f, y^\epsilon \rangle \rightarrow \langle f, y \rangle \quad \text{for any } f \in H^{-1}(\Omega),$$

where $\langle \cdot, \cdot \rangle$ is the usual duality product on $H^1(\Omega)$.

Since we seek the Γ -limit of the energy functionals ϵE^ϵ as defined in (2.2), we need to ensure they are defined over the same space. Following the approach taken in [BDMG99], we associate any discrete deformation y^ϵ with a piecewise linear interpolant defined everywhere on Ω ,

$$y^\epsilon(x) := y_i^\epsilon + D_1 y_i^\epsilon (x - x_i) \quad \text{for any } x \in (x_i, x_{i+1}),$$

where we recall the definition of $D_1 y_i$ from (2.1). For each choice of ϵ , these linear interpolants lie in the spaces

$$P_\epsilon^1(\Omega) := \{y \in W^{1,\infty}(\Omega) : y \text{ is affine on } (x_i, x_{i+1}), x_i, x_{i+1} \in \Omega_\epsilon\}.$$

The admissible deformations $\mathcal{A}^\epsilon(L)$ are defined to be the set of such interpolants with the correct boundary conditions,

$$\mathcal{A}^\epsilon(L) := \{y \in P_\epsilon^1(\Omega) : y(-\tfrac{1}{2}) = 0, y(\tfrac{1}{2}) = L\}.$$

For any ϵ ,

$$\mathcal{A}^\epsilon(L) \subset \mathcal{A}(L) := \{y \in H^1(\Omega) : y(-\tfrac{1}{2}) = 0, y(\tfrac{1}{2}) = L\};$$

in fact, by the properties of linear interpolation, (see Chapter 4 of [BS08]),

$$\mathcal{A}(L) \subseteq \text{clos}\left(\bigcup_{N=1}^{\infty} \mathcal{A}^\epsilon(L)\right),$$

where $\text{clos}(A)$ denotes the closure of a set A in the strong topology on $H^1(\Omega)$. Since $\mathcal{A}(L)$ is convex,

$$\mathcal{A}(L) \subseteq \text{clos}\left(\bigcup_{N=1}^{\infty} \mathcal{A}^\epsilon(L)\right) \subseteq \text{w-clos}\left(\bigcup_{N=1}^{\infty} \mathcal{A}^\epsilon(L)\right) \subseteq \text{w-clos}(\mathcal{A}(L)) = \mathcal{A}(L),$$

where $\text{w-clos}(A)$ denotes sequential closure of a set A in the weak topology on $H^1(\Omega)$. In §2.4.1, we will see that the weak topology on H^1 ends up being the ‘natural’ topology for this problem due to the assumptions made in §2.2.3, even though the Γ -convergence results proven are always phrased in terms of the less restrictive convergence in the L^2 metric on $\mathcal{A}(L)$. It may be checked directly that $\mathcal{A}(L)$ endowed with the metric induced by the L^2 norm is a metric space, and so Γ -convergence is well-defined for functionals defined on this space.

As $H^1(\Omega)$ embeds in $C^0(\Omega)$, we define a projection operator $\mathcal{T}^\epsilon : \mathcal{A}(L) \rightarrow \mathcal{A}^\epsilon(L)$,

$$(\mathcal{T}^\epsilon y)(x) := y_i + D_1 y_i (x - x_i) \quad \text{for any } x \in (x_i, x_{i+1}),$$

where $y_i = y(x_i)$ as before.

We are now in a position to extend the definition of ϵE^ϵ to carry out our Γ -convergence analysis. Guided by other work for similar models (amongst others, see those used in [BC07], [BG02] and [BDMG99]), we define $\mathcal{F}^\epsilon : \mathcal{A}(L) \rightarrow \mathbb{R}$ to be

$$\mathcal{F}^\epsilon(y) := \begin{cases} \epsilon E^\epsilon(y) & y \in \mathcal{A}^\epsilon(L) \\ +\infty & \text{otherwise.} \end{cases} \quad (2.7)$$

We may now state the main result of this chapter.

Theorem 2.3.3. *Suppose that $\mathcal{F}^\epsilon : \mathcal{A}(L) \rightarrow \mathbb{R}$ is as given in (2.7). Then, with respect to the L^2 metric on $\mathcal{A}(L)$,*

$$\mathcal{F}^\epsilon(y) \stackrel{\Gamma}{=} \mathcal{F}_0(y) + \epsilon \mathcal{F}_1(y) + O(\epsilon^2)$$

as $N \rightarrow \infty$, where

$$\begin{aligned} \mathcal{F}_0(y) &:= \int_{\Omega} W(Dy) + f y \, dx, \\ \mathcal{F}_1(y) &:= \begin{cases} \inf_{r \in \ell^2(\mathbb{Z})} \tilde{E}_\infty(r) & y \in \underset{y \in \mathcal{A}(L)}{\operatorname{argmin}} \mathcal{F}_0(y), \\ +\infty & \text{otherwise} \end{cases} \end{aligned}$$

and $\tilde{E}_\infty : \ell^2(\mathbb{Z}) \rightarrow \mathbb{R}$ is defined in (2.18).

The proof of this result is divided into the relevant Γ -convergence results, proved over the course of §§2.4–2.7.

2.4 The 0th-order Γ -limit

Our first result gives the first term in the Γ -expansion of $\mathcal{F}^\epsilon$.

Theorem 2.4.1. *With respect to convergence in L^2 ,*

$$\Gamma\text{-}\lim_{\epsilon \rightarrow 0} \mathcal{F}^\epsilon(y) = \mathcal{F}_0(y) := \int_{\Omega} W(Dy) + f(y - L(x + \tfrac{1}{2})) \, dx.$$

The Γ -convergence of the internal energy in this result is already covered by Theorem 3.2 in [BC07], but we present a complete proof here in order to demonstrate the special structure of the Confined Lennard-Jones model described in §2.2.3. By exploiting the convexity and concavity of the potentials, we do not have to resort to a homogenisation formula to prove the liminf inequality.

2.4.1 The liminf inequality

The following lemma provides both a statement of equicoercivity and the liminf inequality.

Lemma 2.4.1. *Suppose (y^ϵ) is a sequence in $\mathcal{A}^\epsilon(L)$ such that $y^\epsilon \rightarrow y$ in L^2 : then*

1. *if $\mathcal{F}^\epsilon(y^\epsilon)$ is uniformly bounded for all $\epsilon > 0$, $y^\epsilon \rightharpoonup y$ in H^1 , and*
2. $\liminf_{\epsilon \rightarrow 0} \mathcal{F}^\epsilon(y^\epsilon) \geq \mathcal{F}_0(y).$

The proof of this result relies upon the growth assumptions and estimates made in §2.2.3, and is inspired by the argument used in the proof of Theorem 4.5 in [Bra02].

Proof. We construct a lower bound on the energy functional from which statement 1 follows. We begin by estimating the energy due to atoms away from the defect from below. Let

$$P_\epsilon := \{-N, \dots, N-1\} \setminus \{-2, -1, 0\},$$

i.e. the set of indices which have only pure-type interactions with their two neighbours on the right. (2.5) and the l -convexity of W imply that for any $y \in \mathcal{A}^\epsilon(L)$,

$$\begin{aligned} \sum_{i \in P_\epsilon} \frac{1}{2} \phi_1(D_1 y_i) + \phi_2(D_2 y_i) + \frac{1}{2} \phi_1(D_1 y_{i+1}) &\geq \sum_{i \in P_\epsilon} \frac{1}{2} W(D_1 y_i) + \frac{1}{2} W(D_1 y_{i+1}), \\ &\geq \sum_{i \in P_\epsilon} \frac{1}{4} l \left(|D_1 y_i|^2 + |D_1 y_{i+1}|^2 \right) + C. \end{aligned} \quad (2.8)$$

For the remaining indices, (2.6) implies that

$$\begin{aligned} \frac{1}{2} \phi_1(D_1 y_{-2}) + \psi_2(D_2 y_{-2}) + \psi_1(D_1 y_{-1}) + \phi_2(D_2 y_{-1}) + \psi_1(D_1 y_0) \\ + \psi_2(D_2 y_0) + \frac{1}{2} \phi_1(D_1 y_1) &\geq \sum_{i=-2}^0 \frac{1}{4} l \left(|D_1 y_i|^2 + |D_1 y_{i+1}|^2 \right) + C, \end{aligned} \quad (2.9)$$

and hence

$$\epsilon E_p^\epsilon(y^\epsilon) + \epsilon E_d(y^\epsilon) \geq \epsilon \sum_{i=-N}^{N-1} \left(\frac{1}{2} l |D_1 y_i^\epsilon|^2 + C \right) = \frac{1}{2} l \|Dy^\epsilon\|_2^2 + C. \quad (2.10)$$

Finally, Lemma 5.3 in [BDMG99] implies that

$$\epsilon E_f^\epsilon(y^\epsilon) \rightarrow \int_{\Omega} f\left(y - L\left(x + \frac{1}{2}\right)\right) dx,$$

so $\epsilon E_f^\epsilon(y^\epsilon)$ is uniformly bounded, and thus

$$\sup_{\epsilon > 0} \|Dy^\epsilon\|_2 < +\infty,$$

so statement 1 follows via the standard result that $y^\epsilon \rightharpoonup y$ in H^1 if and only if $\|y^\epsilon\|_{1,2}$ is uniformly bounded and $y^\epsilon \rightarrow y$ in $L^2(\Omega)$.

To prove the second statement, we note that as W is l -convex, the map

$$y \mapsto \int_{\Omega} W(Dy) dx \quad (2.11)$$

is lower semicontinuous with respect to weak convergence in $H^1(\Omega)$ (see for example Corollary 2.31 in [Bra02]). Fix $\delta > 0$. The estimates made in (2.8) and (2.9) imply that

$$\epsilon E_p^\epsilon(y^\epsilon) + \epsilon E_d(y^\epsilon) \geq \int_{\Omega \setminus (-\delta, \delta)} W(Dy^\epsilon) dx + C \delta.$$

Using the first statement and the weak lower semicontinuity of (2.11), we have that

$$\begin{aligned} \liminf_{\epsilon \rightarrow 0} (\epsilon E_p^\epsilon(y^\epsilon) + \epsilon E_d(y^\epsilon)) &\geq \liminf_{\epsilon \rightarrow 0} \int_{\Omega \setminus (-\delta, \delta)} W(Dy^\epsilon) dx + C \delta, \\ &\geq \int_{\Omega \setminus (-\delta, \delta)} W(Dy) dx + C \delta. \end{aligned}$$

Since δ was arbitrary, we let $\delta \rightarrow 0$, giving

$$\liminf_{\epsilon \rightarrow 0} (\epsilon E_p^\epsilon(y^\epsilon) + \epsilon E_d(y^\epsilon)) \geq \int_{\Omega} W(Dy) dx. \quad (2.12)$$

Convergence of the external force term is a consequence of Lemma 5.3 in [BDMG99], the result of which implies that if $y^\epsilon \rightarrow y$ in $L^2(\Omega)$ and $\|Dy^\epsilon\|_2$ is uniformly bounded, then

$$\epsilon E_f^\epsilon(y^\epsilon) \rightarrow \int_{\Omega} f(y - L(x + \tfrac{1}{2})) dx. \quad (2.13)$$

Combining (2.12) and (2.13) completes the proof. $\square$

2.4.2 The limsup inequality

We now prove the following lemma to complete the proof of Theorem 2.4.1.

Lemma 2.4.2. *For any $y \in \mathcal{A}(L)$, there exists a sequence of $y^\epsilon \in \mathcal{A}^\epsilon(L)$ such that $y^\epsilon \rightarrow y$ in L^2 and*

$$\limsup_{\epsilon \rightarrow 0} \mathcal{F}^\epsilon(y^\epsilon) \leq \mathcal{F}_0(y).$$

The construction of the sequence y^ϵ requires a diagonal argument, which proceeds in two steps. In the first step, the convexity of W is exploited to show that a naive approximation of $y \in \mathcal{A}(L)$ by $\mathcal{T}^\epsilon y$ works for the ‘pure’ part of the energy. By linearising deformations near the defect, and therefore controlling the behaviour of the energy there, we can take a diagonal sequence to arrive at the correct inequality. Note that the inequality is trivial if $\mathcal{F}_0(y) = +\infty$, so we only need consider $y \in \mathcal{A}(L)$ such that $\mathcal{F}_0(y) < +\infty$.

Proof. Fix $y \in \mathcal{A}(L)$, and define the integrand

$$W_\epsilon(x) := \sum_{i=-N}^{N-1} \left(\frac{1}{2}\phi_2(D_2y_{i-1}) + \phi_1(D_1y_i) + \frac{1}{2}\phi_2(D_2y_i) \right) \chi_i(x),$$

where $\chi_i(x)$ is the indicator function for the interval (x_i, x_{i+1}) . Note that by construction,

$$\int_{\Omega} W_\epsilon(x) dx = \epsilon E_p^\epsilon(y).$$

We will apply Fatou's lemma to the functions W_ϵ .

Almost everywhere convergence of W_ϵ . Define the sequence $i_\epsilon := \lfloor Nx \rfloor \in \mathbb{Z}$ for fixed $x \in \Omega$, so that $x_\epsilon := \epsilon i_\epsilon \rightarrow x$ as $\epsilon \rightarrow 0$. Lebesgue's Differentiation Theorem (see for example Corollary 2 in §1.7 of [EG92]) entails that, as $\epsilon \rightarrow 0$,

$$D_j y_{i_\epsilon} = \oint_{x_\epsilon}^{x_\epsilon + j\epsilon} Dy(t) dt \rightarrow Dy(x) \quad \text{for almost every } x \in \Omega.$$

The continuity of the potentials ϕ_i therefore implies that $W_\epsilon(x) \rightarrow W(Dy(x))$ for almost every $x \in \Omega$.

Pointwise upper bound on W_ϵ . Fix a point $x \in \Omega$ and the sequence i_ϵ as above. Dropping the subscript, we estimate

$$\begin{aligned} W_\epsilon(x) &\leq \frac{1}{2}\phi_2(D_2y_{i-1}) + \frac{1}{2}\phi_1(D_2y_{i-1}) + \phi_1(D_1y_i) + \frac{1}{2}\phi_1(D_2y_i) + \frac{1}{2}\phi_2(D_2y_i) + C, \\ &= \frac{1}{2}W(D_2y_{i-1}) + \phi_1(D_1y_i) + \frac{1}{2}W(D_2y_i) + C, \end{aligned}$$

where $-C \in \mathbb{R}$ is a lower bound for ϕ_1 . Next, Assumption 4 in §2.2.3 implies that for some $C \in \mathbb{R}$,

$$\frac{1}{1-\alpha}W(t) + C \geq \phi_1(t).$$

Hence, letting $A := \max\{\frac{1}{2}, \frac{1}{1-\alpha}\}$, and applying Jensen's inequality,

$$\begin{aligned} W_\epsilon(x) &\leq A \left(W(D_2y_{i-1}) + W(D_1y_i) + W(D_2y_i) \right) + C, \\ &\leq A \left(\oint_{x_{i-1}}^{x_{i+1}} W(Dy) dx + \oint_{x_i}^{x_{i+1}} W(Dy) dx + \oint_{x_i}^{x_{i+2}} W(Dy) dx \right) + C. \end{aligned}$$

Since W is bounded below, we can extend the domain of integration for each integral, to reach the upper bound

$$W_\epsilon(x) \leq g_\epsilon(x) := 3A \oint_{x-2\epsilon}^{x+2\epsilon} W(Dy) dt + C.$$

Convergence of g_ϵ . As $\mathcal{F}_0(y)$ is bounded, $W(Dy)$ is integrable and so another application of Lebesgue's Differentiation Theorem implies that

$$g_\epsilon(x) \rightarrow g(x) := 3AW(Dy(x)) + C$$

almost everywhere as $\epsilon \rightarrow 0$. Furthermore, g_ϵ may be expressed as the convolution $g_\epsilon = g * \rho_\epsilon$, where ρ_ϵ is an approximation to a Dirac mass given by

$$\rho_\epsilon(x) := \frac{1}{4\epsilon} \rho\left(\frac{x}{4\epsilon}\right), \quad \text{where} \quad \rho(x) = \chi_\Omega(x).$$

Since $g \in L^1(\Omega)$ and $\rho_\epsilon \in L^\infty(\Omega)$ it follows that $g_\epsilon \in L^1(\Omega)$, and by a standard argument

$$\int_\Omega g_\epsilon(x) dx \rightarrow \int_\Omega g(x) dx$$

as $\epsilon \rightarrow 0$. We can now apply Fatou's Lemma to $g_\epsilon - W_\epsilon$, which is positive, measurable, and converges almost everywhere, so

$$\int_\Omega g dx - \limsup_{\epsilon \rightarrow 0} \int_\Omega W_\epsilon dx = \liminf_{\epsilon \rightarrow 0} \int_\Omega g_\epsilon - W_\epsilon dx \geq \int_\Omega g - W(Dy) dx.$$

A rearrangement of this inequality allows us to conclude that

$$\limsup_{N \rightarrow \infty} \epsilon E_p^\epsilon(y^\epsilon) = \limsup_{N \rightarrow \infty} \int_\Omega W_\epsilon dx \leq \int_\Omega W(Dy) dx. \quad (2.14)$$

Controlling the energy near the defect. For any $y \in \mathcal{A}(L)$ and $\delta > 0$, let y^δ be a linearisation close to 0 of $y \in \mathcal{A}(L)$ given by

$$y^\delta(x) := \begin{cases} y(-\delta) + \frac{y(\delta) - y(-\delta)}{2\delta}(x + \delta) & \text{when } |x| < \delta, \\ y(x) & \text{otherwise.} \end{cases}$$

Let $F^\delta := Dy^\delta(0)$. For ϵ sufficiently small, the defect energy for $\mathcal{T}^\epsilon y^\delta$ is:

$$\epsilon E_d(\mathcal{T}^\epsilon y^\delta) = 2\epsilon(\psi_2(F^\delta) - \phi_2(F^\delta) + \psi_1(F^\delta) - \phi_1(F^\delta)) \leq C(\delta)\epsilon \quad (2.15)$$

with δ fixed. To control ϵE_f^ϵ , we can once again employ the estimate that was proven in (2.13), since the argument used was for a more general sequence than that chosen here. Therefore, combining (2.13), (2.14) and (2.15), we deduce that

$$\limsup_{\epsilon \rightarrow 0} \mathcal{F}^\epsilon(\mathcal{T}^\epsilon y^\delta) \leq \mathcal{F}_0(y^\delta).$$

Since $y^\delta \rightarrow y$ in L^2 as $\delta \rightarrow 0$, we wish to show that $\mathcal{F}_0(y^\delta) \rightarrow \mathcal{F}_0(y)$ as $\delta \rightarrow 0$ in order to use a diagonalisation argument. This follows from the observation that

$$2\delta \cdot C \leq \int_{-\delta}^{\delta} W(Dy^\delta) \, dx \leq \int_{-\delta}^{\delta} W(Dy) \, dx,$$

since W is bounded below and convex. Both the left- and right-hand sides tend to 0 as $\delta \rightarrow 0$, so we deduce that

$$\begin{aligned} \mathcal{F}_0(y^\delta) &= \int_{\Omega} W(Dy^\delta) + f(y^\delta - L(x + \tfrac{1}{2})) \, dx, \\ &\leq \int_{\Omega \setminus (-\delta, \delta)} W(Dy) \, dx + \int_{-\delta}^{\delta} W(Dy^\delta) + \int_{\Omega} f u \, dx + \|f\|_2 \|y^\delta - y\|_2, \\ &\rightarrow \mathcal{F}_0(y) \end{aligned}$$

as $\delta \rightarrow 0$, where $u(x) := y(x) - L(x + \frac{1}{2})$.

Conclusion. By taking a diagonal sequence from the collection of $\mathcal{T}^\epsilon y^\delta$, there exists a sequence $\mathcal{T}^\epsilon y^{\delta_\epsilon} \rightarrow y$ in L^2 , along which

$$\limsup_{\epsilon \rightarrow 0} \mathcal{F}^\epsilon(\mathcal{T}^\epsilon y^{\delta_\epsilon}) \leq \mathcal{F}_0(y),$$

proving the statement, and thus concluding the proof of Theorem 2.4.1. $\square$

Remark 2.4.1. The defect does not introduce a perturbation to the Γ -limit at this order: see Theorem 3.2 in [BC07] for the Γ -limit of this problem without a defect. This is to be expected, since the ‘defect set’ is null in the limit as $\epsilon \rightarrow 0$, and hence it becomes reasonable to ask whether there is a higher order change in the energy.

2.5 Properties of $\mathcal{F}_0$

The functional $\mathcal{F}_0$ is of a well-studied form, and the analysis of the minimum problem is classical. The following lemma collects relevant results regarding the functional and its minimisers which we will invoke in the following sections.

Lemma 2.5.1. *The variational problem*

$$\operatorname{argmin}_{y \in \mathcal{A}(L)} \mathcal{F}_0(y)$$

has a unique solution $\bar{y}$, which has the following properties:

1. $\bar{y}$ satisfies the Euler–Lagrange equation for this problem,

2. $\bar{y} \in C^2(\Omega)$.

Proof. The existence part of this result is completely classical, and a proof may be found in [Dac08] for example. If we suppose for the moment that minimisers are in $W^{1,\infty}(\Omega)$ and satisfy the condition

$$D\bar{y}(x) \geq \delta > 0$$

for almost every $x \in \Omega$, it is also easy to show that they satisfy

$$\int_{\Omega} [W'(D\bar{y}) - \sigma] Dv \, dx = 0 \quad \forall v \in W_0^{1,\infty}(\Omega), \quad (2.16)$$

where $\sigma(x) := \int_0^x f(t) \, dt$. Since W is l -convex, $W' : \mathbb{R}^+ \rightarrow \mathbb{R}$ is strictly increasing and is a C^1 diffeomorphism. If $(W')^{-1}$ is the inverse of W' , it is possible to ‘explicitly’ define a solution of the Euler–Lagrange equations

$$\bar{y}(x) := \int_{-\frac{1}{2}}^x (W')^{-1}(\sigma(t) + \Sigma) \, dt,$$

where Σ is the solution of the following implicit equation:

$$\int_{\Omega} (W')^{-1}(\sigma(t) + \Sigma) \, dt = L.$$

It may be shown that this equation has a unique solution by regarding the left-hand side as a function of Σ , showing this function is C^1 , has a strictly positive derivative, and tends to 0 as $\Sigma \rightarrow -\infty$ so attains all possible values $L > 0$ only once. It is now simple to verify that $\bar{y}$ is C^2 and satisfies the pointwise Euler–Lagrange equation, that is

$$\frac{d}{dx} W'(D\bar{y}(x)) = f(x) \quad \Rightarrow \quad W'(D\bar{y}(x)) = \sigma(x) + \Sigma, \quad (2.17)$$

so all that remains to do is show that $\bar{y}$ is in fact the minimiser. Suppose that $\tilde{y} \in \mathcal{A}(L)$ minimises $\mathcal{F}_0$ and is not equal to $\bar{y}$; then

$$\begin{aligned} 0 &\geq \int_{\Omega} W(D\tilde{y}) - W(D\bar{y}) + f(\tilde{y} - \bar{y}) \, dx, \\ &= \int_{\Omega} W(D\tilde{y}) - W(D\bar{y}) - \sigma(D\tilde{y} - D\bar{y}) \, dx, \\ &\geq \int_{\Omega} [W'(D\bar{y}) - \sigma] \cdot (D\tilde{y} - D\bar{y}) \, dx + \frac{1}{2}l \|D\tilde{y} - D\bar{y}\|_2^2, \end{aligned}$$

where we have integrated by parts and used the fact that W is l -convex. Since $\bar{y}$ has been constructed to solve the pointwise Euler–Lagrange equation (2.17), the integrand in the first term vanishes, and hence $\tilde{y} = \bar{y}$. This argument clearly also implies uniqueness of solutions. $\square$

2.6 The 1st-order Γ -limit

The approach taken in §2.4.2 gives an indication of the scaling of the next term in an asymptotic expansion of the energy: (2.15) suggests that the extra energy from the defect is only coming from a set near the defect that is of size $O(\epsilon)$ since the minimiser of $\mathcal{F}_0$ is C^2 at 0. §2.5 shows that we have a very clear understanding of the properties of $\bar{y}$, and thus we can reasonably hope to derive a good characterisation of the next term in the asymptotic expansion as in [SSZ11, BC07].

For this purpose, we define some additional notation. Recalling from §2.5 that

$$\bar{y} = \operatorname{argmin}_{y \in \mathcal{A}(L)} \mathcal{F}_0(y),$$

the functional from which we obtain the first-order limit is

$$\mathcal{F}_1^\epsilon(y) := \frac{\mathcal{F}^\epsilon(y) - \mathcal{F}_0(\bar{y})}{\epsilon}.$$

To make the notation used in this section more concise, we let $F_0 := D\bar{y}(0)$ as in §2.2.2, and define

$$\begin{aligned} \Phi_1(t) &:= \phi_1(F_0 + t) - \phi_1(F_0) - \phi'_1(F_0)t, \\ \Psi_1(t) &:= \psi_1(F_0 + t) - \phi_1(F_0) - \phi'_1(F_0)t, \\ \Phi_2(t) &:= \phi_2(F_0 + t) - \phi_2(F_0) - \phi'_2(F_0)t, \\ \Psi_2(t) &:= \psi_2(F_0 + t) - \phi_2(F_0) - \phi'_2(F_0)t. \end{aligned}$$

We will show that the first-order Γ -limit can be written in terms of the infinite cell problem

$$\inf_{r \in \ell^2(\mathbb{Z})} \tilde{E}_\infty(r),$$

where $\tilde{E}_\infty : \ell^2(\mathbb{Z}) \rightarrow \mathbb{R} \cup \{+\infty\}$ is defined to be

$$\tilde{E}_\infty(r) := \begin{cases} \sum_{i=-\infty}^{\infty} \Phi_1(r_i) + \Phi_2\left(\frac{r_{i+1}+r_i}{2}\right) + \tilde{E}_d(r), & F_0 + r_i > 0 \text{ for all } i \in \mathbb{N}, \\ +\infty & \text{otherwise,} \end{cases} \quad (2.18)$$

and we replace ϕ_i by ψ_i in the relevant places by setting $\tilde{E}_d : \ell^\infty(\mathbb{Z}) \rightarrow \mathbb{R}$ to be

$$\begin{aligned} \tilde{E}_d(r) &:= \psi_2\left(F_0 + \frac{r_{-2}+r_{-1}}{2}\right) - \phi_2\left(F_0 + \frac{r_{-2}+r_{-1}}{2}\right) + \psi_1(F_0 + r_{-1}) - \phi_1(F_0 + r_{-1}) \\ &\quad + \psi_1(F_0 + r_0) - \phi_1(F_0 + r_0) + \psi_2\left(F_0 + \frac{r_0+r_1}{2}\right) - \phi_2\left(F_0 + \frac{r_0+r_1}{2}\right). \end{aligned}$$

We briefly show that $\tilde{E}_\infty$ is well-defined. It is straightforward to check that Φ_2 is concave because ϕ_2 is concave, hence

$$\tilde{E}_\infty(r) \geq \sum_{i=-\infty}^{\infty} \Phi_1(r_i) + \Phi_2(r_i) + \tilde{E}_d(r).$$

Furthermore, the fact that W is l -convex implies

$$\Phi_1(t) + \Phi_2(t) = W(F_0 + t) - W(F_0) - W'(F_0)t \geq \frac{1}{2}l t^2, \quad (2.19)$$

and for $i = -2, -1, 0, 1$, as in (2.9), there exists some constant $C \in \mathbb{R}$ such that

$$\sum_{i=-2}^1 \left(\frac{1}{2}\Phi_1(r_i) + \frac{1}{2}\Phi_1(r_{i+1}) + \Phi_2\left(\frac{r_i+r_{i+1}}{2}\right) \right) + \tilde{E}_d(r) \geq \sum_{i=-2}^1 \frac{1}{2}l |r_i|^2 + C.$$

Hence we have that

$$\tilde{E}_\infty(r) \geq \frac{1}{2}l \|r\|_{\ell^2(\mathbb{Z})}^2 + C, \quad (2.20)$$

and $\tilde{E}_\infty$ is well-defined as a function mapping $\ell^2(\mathbb{Z})$ into $\mathbb{R} \cup \{+\infty\}$.

We now state the Γ -convergence result for the second term in the expansion.

Theorem 2.6.1. *With respect to convergence in L^2 ,*

$$\Gamma\text{-}\lim_{\epsilon \rightarrow 0} \mathcal{F}_1^\epsilon(y) = \mathcal{F}_1(y) := \begin{cases} \inf_{r \in \ell^2(\mathbb{Z})} \tilde{E}_\infty(r) & y = \bar{y}, \\ +\infty & y \neq \bar{y}. \end{cases}$$

In contrast to the results of [SSZ11] and [BC07], we emphasise that we have an explicit representation of the 1st-order limit in terms of a minimisation problem in an infinite cell.

2.6.1 The liminf inequality

The liminf inequality is the following statement.

Lemma 2.6.1. *If $y^\epsilon \rightarrow y$ in L^2 , then*

$$\liminf_{\epsilon \rightarrow 0} \mathcal{F}_1^\epsilon(y^\epsilon) \geq \mathcal{F}_1(y).$$

As in the proof of Lemma 2.4.1, we use a coercivity result which says uniform boundedness of $\mathcal{F}_1^\epsilon(y^\epsilon)$ implies a form of compactness for the sequence y^ϵ . In this proof, there are two such results, which are employed at crucial steps in the main argument. The first of these results, Lemma 2.6.2, states that if $\mathcal{F}_1^\epsilon(y^\epsilon)$ is uniformly

bounded then the weak convergence of y^ϵ in H^1 proven in Lemma 2.4.1 improves to strong convergence in H^1 . The second, Lemma 2.6.4, describes coercivity in a topology which we use to describe perturbations to the minimiser of $\mathcal{F}_0$ close to the defect. Once these results have been obtained, the main argument will follow by applying Fatou's Lemma to a suitable reinterpretation of $\mathcal{F}_1^\epsilon(y^\epsilon)$.

We remark here that to simplify the notation, we write u , u^ϵ and $\bar{u}$ in place of $y - L(x + \frac{1}{2})$, $y^\epsilon - L(x + \frac{1}{2})$ and $\bar{y} - L(x + \frac{1}{2})$ respectively.

A key step before proving the coercivity results is to rewrite $\mathcal{F}_1^\epsilon(y^\epsilon)$ and $\mathcal{F}_0(\bar{y})$ by using integration by parts on the external force terms, giving

$$\int_{\Omega} f \bar{u} \, dx = - \int_{\Omega} \sigma \, D \bar{u} \, dx,$$

using the boundary conditions and defining $\sigma(x) := \int_{-1/2}^x f(t) \, dt$ as in §2.2.2. Analogously, we recursively define

$$\sigma_{-N}^\epsilon := -\frac{1}{2}\epsilon f_{-N} \quad \text{and} \quad \sigma_i^\epsilon := \sigma_{i-1}^\epsilon + \epsilon f_{i-1},$$

which leads to the representation

$$\sum_{i=-N}^{N-1} f_i u_i = \sum_{i=-N}^{N-1} \frac{\sigma_{i+1}^\epsilon - \sigma_i^\epsilon}{\epsilon} u_i = - \sum_{i=-N}^{N-1} \sigma_{i+1}^\epsilon D_1 u_i.$$

As remarked in §2.2.2, the definition of σ_{-N}^ϵ can be left free to carry out this summation by parts; however, the particular choice of σ_{-N}^ϵ given here will be exploited to obtain (2.26), a pointwise estimate on $\sigma - \sigma^\epsilon$ during the proof of Lemma 2.6.2.

Define the step function $\sigma^\epsilon : \Omega \rightarrow \mathbb{R}$

$$\sigma^\epsilon(x) := \sum_{i=-N}^{N-1} \sigma_{i+1}^\epsilon \chi_{(x_i, x_{i+1})}(x),$$

so that if $y \in \mathcal{A}^\epsilon(L)$,

$$\epsilon E_f^\epsilon(y) = - \int_{\Omega} \sigma^\epsilon \, D u \, dx.$$

Using these definitions, we perform careful estimates of $\mathcal{F}_1^\epsilon(y^\epsilon)$ by splitting the domain of integration over the intervals (x_i, x_{i+2}) . For $y^\epsilon \in \mathcal{A}^\epsilon(L)$, let

$$\begin{aligned} s_i^\epsilon &:= \phi_2(D_2 y_i^\epsilon) + \frac{1}{2} \phi_1(D_1 y_i^\epsilon) + \frac{1}{2} \phi_1(D_1 y_{i+1}^\epsilon) - \frac{1}{2} \sigma_{i+1}^\epsilon D_1 u_i^\epsilon - \frac{1}{2} \sigma_{i+2}^\epsilon D_1 u_{i+1}^\epsilon \\ &\quad - \int_{x_i}^{x_{i+2}} W(D \bar{y}) - \sigma \, D \bar{u} + \Sigma(D y^\epsilon - D \bar{y}) \, dx \end{aligned} \quad (2.21)$$

if $i \in \{-N, \dots, N-1\}$, and set $s_i^\epsilon := 0$ otherwise. Then it is easy to check that

$$\mathcal{F}_1^\epsilon(y^\epsilon) = \sum_{i=-\infty}^{\infty} s_i^\epsilon + \tilde{E}_d(D_1 y^\epsilon - F_0), \quad (2.22)$$

where $D_1 y^\epsilon - F_0 \in \ell^\infty(\mathbb{Z})$ is

$$(D_1 y^\epsilon - F_0)_i := \begin{cases} D_1 y_i^\epsilon - F_0, & i = -N, \dots, N-1, \\ 0 & \text{otherwise.} \end{cases}$$

We are now in a position to state and prove the necessary coercivity results.

Lemma 2.6.2. *If $y^\epsilon \rightarrow y$ in L^2 and $\mathcal{F}_1^\epsilon(y^\epsilon)$ is uniformly bounded for all $\epsilon > 0$, then $y^\epsilon \rightarrow \bar{y}$ in H^1 .*

Proof. Since $\mathcal{F}_1^\epsilon(y^\epsilon)$ is uniformly bounded, we know that for some $C \in \mathbb{R}$,

$$|\mathcal{F}^\epsilon(y^\epsilon) - \mathcal{F}_0(\bar{y})| \leq C\epsilon,$$

which immediately implies that $\mathcal{F}^\epsilon(y^\epsilon) \rightarrow \mathcal{F}_0(\bar{y})$ as $\epsilon \rightarrow 0$. Consequently, Lemma 2.4.1 applies and so $\|Dy^\epsilon\|_2$ is uniformly bounded. Let $i \in \{-N, \dots, N-1\}$. We estimate s_i^ϵ below:

$$\begin{aligned} s_i^\epsilon &\geq \int_{x_i}^{x_{i+2}} W(Dy^\epsilon) - W(D\bar{y}) - \sigma^\epsilon Du^\epsilon + \sigma D\bar{u} - \Sigma(Dy^\epsilon - D\bar{y}) \, dx, \\ &\geq \int_{x_i}^{x_{i+2}} W'(D\bar{y})(Dy^\epsilon - D\bar{y}) + \frac{1}{2}l|Dy^\epsilon - D\bar{y}|^2 \\ &\quad - \sigma^\epsilon Du^\epsilon + \sigma D\bar{u} - \Sigma(Dy^\epsilon - D\bar{y}) \, dx, \end{aligned}$$

using the concavity of ϕ_2 on the first line, and the l -convexity of W on the second. Next, as $\bar{y}$ satisfies the pointwise Euler–Lagrange equation (2.17),

$$\begin{aligned} s_i^\epsilon &\geq \int_{x_i}^{x_{i+2}} \left(\sigma(Dy^\epsilon - D\bar{y}) + \frac{1}{2}l|Dy^\epsilon - D\bar{y}|^2 - \sigma^\epsilon Du^\epsilon + \sigma D\bar{u} \right) dx, \\ &\geq \int_{x_i}^{x_{i+2}} \left((\sigma - \sigma^\epsilon) Du^\epsilon + \frac{1}{2}l|Dy^\epsilon - D\bar{y}|^2 \right) dx. \end{aligned} \quad (2.23)$$

The latter term in the above integral is of the form we seek, so it remains to show that the other term vanishes in the limit. Once this is done, we must then show that the defect energy is also suitably bounded below.

Pointwise estimate on $\sigma - \sigma^\epsilon$. Noting that Du^ϵ is constant on the intervals (x_i, x_{i+1}) and using the definitions of σ and σ^ϵ , we rewrite

$$\begin{aligned} \int_{x_i}^{x_{i+1}} (\sigma - \sigma^\epsilon) \, dx &= \int_{x_i}^{x_{i+1}} \left(\int_{-1/2}^x f(t) \, dt - \epsilon \sum_{j=-N}^{i-1} \frac{1}{2}(f_j + f_{j+1}) - \frac{1}{2}\epsilon f_i \right) dx, \\ &= \int_{-1/2}^{x_i} \left(f(t) - (\mathcal{T}^\epsilon f)(t) \right) dt + \int_{x_i}^{x_{i+1}} \left(\int_{x_i}^x f(t) \, dt - \frac{1}{2}\epsilon f_i \right) dx. \end{aligned}$$

Since we know that $f \in C^2$, standard results about interpolation error (see for example [SM03]) imply that

$$\left| \int_{-1/2}^{x_i} \left(f(t) - (\mathcal{T}^\epsilon f)(t) \right) dt \right| \leq \frac{1}{12} \epsilon^2 \|f''\|_\infty. \quad (2.24)$$

For the other term, we Taylor expand $f(t)$ at x_i , then evaluate integrals to show that

$$\left| \int_{x_i}^{x_{i+1}} f(t) dt - \frac{1}{2} \epsilon f_i dx \right| \leq \frac{1}{6} \epsilon^2 \|f'\|_\infty. \quad (2.25)$$

Combining (2.24) and (2.25), we have

$$\begin{aligned} \left| \int_{x_i}^{x_{i+2}} (\sigma - \sigma^\epsilon) Du^\epsilon dx \right| &\leq \left(\frac{1}{12} \epsilon^2 \|f''\|_\infty + \frac{1}{6} \epsilon^2 \|f'\|_\infty \right) \frac{|D_1 u_i^\epsilon| + |D_1 u_{i+1}^\epsilon|}{2}, \\ &\lesssim \epsilon^2 (|D_1 u_i^\epsilon|^2 + |D_1 u_{i+1}^\epsilon|^2)^{1/2}, \\ &\lesssim \epsilon^{3/2} \|Du^\epsilon\|_2, \end{aligned} \quad (2.26)$$

where we have used Jensen's inequality, and then added further positive terms inside the brackets on the second line. This estimate can be inserted into (2.23) to give

$$s_i^\epsilon \geq -C\epsilon^{3/2} \|Du^\epsilon\|_2 + \frac{1}{2} l \int_{x_i}^{x_{i+2}} |Dy^\epsilon - D\bar{y}|^2 dx. \quad (2.27)$$

Lower bound on defect energy. Using (2.9), the fact that $W(D\bar{y}) - (\sigma + \Sigma)D\bar{u}$ is finite, and estimate (2.26),

$$\begin{aligned} \sum_{i=-2}^0 s_i^\epsilon + \tilde{E}_d(Dy^\epsilon - F_0) &\geq \sum_{i=-2}^0 \frac{1}{4} l (|D_1 y_i^\epsilon|^2 + |D_1 y_{i+1}^\epsilon|^2) - \int_{x_i}^{x_{i+2}} \sigma^\epsilon Du^\epsilon + \Sigma Du^\epsilon dx + C, \\ &= \sum_{i=-2}^0 \int_{x_i}^{x_{i+2}} \frac{1}{2} l |Dy^\epsilon|^2 - \sigma Du^\epsilon - (\sigma^\epsilon - \sigma) Du^\epsilon - \Sigma Du^\epsilon dx + C, \\ &\geq \sum_{i=-2}^0 \int_{x_i}^{x_{i+2}} \frac{1}{2} l |Dy^\epsilon|^2 - \|\sigma + \Sigma\|_\infty |Du^\epsilon| + C dx - C\epsilon^{3/2} \|Dy^\epsilon\|_2. \end{aligned}$$

Since $D\bar{y}$ is bounded above and below,

$$\sum_{i=-2}^0 s_i^\epsilon + \tilde{E}_d(Dy^\epsilon - F_0) \geq \sum_{i=-2}^0 \int_{x_i}^{x_{i+2}} \frac{1}{2} l |Dy^\epsilon - D\bar{y}|^2 dx + C - C\epsilon^{3/2} \|Dy^\epsilon\|_2. \quad (2.28)$$

Conclusion of the argument. Summing over i in (2.27), and applying (2.28) and the fact that $\|Dy^\epsilon\|_2$ is uniformly bounded, we have shown that

$$\mathcal{F}_1^\epsilon(y^\epsilon) \geq -C\epsilon^{1/2} + \frac{1}{2} l \sum_{i=-N}^{N-1} \int_{x_i}^{x_{i+1}} |Dy^\epsilon - D\bar{y}|^2 dx + C.$$

Multiplying this inequality by ϵ and using the assumption that $\mathcal{F}_1^\epsilon(y^\epsilon)$ is uniformly bounded, we have

$$C\epsilon \geq \frac{1}{2}l\|Dy^\epsilon - D\bar{y}\|_2^2, \quad (2.29)$$

which proves the result. $\square$

To state the second coercivity result, let $\mathcal{P}_\epsilon : \mathcal{A}^\epsilon(L) \rightarrow \ell^2(\mathbb{Z})$ be the sequence of operators

$$(\mathcal{P}_\epsilon y)_i := \begin{cases} D_1 y_i - D_1 \bar{y}_i & i \in \{-N, \dots, N-1\} \\ 0 & \text{otherwise.} \end{cases}$$

Clearly $\mathcal{P}_\epsilon$ is well-defined as a map into $\ell^2(\mathbb{Z})$, since $\mathcal{P}_\epsilon y$ is always compactly supported.

Lemma 2.6.3. *If $\mathcal{F}_1^\epsilon(y^\epsilon)$ is uniformly bounded, then there exists a subsequence of $\mathcal{P}_\epsilon y^\epsilon$ which converges weakly in $\ell^2(\mathbb{Z})$.*

Proof. By dividing (2.29) by ϵ and using Jensen's inequality, we have

$$C \geq \frac{1}{2}l \sum_{i=-N}^{N-1} \int_{x_i}^{x_{i+1}} |Dy^\epsilon - D\bar{y}|^2 dx \geq \frac{1}{2}l \sum_{i=-N}^{N-1} \left| \int_{x_i}^{x_{i+1}} Dy^\epsilon - D\bar{y} dx \right|^2 = \frac{1}{2}l \|\mathcal{P}_\epsilon y^\epsilon\|_{\ell^2(\mathbb{Z})}^2.$$

We have shown that the sequence $\mathcal{P}_\epsilon y^\epsilon$ is uniformly bounded in $\ell^2(\mathbb{Z})$, so in particular, it must have a weakly convergent subsequence. $\square$

To conclude the argument which will prove the liminf inequality, we will use the following characterisation of weak convergence in $\ell^2(\mathbb{Z})$ which follows easily from the Riesz Representation Theorem.

Lemma 2.6.4. *A sequence $(r^\epsilon) \subset \ell^2(\mathbb{Z})$ converges weakly to $r \in \ell^2(\mathbb{Z})$ as $\epsilon \rightarrow 0$ if and only if the following two conditions hold:*

1. $\|r^\epsilon\|_{\ell^2}$ is uniformly bounded,
2. $r^\epsilon \rightarrow r$ pointwise (almost everywhere in the counting measure) as $\epsilon \rightarrow 0$.

Proof of Lemma 2.6.1. As indicated at the beginning of this section, we apply Fatou's Lemma to the sum (2.22). Suppose that $\mathcal{F}_1^\epsilon(y^\epsilon)$ is uniformly bounded and $y^\epsilon \rightarrow y$ in L^2 . Take a subsequence y^{ϵ_k} such that

$$\lim_{k \rightarrow \infty} \mathcal{F}_1^{\epsilon_k}(y^{\epsilon_k}) = \liminf_{\epsilon \rightarrow 0} \mathcal{F}_1^\epsilon(y^\epsilon),$$

and then using Lemma 2.6.3, a further subsequence (which we do not relabel) such that $\mathcal{P}_{\epsilon_k} y^{\epsilon_k}$ weakly converges to r in $\ell^2(\mathbb{Z})$. Since $\bar{y} \in C^2(\Omega)$, we have that

$$D_1 \bar{y}_i = \int_{x_i}^{x_{i+1}} D\bar{y} \, dx \rightarrow F_0 := D\bar{y}(0)$$

as $\epsilon \rightarrow 0$. Fixing an index $i \in \mathbb{Z}$, Lemma 2.6.4 implies that

$$(\mathcal{P}_{\epsilon_k} y^{\epsilon_k})_i = D_1 y_i^{\epsilon_k} - D_1 \bar{y}_i \rightarrow F_0 + r_i - F_0$$

as $k \rightarrow \infty$, so that we may view r as a perturbation to the deformation gradient in an ‘infinitesimal’ neighbourhood of the defect. (2.27) implies that $s_i^\epsilon + C\epsilon^{3/2} \geq 0$ for $i = -N, \dots, N-1$, so that

$$\liminf_{k \rightarrow \infty} \sum_{i=-N_k}^{N_k-1} s_i^{\epsilon_k} + C\epsilon_k^{3/2} \geq \sum_{i=-\infty}^{\infty} \liminf_{k \rightarrow \infty} (s_i^{\epsilon_k} + C\epsilon_k^{3/2}). \quad (2.30)$$

Since the potentials ϕ_i are continuous and $\sigma_i^\epsilon \rightarrow \sigma(0)$ as $\epsilon \rightarrow 0$ with i fixed, we have that

$$\begin{aligned} \liminf_{k \rightarrow \infty} (s_i^{\epsilon_k} + \epsilon_k^{3/2}) &= \phi_2\left(F_0 + \frac{r_i + r_{i+1}}{2}\right) + \frac{1}{2}\phi_1(F_0 + r_i) + \frac{1}{2}\phi_1(F_0 + r_{i+1}) \\ &\quad - W(F_0) - \sigma(0)\left(F_0 + \frac{r_i + r_{i+1}}{2}\right) + \sigma(0)F_0 - \Sigma \frac{r_i + r_{i+1}}{2}, \\ &= \Phi_2(r_i + r_{i+1}) + \frac{1}{2}\Phi_1(r_i) + \frac{1}{2}\Phi_1(r_{i+1}), \end{aligned} \quad (2.31)$$

where we have used the fact that since $\bar{y}$ satisfies (2.17) pointwise, $\sigma(0) = W'(F_0) - \Sigma$. Note that

$$\lim_{k \rightarrow \infty} \sum_{i=-N_k}^{N_k-1} C\epsilon_k^{3/2} = \lim_{k \rightarrow \infty} C\epsilon_k^{1/2} = 0, \quad (2.32)$$

so then combining (2.30), (2.31) and (2.32), we have that

$$\liminf_{k \rightarrow \infty} \sum_{i=-\infty}^{\infty} s_i^{\epsilon_k} \geq \sum_{i=-\infty}^{\infty} \Phi_2\left(\frac{r_i + r_{i+1}}{2}\right) + \frac{1}{2}\Phi_1(r_i) + \frac{1}{2}\Phi_1(r_{i+1}).$$

Finally, by possibly taking further subsequences, we can assume that $(\mathcal{P}_{\epsilon_k} y^{\epsilon_k})_i$ converges uniformly for $i \in \{-2, -1, 0, 1\}$, and so

$$\liminf_{\epsilon \rightarrow 0} \mathcal{F}_1^\epsilon(y^\epsilon) = \liminf_{k \rightarrow \infty} \left(\sum_{i=-\infty}^{\infty} s_i^{\epsilon_k} + \tilde{E}_d(Dy^{\epsilon_k} - F_0) \right) \geq \tilde{E}_\infty(r) \geq \inf_{r \in \ell^2(\mathbb{Z})} \tilde{E}_\infty(r),$$

proving Lemma 2.6.1. □

Note that by the periodicity assumption, we have

$$\sum_{i=-N}^{N-1} (\mathcal{P}_\epsilon y^\epsilon)_i = 0$$

for any $y^\epsilon \in \mathcal{A}^\epsilon(L)$. If $\mathcal{P}_\epsilon y^\epsilon \rightharpoonup r$ in $\ell^1(\mathbb{Z})$, we could conclude that

$$\sum_{i=-\infty}^{\infty} r_i = 0;$$

however, since we have convergence only in $\ell^2(\mathbb{Z})$, this is false in general. As a corollary of the argument contained in the proof of Lemma 2.6.1, we have therefore demonstrated that the set of compactly supported mean zero sequences is dense in the weak topology on $\ell^2(\mathbb{Z})$.

2.6.2 The limsup inequality

The limsup inequality is the following statement.

Lemma 2.6.5. *For every $y \in \mathcal{A}(L)$, there exists a sequence $y^\epsilon \rightarrow y$ in L^2 such that*

$$\limsup_{\epsilon \rightarrow 0} \mathcal{F}_1^\epsilon(y^\epsilon) \leq \mathcal{F}_1(y).$$

This statement is trivial in the case where $y \neq \bar{y}$, so we only need to construct the sequence for $y = \bar{y}$. In order to construct the limsup sequence, we will show that there exists a minimiser of $\tilde{E}_\infty$, and then combine a suitable truncation of this minimiser with $\mathcal{T}^\epsilon \bar{y}$ to get the result.

Lemma 2.6.6. *There exist minimisers $r \in \ell^2(\mathbb{Z})$ of $\tilde{E}_\infty$ which satisfy the infinite system of nonlinear algebraic Euler–Lagrange equations*

$$\frac{1}{2} \Phi_2' \left(\frac{r_{i-1} + r_i}{2} \right) + \Phi_1'(r_i) + \frac{1}{2} \Phi_2' \left(\frac{r_i + r_{i+1}}{2} \right) = 0, \quad i \notin \{-2, -1, 0, 1\}, \quad (2.33a)$$

$$\frac{1}{2} \Phi_2' \left(\frac{r_{-3} + r_{-2}}{2} \right) + \Phi_1'(r_{-2}) + \frac{1}{2} \Psi_2' \left(\frac{r_{-2} + r_{-1}}{2} \right) = 0, \quad (2.33b)$$

$$\frac{1}{2} \Psi_2' \left(\frac{r_{-2} + r_{-1}}{2} \right) + \Psi_1'(r_{-1}) + \frac{1}{2} \Phi_2' \left(\frac{r_{-1} + r_0}{2} \right) = 0, \quad (2.33c)$$

$$\frac{1}{2} \Phi_2' \left(\frac{r_{-1} + r_0}{2} \right) + \Psi_1'(r_0) + \frac{1}{2} \Psi_2' \left(\frac{r_0 + r_1}{2} \right) = 0, \quad (2.33d)$$

$$\frac{1}{2} \Psi_2' \left(\frac{r_0 + r_1}{2} \right) + \Phi_1'(r_1) + \frac{1}{2} \Phi_2' \left(\frac{r_1 + r_2}{2} \right) = 0. \quad (2.33e)$$

Proof. Since $\tilde{E}_\infty(r) < +\infty$ for the constant sequence $r = 0$, $\inf_{r \in \ell^2(\mathbb{Z})} \tilde{E}_\infty(r) < +\infty$. Recall from (2.20) that

$$\tilde{E}_\infty(r) \geq \frac{1}{2}l \|r\|_{\ell^2(\mathbb{Z})}^2 + C.$$

This bound implies that $\tilde{E}_\infty$ is coercive, and applying Fatou's lemma as above with the pointwise lower bound (2.19) implies that $\tilde{E}_\infty$ is weakly lower semicontinuous. A standard application of the Direct Method of the Calculus of Variations now yields existence.

To obtain the Euler–Lagrange equations, suppose r is a minimiser of $\tilde{E}_\infty$. Let $e^i \in \ell^2(\mathbb{Z})$ be the sequence which has

$$e_j^i = \begin{cases} 1 & j = i, \\ 0 & \text{otherwise.} \end{cases}$$

Let $i \neq -2, -1, 0, 1$; for small enough $t > 0$, $\tilde{E}_\infty(r + te^i) < +\infty$, and

$$0 \leq \frac{\tilde{E}_\infty(r + te^i) - \tilde{E}_\infty(r)}{t} = \int_0^1 \frac{1}{2} \Phi_2' \left(\frac{r_{i-1} + r_i + st}{2} \right) + \Phi_1'(r_i + st) + \frac{1}{2} \Phi_2' \left(\frac{r_i + st + r_{i+1}}{2} \right) ds.$$

Applying the Dominated Convergence Theorem and repeating the argument for $t < 0$ now implies that the equations (2.33a) are satisfied. The same argument implies the other equations in (2.33), completing the proof. $\square$

In order to complete the proof of the limsup inequality, we will require a better understanding of minimisers of $\tilde{E}_\infty$, and so we prove the following sequence of results, which amount to regularity results for solutions of the Euler–Lagrange equations (2.33). From now on, we fix $r \in \ell^2(\mathbb{Z})$ to be one particular minimiser of $\tilde{E}_\infty$.

Lemma 2.6.7. *Suppose that $r \in \ell^2(\mathbb{N})$ solves (2.33a) for all $i \geq 2$. Then*

$$\begin{aligned} r_1 \geq 0 & \Rightarrow r_1 = \max_{j \in \mathbb{N}} \{r_j\}; \\ r_1 \leq 0 & \Rightarrow r_1 = \min_{j \in \mathbb{N}} \{r_j\}. \end{aligned}$$

Proof. We prove only the first conclusion, the proof of the second being similar. Suppose for contradiction that $r \in \ell^2(\mathbb{Z})$ solves (2.33a) and $r_1 \neq \max_{j \in \mathbb{N}} \{r_j\}$. Since $r_j \rightarrow 0$ as $j \rightarrow \infty$, it follows that r must have an interior maximum, i.e. there exists r_M with $M > 1$ such that

$$r_M = \max_{j \in \mathbb{N}} \{r_j\} > r_1 \geq 0.$$

Then because Φ_2 is concave, we have that Φ'_2 is monotone decreasing, and hence

$$\begin{aligned}
0 &= \frac{1}{2}\Phi'_2\left(\frac{r_{M-1}+r_M}{2}\right) + \Phi'_1(r_M) + \frac{1}{2}\Phi'_2\left(\frac{r_M+r_{M+1}}{2}\right), \\
&\geq \Phi'_2(r_M) + \Phi'_1(r_M), \\
&= W'(F_0 + r_M) - W'(F_0), \\
&= \int_0^{r_M} W''(F_0 + s) \, ds, \\
&\geq l r_M,
\end{aligned} \tag{2.34}$$

in contradiction to the statement that $r_M > 0$. $\square$

Corollary 2.6.1. *Suppose that $r \in \ell^2(\mathbb{N})$ solves (2.33a) for all $i \geq 2$. Then*

$$\begin{aligned}
r_1 \geq 0 &\Rightarrow r_i \geq r_{i+1} \geq 0 \text{ for all } i \in \mathbb{N}; \\
r_1 \leq 0 &\Rightarrow r_i \leq r_{i+1} \leq 0 \text{ for all } i \in \mathbb{N}.
\end{aligned}$$

Proof. Estimate (2.34) states that if

$$r_i = \max\{r_{i-1}, r_i, r_{i+1}\}, \quad \text{then } r_i \leq 0.$$

Similarly, it is possible to show that if

$$r_i = \min\{r_{i-1}, r_i, r_{i+1}\}, \quad \text{then } r_i \geq 0.$$

Suppose that r has a local maximum $r_M < 0$ with $M > 1$. Then $r_{M+1} \leq r_M < 0$. Since local minima can only occur when $r_i \geq 0$, r_{M+1} cannot be a local minimum, and so $r_{M+2} \leq r_{M+1} < 0$. Proceeding by induction, $r_i \leq r_M < 0$ for all $i \geq M$, which contradicts the fact that $r \in \ell^2(\mathbb{N})$. A similar argument prevents the existence of local minima r_M with $r_M > 0$.

Next suppose that $r_M = 0$ is a local maximum for $M > 1$. If $r_{M+1} < 0$, then the previous argument applies. If $r_{M+1} = 0$, then it too must be a local maximum or minimum, depending on the sign of r_{M+2} . If $r_{M+2} \neq 0$, then we can apply the previous arguments again to arrive at a contradiction, so by induction we have that $r_i = 0$ for all $i \geq M$.

We have therefore shown that there can be no internal maxima, unless they are degenerate in the sense that r is identically 0 after the maximum, and by a similar argument, we can show that there can be no internal minima except if they are degenerate in the same sense. We can now conclude that any solution of (2.33a) must be decreasing if $r_1 \geq 0$, or increasing if $r_1 \leq 0$, which concludes the proof. $\square$

Finally, we prove that minimisers exhibit exponential decay.

Lemma 2.6.8. *Suppose that $r \in \ell^2(\mathbb{N})$ solves (2.33a) for all $i \geq 2$. If $C \geq 0$ is a constant such that $0 \geq \Phi_2''(t) \geq -C$ for all $t \in [\inf r_j, \sup r_j]$, then setting $\lambda := \frac{C}{l+C}$, we have that*

$$|r_i| \leq \lambda^{i-1} |r_1| \quad (2.35)$$

for all $i \geq 2$.

Proof. We will only prove the result for $r_1 \geq 0$, since the other case is similar. Corollary 2.6.1 implies that $\sup r_j = r_1$ and $\inf r_j = 0$. By using the definitions of Φ_1 and Φ_2 and the Fundamental Theorem of Calculus, we may rewrite (2.33a) as

$$\begin{aligned} 0 &= \frac{1}{2} \Phi_2' \left(\frac{r_{i-1} + r_i}{2} \right) + \Phi_1'(r_i) + \frac{1}{2} \Phi_2' \left(\frac{r_i + r_{i+1}}{2} \right), \\ &= \frac{1}{2} \phi_2' \left(F_0 + \frac{r_{i-1} + r_i}{2} \right) + \phi_1'(F_0 + r_i) + \frac{1}{2} \phi_2' \left(F_0 + \frac{r_i + r_{i+1}}{2} \right) - W'(F_0), \\ &= \frac{1}{2} \left(\phi_2' \left(F_0 + \frac{r_{i-1} + r_i}{2} \right) - \phi_2'(F_0 + r_i) \right) + \frac{1}{2} \left(\phi_2' \left(F_0 + \frac{r_i + r_{i+1}}{2} \right) - \phi_2'(F_0 + r_i) \right) \\ &\quad + W'(F_0 + r_i) - W'(F_0), \\ &= \int_{r_i}^{r_{i-1}} \Phi_2'' \left(\frac{r_i + t}{2} \right) dt + \int_{r_i}^{r_{i+1}} \Phi_2'' \left(\frac{r_i + t}{2} \right) dt + \int_0^{r_i} W''(F_0 + t) dt. \end{aligned}$$

Using the conclusion of Corollary 2.6.1 once more, $r_{i-1} \geq r_i \geq r_{i+1}$, so we have

$$\begin{aligned} 0 &= \int_{r_i}^{r_{i-1}} \Phi_2'' \left(\frac{r_i + t}{2} \right) dt - \int_{r_{i+1}}^{r_i} \Phi_2'' \left(\frac{r_i + t}{2} \right) dt + \int_0^{r_i} W''(F_0 + t) dt, \\ &\geq - \int_{r_i}^{r_{i-1}} C dt + \int_0^{r_i} l dt, \end{aligned}$$

which following from the assumed bound on the second derivative of Φ_2 , and the l -convexity of W . Evaluating the integrals and rearranging gives

$$\lambda r_{i-1} \geq r_i,$$

which holds for any $i \geq 2$, and the decay estimate now follows by induction. $\square$

It should immediately be noted that since r_i converges to zero exponentially as $i \rightarrow \pm\infty$, $r \in \ell^1(\mathbb{Z})$: this fact will be crucial in what follows. This characterisation of the minimisers of $\tilde{E}_\infty$ is now employed to complete the proof of Lemma 2.6.5.

Proof of Lemma 2.6.5. Let the sequence of functions $y^{\epsilon, \delta}$ be given by

$$y^{\epsilon, \delta}(x) := \int_{-1/2}^x Dy^{\epsilon, \delta}(t) dt, \quad (2.36)$$

where we have set

$$Dy^{\epsilon, \delta}(x) := \begin{cases} D_1 \bar{y}_i + r_i - \bar{r}^\delta & x \in (x_i, x_{i+1}), i \in \{-K, \dots, K-1\}, \\ D_1 \bar{y}_i & x \in (x_i, x_{i+1}), i \notin \{-K, \dots, K-1\}, \end{cases}$$

$$\bar{r}^\delta := \delta \sum_{i=-K}^{K-1} r_i, \quad \text{and} \quad \delta := \frac{1}{2K}.$$

We will prove estimates for $y^{\epsilon, \delta}$, and then set δ as a function of ϵ in order to obtain the recovery sequence. Since $r \in \ell^1(\mathbb{Z})$, we have that

$$|\bar{r}^\delta| \leq \delta \sum_{i=-K}^{K-1} |r_i| \leq \delta \|r\|_{\ell^1(\mathbb{Z})}. \quad (2.37)$$

By construction, $y^{\epsilon, \delta} \in \mathcal{A}^\epsilon(L)$ as long as $\delta \geq \epsilon$, i.e. $K \leq N$, and it is straightforward to check that $y^{\epsilon, \delta(\epsilon)} \rightarrow \bar{y}$ in L^2 as $\epsilon \rightarrow 0$ for any sequence $\delta(\epsilon)$ such that $\epsilon \leq \delta(\epsilon) \leq 1$ for all ϵ .

Ensuring $W(Dy^{\epsilon, \delta})$ is well-defined. The first step we take is to check that $W(D_1 y_i^{\epsilon, \delta})$ is well-defined. Since $\tilde{E}_\infty(r) < +\infty$, for each $i \in \mathbb{Z}$

$$W(F_0 + r_i) < +\infty, \quad \text{and hence} \quad F_0 + r_i > 0.$$

Recalling from §2.5 that $F_0 = D\bar{y}(0) > 0$, and as $r \in \ell^2(\mathbb{Z})$, $r_i \rightarrow 0$ as $i \rightarrow \infty$, it follows that $F_0 + r_i$ is uniformly bounded away from 0. Next, by using the Mean Value Theorem and (2.37), we estimate for $i \in \{-K, \dots, K-1\}$ that

$$\begin{aligned} |D_1 y_i^{\epsilon, \delta} - F_0 - r_i| &= \left| \int_{x_i}^{x_{i+1}} D\bar{y} \, dx - \bar{r}^\delta - D\bar{y}(0) \right|, \\ &= |D\bar{y}(\xi) - \bar{r}^\delta - D\bar{y}(0)|, \\ &\leq \left| \int_0^\xi D^2 \bar{y}(x) \, dx \right| + \delta \|r\|_{\ell^1(\mathbb{Z})}, \\ &\leq |\xi| \|D^2 \bar{y}\|_\infty + \delta \|r\|_{\ell^1(\mathbb{Z})}, \\ &\leq \frac{\epsilon}{2\delta} \|D^2 \bar{y}\|_\infty + \delta \|r\|_{\ell^1(\mathbb{Z})}. \end{aligned}$$

Here, ξ is some point in (x_i, x_{i+1}) for which $|\xi| \leq K\epsilon = \frac{\epsilon}{2\delta}$. For fixed i , it is now clear that since $W(t)$ is Lipschitz for $t > 0$,

$$|W(D_1 y_i^{\epsilon, \delta}) - W(F_0 + r_i)| \leq C\left(\frac{\epsilon}{\delta} + \delta\right),$$

therefore $W(D_1 y_i^{\epsilon, \delta})$ is finite when $\epsilon \ll \delta \ll 1$. We can additionally estimate

$$\begin{aligned} |D_1 y_i^{\epsilon, \delta} - D\bar{y}(x)| &= \left| \int_{x_i}^{x_{i+1}} D\bar{y} \, dx - \bar{r}^\delta - D\bar{y}(x) \right|, \\ &\leq \epsilon \|D^2 \bar{y}\|_\infty + \delta \|r\|_{\ell^2(\mathbb{Z})}. \end{aligned} \quad (2.38)$$

Pointwise upper bounds on $s_i^{\epsilon, \delta}$. Next, we define $s_i^{\epsilon, \delta}$ in a similar fashion to (2.21), but adding and subtracting an extra $\phi_1(D_2 y_i^{\epsilon, \delta})$ term, we have

$$\begin{aligned} s_i^{\epsilon, \delta} &= \left(W(D_2 y_i^{\epsilon, \delta}) - \int_{x_i}^{x_{i+2}} W(D\bar{y}) \, dx \right) \\ &\quad + \left(\frac{1}{2} \phi_1(D_1 y_i^{\epsilon, \delta}) + \frac{1}{2} \phi_1(D_1 y_{i+1}^{\epsilon, \delta}) - \phi_1(D_2 y_i^{\epsilon, \delta}) \right) \\ &\quad + \int_{x_i}^{x_{i+2}} \left(\sigma D\bar{u} - \sigma^\epsilon D u^{\epsilon, \delta} - \Sigma(D y^{\epsilon, \delta} - D\bar{y}) \right) dx, \\ &=: T_1 + T_2 + T_3. \end{aligned} \tag{2.39}$$

T_1 can be treated using Jensen's inequality and the convexity of W :

$$\begin{aligned} T_1 &= W(D_2 y_i^{\epsilon, \delta}) - \int_{x_i}^{x_{i+2}} W(D\bar{y}) \, dx \\ &\leq \frac{1}{2} W(D_1 y_i^{\epsilon, \delta}) + \frac{1}{2} W(D_1 y_{i+1}^{\epsilon, \delta}) - \int_{x_i}^{x_{i+1}} W(D\bar{y}) \, dx, \\ &\leq \int_{x_i}^{x_{i+2}} W(D y^{\epsilon, \delta}) - W(D\bar{y}) \, dx, \\ &\leq \int_{x_i}^{x_{i+1}} W'(D y^{\epsilon, \delta})(D y^{\epsilon, \delta} - D\bar{y}) \, dx. \end{aligned} \tag{2.40}$$

The final integral term, T_3 , is bounded by

$$\begin{aligned} T_3 &= \int_{x_i}^{x_{i+2}} \sigma D\bar{u} - \sigma^\epsilon D u^{\epsilon, \delta} - \Sigma(D u^{\epsilon, \delta} - D\bar{u}) \, dx \\ &= \int_{x_i}^{x_{i+2}} (\sigma + \Sigma)(D\bar{u} - D u^{\epsilon, \delta}) + (\sigma - \sigma^\epsilon) D u^{\epsilon, \delta} \, dx, \\ &\leq \int_{x_i}^{x_{i+2}} W'(D\bar{y})(D\bar{y} - D y^{\epsilon, \delta}) \, dx + C\epsilon^{3/2} \|D u^{\epsilon, \delta}\|_2, \end{aligned} \tag{2.41}$$

using the Euler–Lagrange equations and the estimate proved in (2.26). The remaining part of the expression, T_2 , can then be estimated as follows:

$$\begin{aligned} T_2 &= \frac{1}{2} \phi_1(D_1 y_i^{\epsilon, \delta}) + \frac{1}{2} \phi_1(D_1 y_{i+1}^{\epsilon, \delta}) - \phi_1(D_2 y_i^{\epsilon, \delta}) \\ &= \frac{1}{4} \int_{D_1 y_i^{\epsilon, \delta}}^{D_1 y_{i+1}^{\epsilon, \delta}} \int_{D_1 y_i^{\epsilon, \delta}}^{D_1 y_{i+1}^{\epsilon, \delta}} \phi_1''\left(\frac{s+t}{2}\right) \, ds \, dt, \\ &\lesssim |D_1 y_{i+1}^{\epsilon, \delta} - D_1 y_i^{\epsilon, \delta}|^2, \end{aligned}$$

where we have used the fact that ϕ_1'' is bounded on the domain of integration for sufficiently small ϵ and δ , and $\phi_1 \in C^2$. If $i \in \{-K, \dots, K-1\}$, then applying the

Mean Value Theorem with $\xi \in (x_i, x_{i+1})$ and $\zeta \in (x_{i+1}, x_{i+2})$ gives

$$\begin{aligned} \frac{1}{2}\phi_1(D_1y_i^{\epsilon,\delta}) + \frac{1}{2}\phi_1(D_1y_{i+1}^{\epsilon,\delta}) - \phi_1(D_2y_i^{\epsilon,\delta}) &\lesssim |D\bar{y}(\xi) - D\bar{y}(\zeta) + r_{i+1} - r_i|^2, \\ &\lesssim (\|D^2\bar{y}\|_\infty\epsilon + |r_i| + |r_{i+1}|)^2, \\ &\lesssim \|D^2\bar{y}\|_\infty^2\epsilon^2 + |r_i|^2 + |r_{i+1}|^2. \end{aligned} \quad (2.42)$$

In the case where $i \notin \{-K, \dots, K-1\}$, we obtain

$$\frac{1}{2}\phi_1(D_1y_i^{\epsilon,\delta}) + \frac{1}{2}\phi_1(D_1y_{i+1}^{\epsilon,\delta}) - \phi_1(D_2y_i^{\epsilon,\delta}) \lesssim \epsilon^2 \|D^2\bar{y}\|_\infty.$$

Adding together (2.40), (2.41) and (2.42), for $i \in \{-K-1, \dots, K-1\}$ we have

$$\begin{aligned} s_i^{\epsilon,\delta} &\leq \int_{x_i}^{x_{i+2}} (W'(Dy^{\epsilon,\delta}) - W'(D\bar{y}))(Dy^{\epsilon,\delta} - D\bar{y}) \, dx + C\epsilon^{3/2}\|Du^{\epsilon,\delta}\|_2 \\ &\quad + C\epsilon^2 + C(|r_i|^2 + |r_{i+1}|^2), \\ &\lesssim \int_{x_i}^{x_{i+2}} |Dy^{\epsilon,\delta} - D\bar{y}|^2 \, dx + \epsilon^{3/2} + \epsilon^2 + |r_i|^2 + |r_{i+1}|^2, \\ &\lesssim (\epsilon + \delta)^2 + \epsilon^{3/2} + \epsilon^2 + |r_i|^2 + |r_{i+1}|^2, \\ &\lesssim \delta^2 + \epsilon^{3/2} + \epsilon^2 + |r_i|^2 + |r_{i+1}|^2, \end{aligned}$$

using $W' \in C^1$, estimate (2.38) and Jensen's inequality. For the other indices, we obtain

$$s_i^{\epsilon,\delta} \leq \int_{x_i}^{x_{i+2}} (W'(Dy^{\epsilon,\delta}) - W'(D\bar{y}))(Dy^{\epsilon,\delta} - D\bar{y}) \, dx + C\epsilon^{3/2}\|Du^{\epsilon,\delta}\|_2 \lesssim \epsilon^2 + \epsilon^{3/2}.$$

Conclusion of the argument. The two pointwise estimates just obtained imply

$$\sum_{i=-\infty}^{\infty} s_i^{\epsilon,\delta} \lesssim \sum_{i=-N}^{N-1} \epsilon^{3/2} + \sum_{i=-K}^K (|r_i|^2 + \delta^2) \lesssim \epsilon^{1/2} + \|r\|_{\ell^2(\mathbb{Z})}^2 + \delta.$$

By choosing $K = \lfloor \sqrt{N} \rfloor$, we have that $\delta \lesssim \epsilon^{1/2}$, and so an application of Fatou's Lemma with the pointwise upper bound we have just proven implies that

$$\limsup_{\epsilon \rightarrow 0} \sum_{i=-\infty}^{\infty} s_i^{\epsilon,\delta} + \tilde{E}_d(Dy^{\epsilon,\delta} - F_0) \leq \sum_{i=-\infty}^{\infty} \limsup_{\epsilon \rightarrow 0} s_i^{\epsilon,\delta} + \lim_{\epsilon \rightarrow 0} \tilde{E}_d(Dy^{\epsilon,\delta} - F_0) = \tilde{E}_\infty(r).$$

This now proves Lemma 2.6.5, and concludes the proof of Theorem 2.6.1. $\square$

2.7 Higher order contributions

To complete our study of the energy $\mathcal{F}^\epsilon$, and the proof of Theorem 2.3.3, we prove the final Γ -convergence result concerning the order of the next term in the asymptotic expansion. In order to do so, we consider the functional

$$\mathcal{F}_{1+\alpha}^\epsilon(y) := \frac{\mathcal{F}^\epsilon(y) - \mathcal{F}_0(\bar{y}) - \epsilon \mathcal{F}_1(\bar{y})}{\epsilon^{1+\alpha}},$$

where $\bar{y} = \operatorname{argmin}_{y \in \mathcal{A}(L)} \mathcal{F}_0(y)$.

Lemma 2.7.1. *Suppose that $r \in \operatorname{argmin}_{r \in \ell^2(\mathbb{Z})} \tilde{E}_\infty(r)$, and define $R := \sum_{i=-\infty}^{\infty} r_i$. Then*

$$\Gamma\text{-}\lim_{\epsilon \rightarrow 0} \mathcal{F}_{1+\alpha}^\epsilon(y) = \begin{cases} 0 & y = \bar{y}, \\ +\infty & \text{otherwise,} \end{cases}$$

if $R \neq 0$ and $\alpha \in [0, 1)$, and hence

$$\mathcal{F}^\epsilon(y) \stackrel{\Gamma}{=} \mathcal{F}_0(y) + \epsilon \mathcal{F}_1(y) + O(\epsilon^2).$$

Furthermore, in the case where $R = 0$ and $f = 0$, we have the stronger result that

$$\mathcal{F}^\epsilon(y) \stackrel{\Gamma}{=} \mathcal{F}_0(y) + \epsilon \mathcal{F}_1(y) + O(\lambda^{2/\epsilon}),$$

where $\lambda \in (0, 1)$ is the constant in (2.35).

Proof. First, begin by considering a sequence y^ϵ such that $\mathcal{F}_{1+\alpha}^\epsilon(y^\epsilon)$ is uniformly bounded for some $\alpha \in (0, 1)$. Writing

$$|\mathcal{F}_{1+\alpha}^\epsilon(y^\epsilon)| = \epsilon^{-\alpha} |\mathcal{F}_1^\epsilon(y^\epsilon) - \epsilon \tilde{E}_\infty(r)| \leq C,$$

it is clear that such sequences satisfy the hypothesis of Lemma 2.6.3, and hence there exists a subsequence which we do not relabel such that $\mathcal{P}_\epsilon y^\epsilon$ converges weakly to some $r \in \ell^2(\mathbb{Z})$. As a corollary of this result, it follows that along this subsequence $\mathcal{P}_\epsilon y^\epsilon$ is uniformly bounded in $\ell^2(\mathbb{Z})$, and hence in $\ell^\infty(\mathbb{Z})$; furthermore, as

$$(\mathcal{P}_\epsilon y^\epsilon)_i = D_1 y_i^\epsilon - D_1 \bar{y}_i$$

and $\bar{y} \in C^2(\Omega)$, it follows that Dy^ϵ is bounded in $L^\infty(\Omega)$.

We now proceed to prove the liminf inequality. Note that as in the proof of Lemma 2.6.1, we need only suppose that $y^\epsilon \rightarrow \bar{y}$ in L^2 , as in any other case the result is trivial.

Fixing N for now, let $K \in \{0, \dots, N\}$ and $\delta = 1/2K$, an additional length-scale centred at the defect. We may then write

$$\mathcal{F}_{1+\alpha}^\epsilon(y^\epsilon) = \epsilon^{-\alpha} \left(\sum_{i=-N}^{N-1} s_i^\epsilon - \tilde{E}_\infty(r) \right),$$

where s_i^ϵ was defined in (2.21). For $i \in \{-N, \dots, -K-1\} \cup \{K, \dots, N-1\}$, we may follow an almost identical argument to that given in the proof of Lemma 2.6.2 to bound s_i^ϵ below, but noting that $\|Du^\epsilon\|_\infty$ is uniformly bounded, (2.26) improves to give

$$\left| \int_{x_i}^{x_{i+2}} (\sigma - \sigma^\epsilon) Du^\epsilon dx \right| \lesssim \epsilon^2 \|Du^\epsilon\|_\infty, \quad (2.43)$$

and hence

$$s_i^\epsilon \geq \frac{1}{2} l \int_{x_i}^{x_{i+2}} |Dy^\epsilon - D\bar{y}|^2 dx - C\epsilon^2 \|Du^\epsilon\|_\infty. \quad (2.44)$$

Next consider the sum

$$S := \epsilon^{-\alpha} \left(\sum_{i=-K}^{K-1} s_i^\epsilon - \tilde{E}_\infty(r) \right).$$

Defining $\mathcal{P}_\delta y^\epsilon$ by

$$\mathcal{P}_\delta y^\epsilon = \begin{cases} D_1 y_i^\epsilon - F_0 & i \in \{-K, \dots, K-1\}, \\ 0 & \text{otherwise} \end{cases}$$

and using the definition of Φ_i and Ψ_i , we may now write

$$\begin{aligned} S &= \frac{1}{\epsilon^\alpha} \left(\tilde{E}_\infty(\mathcal{P}_\delta y^\epsilon) - \tilde{E}_\infty(r) + \sum_{i=-K}^{K-1} \left(W(F_0) + W'(F_0)(\mathcal{P}_\delta y^\epsilon)_i - \int_{x_i}^{x_{i+1}} W(D\bar{y}) dx \right) \right. \\ &\quad \left. - \sum_{i=-K}^{K-1} \left(\frac{1}{2} \sigma_{i+1}^\epsilon D_1 u_i^\epsilon + \frac{1}{2} \sigma_{i+2}^\epsilon D_1 u_{i+1}^\epsilon - \int_{x_i}^{x_{i+1}} \sigma D\bar{u} - \Sigma(Dy^\epsilon - D\bar{y}) dx \right) \right), \quad (2.45) \\ &=: \epsilon^{-\alpha} (T_1 + T_2 + T_3). \end{aligned}$$

Since $\tilde{E}_\infty(\mathcal{P}_\delta y^\epsilon) \geq \tilde{E}_\infty(r)$, it follows that $T_1 \geq 0$. Taylor expanding under the integral sign in T_2 and using the Euler–Lagrange equation (2.17),

$$\begin{aligned} T_2 &= \sum_{i=-K}^{K-1} \left(W'(F_0)(D_1 y_i^\epsilon - D_1 \bar{y}_i) - \int_{x_i}^{x_{i+1}} \frac{1}{2} W''(\theta_i) (D\bar{y} - F_0)^2 dx \right) \\ &\geq \sum_{i=-K}^{K-1} W'(F_0)(D_1 u_i^\epsilon - D_1 \bar{u}_i) - C\epsilon^{-1} \int_{-\delta}^{\delta} \left(\int_0^x D^2 \bar{y} dt \right)^2 dx, \\ &\geq \sum_{i=-K}^{K-1} (\sigma(0) + \Sigma)(D_1 u_i^\epsilon - D_1 \bar{u}_i) - C\delta^3 \epsilon^{-1} \|D^2 \bar{y}\|_\infty. \end{aligned}$$

Adding this estimate to T_3 , the terms involving Σ cancel, and we obtain

$$T_2 + T_3 \geq \sum_{i=-K}^{K-1} \int_{x_i}^{x_{i+1}} (\sigma - \sigma(0)) (D\bar{u} - Du^\epsilon) + (\sigma - \sigma^\epsilon) Du^\epsilon dx - C\delta^3 \epsilon^{-1}.$$

Taylor expanding σ at 0 under the integral sign and employing (2.43), we have

$$\begin{aligned} T_2 + T_3 &\geq \epsilon^{-1} \int_{-\delta}^{\delta} (D\bar{u} - Du^\epsilon) \sigma'(0) x dx - C\epsilon^2 \|Du^\epsilon\|_\infty - C\delta^3 \epsilon^{-1}, \\ &\geq f(0) \delta^2 \epsilon^{-1} \|D\bar{u} - Du^\epsilon\|_\infty - C\epsilon^2 \|Du^\epsilon\|_\infty - C\delta^3 \epsilon^{-1}. \end{aligned}$$

Combining the estimates for T_1 , T_2 and T_3 with (2.44), we have shown that

$$\mathcal{F}_{1+\alpha}^\epsilon(y^\epsilon) \geq -C\epsilon^{1-\alpha} \|Du^\epsilon\|_\infty - C\delta^3 \epsilon^{-1-\alpha} - f(0) \delta^2 \epsilon^{-1-\alpha} \|D\bar{u} - Du^\epsilon\|_\infty,$$

and hence setting $K = \lfloor N^\beta \rfloor$ where $\beta \in (\frac{\alpha+1}{2}, 1)$ implies that

$$\liminf_{\epsilon \rightarrow 0} \mathcal{F}_{1+\alpha}^\epsilon(y^\epsilon) \geq 0 \quad \text{for any } \alpha \in [0, 1),$$

completing the proof of the liminf inequality.

To prove the corresponding limsup inequality, let $y^{\epsilon, \delta}$ be defined as in (2.36). Defining $s_i^{\epsilon, \delta}$ as in (2.39),

$$\mathcal{F}_{1+\alpha}^\epsilon(y^{\epsilon, \delta}) = \epsilon^{-\alpha} \left(\sum_{i=-N}^{N-1} s_i^{\epsilon, \delta} - \tilde{E}_\infty(r) \right).$$

For $i \notin \{-K, \dots, K-1\}$, we obtain that

$$s_i^{\epsilon, \delta} \lesssim \epsilon^2 \|Du^{\epsilon, \delta}\|_\infty$$

by using (2.43). Next, recall the definition of S and T_1 , T_2 and T_3 in (2.45). Taylor expanding $\tilde{E}_\infty$ at r to second-order and using the Euler-Lagrange equations (2.33),

$$\begin{aligned} T_1 &= \tilde{E}_\infty(\mathcal{P}_\delta y^{\epsilon, \delta}) - \tilde{E}_\infty(r), \\ &\lesssim \sum_{i=-K}^{K-1} \left| \int_{x_i}^{x_{i+1}} D\bar{y}_i - F_0 dx - \bar{r}^\delta \right|^2 + \sum_{i \leq -K-1} |r_i|^2 + \sum_{i \geq K} |r_i|^2, \\ &\lesssim \epsilon^{-1} \int_{-\delta}^{\delta} |D\bar{y} - F_0|^2 dx + \sum_{i=-K}^{K-1} |\bar{r}^\delta|^2 + \lambda^{2/\delta}, \\ &\lesssim \delta^3 \epsilon^{-1} + \delta (R - \lambda^{1/\delta})^2 + \lambda^{2/\delta}. \end{aligned}$$

Since W is convex, it is straightforward to check that $T_2 \leq 0$, and a similar argument to that used above implies that

$$T_3 \leq f(0) \delta^2 \epsilon^{-1} \|Du^{\epsilon, \delta} - D\bar{u}\|_\infty + C\epsilon^2 \|Du^{\epsilon, \delta}\|_\infty + C\delta^3 \epsilon^{-1}.$$

Setting $\delta = \epsilon^\beta$, with $\beta \in (\frac{\alpha+1}{2}, 1)$, these estimates imply that

$$\limsup_{\epsilon \rightarrow 0} \mathcal{F}_{1+\alpha}^\epsilon(y^{\epsilon, \delta}) \leq 0,$$

which completes the proof of the first part of the statement.

To prove the second part of the statement, we note that in this case the situation simplifies considerably, so that for any function $0 < \omega(\epsilon) \ll \lambda^{2/\epsilon}$ as $\epsilon \rightarrow 0$,

$$\mathcal{F}_{\omega(\epsilon)}^\epsilon(y^\epsilon) = \frac{\tilde{E}_\infty(\mathcal{P}_\epsilon y^\epsilon) - \tilde{E}_\infty(r)}{\omega(\epsilon)} \geq 0;$$

this provides an immediate proof of the liminf inequality in this case. For the limsup inequality, taking $y^{\epsilon, \delta}$ as the recovery sequence as before, but this time with $\delta = \epsilon$, and taking T_1 , T_2 and T_3 as before, it can be checked directly that

$$T_1 \lesssim \delta(R - \lambda^{1/\epsilon})^2 + \lambda^{2/\epsilon} \lesssim \lambda^{2/\epsilon}, \quad T_2 \leq 0 \quad \text{and} \quad T_3 = 0.$$

Thus $\limsup_{\epsilon \rightarrow 0} \mathcal{F}_{\omega(\epsilon)}^\epsilon(y^{\epsilon, \epsilon}) = 0$ for any $\omega(\epsilon) \ll \lambda^{2/\epsilon}$, completing the proof of the result. $\square$

Lemma 2.7.1 provides a characterisation of the order of the next term in the Γ -expansion: we do not attempt to explicitly calculate the Γ -limit here, but briefly comment on the likely dependence of such a term if it were to exist.

To obtain the Γ -limit at the next order, we would need to fix $K = \lfloor \alpha N \rfloor$ for some $\alpha \in (0, 1)$ in the proof of Lemma 2.7.1 given above. It can then be seen that the leading order terms depend on the volume change introduced by the defect, R , and on the discretisation error $\sigma^\epsilon - \sigma$. The former contribution arises since the volume is constrained by the periodic boundary conditions along the sequence, but is unconstrained in the variational problem for $\tilde{E}_\infty$, while the latter contribution depends on the behaviour of f . Both are related to the ‘bending’ of the lattice through the strain gradient $D^2 \bar{y}$, and so it seems likely that the next term in the asymptotic expansion will depend upon the strain gradient in some way.

2.8 Discussion

In this chapter, we presented an analysis of a model for a point defect in a 1D chain of atoms interacting under assumptions which attempt to replicate a Lennard-Jones type interaction in an elastic regime. In so doing, we proved Lemma 2.6.8, which may be interpreted as showing that the perturbation to the minimiser from the continuum

model due to the defect is confined to an exponentially thin boundary layer. This exponential decay suggests that any interaction between defects of the type described here is likely to ‘decouple’ if one were to study a situation in which there were multiple defects which remain well-separated in the limit $\epsilon \rightarrow 0$.

We note here that this model concerns a codimension 1 defect, and so as remarked at the beginning of §1.2, the conclusions of this analysis should not be extrapolated to point defects in three dimensions, where they are codimension 3 defects. Rather, it would seem to be more analogous to the behaviour observed near crystalline twin boundaries. These are codimension 1 defects at which the lattice changes orientation abruptly, but where the strain required to accommodate this change remains small enough that the interface appears sharp (see for example [BSB03]). Such interfaces would seem to be consistent with exponential decay of the perturbation in the direction normal to the defect, as observed here.

Chapter 3

An anti-plane lattice model for screw dislocations in a BCC crystal

This chapter presents the model which is the second main topic of this work: an anti-plane lattice model describing the energy per unit length of $\frac{1}{2}[111]$ screw dislocations in a BCC lattice. This class of dislocations is one of the few found in nature which is of a ‘pure’ edge or ‘pure’ screw type; most dislocations observed have a Burgers vector which is neither parallel nor perpendicular to the dislocation line.

We begin in §3.1 by providing a kinematic description of dislocations in this context, allowing us to define what it means for an anti-plane deformation to contain a dislocation. §3.2 then discusses the class of finite domains considered in Chapter 5, and in §3.3, we define the energy difference functional which is analysed in detail in the two subsequent chapters.

3.1 A kinematic description of screw dislocations

3.1.1 Anti-plane displacements in a BCC crystal

Here, we will consider the body-centred cubic (BCC) lattice, which may be defined by

$$\mathcal{L} := B\mathbb{Z}^3 \quad \text{where} \quad B := s \begin{bmatrix} \sqrt{8/9} & \sqrt{2/9} & 0 \\ 0 & \sqrt{2/3} & 0 \\ 1/3 & -1/3 & 1 \end{bmatrix}$$

and $s > 0$ is a scaling factor that we leave undefined for now.

To define anti-plane displacements, we fix the lattice vector $\nu := [0, 0, s]$ and define the projection

$$\Pi_\nu := I - \frac{\nu}{|\nu|} \otimes \frac{\nu}{|\nu|},$$

which ‘flattens’ the Bravais lattice $\mathcal{L}$ onto the lattice plane with normal ν ; see Figure 3.1a. It is straightforward to check that the set $\Pi_\nu(\mathcal{L})$ is a two-dimensional triangular lattice embedded in $\mathbb{R}^3$ with lattice constant $s\sqrt{8/9}$; we will choose $s = \sqrt{9/8}$ so that the planar lattice constant is 1. We further shift the origin so that the projected set may be identified with

$$\Lambda := \left(\frac{1}{2}, \frac{\sqrt{3}}{6}\right)^T + [a_1, a_2] \cdot \mathbb{Z}^2, \quad \text{where } a_1 = (1, 0)^T \text{ and } a_2 = \left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right)^T.$$

An *anti-plane displacement* in the direction ν (or more simply, a *displacement*), is a map $y : \Lambda \rightarrow \mathbb{R}$. The set of all displacements is denoted $\mathscr{W}(\Lambda)$. A displacement y gives rise to a lattice *deformation* $Y : \mathcal{L} \rightarrow \mathbb{R}^3$,

$$Y(\eta) := \eta + y\left(\left(\frac{1}{2}, \frac{\sqrt{3}}{6}\right)^T + \Pi_\nu \eta\right)\nu, \quad \eta \in \mathcal{L}.$$

Let $y, \tilde{y}$ be displacements and $Y, \tilde{Y}$ the associated deformations. We say that $y, \tilde{y}$ are equivalent if $Y(\mathcal{L}) = \tilde{Y}(\mathcal{L})$ (i.e., they describe the same atomistic configurations). It is easy to see that $y, \tilde{y}$ are equivalent if and only if $(y - \tilde{y})(\Lambda) \subseteq \mathbb{Z}$.

In addition to displacements defined over the whole lattice Λ , we also consider displacements $y : \Omega \rightarrow \mathbb{R}$ of crystals with finite cross-section $\Omega \subset \Lambda$, and denote the set of such maps $\mathscr{W}(\Omega)$.

3.1.2 Bonds and bond lengths

Each $\xi \in \Lambda$ has six nearest neighbours in the full lattice, $\xi + a_i$, $i = 1, \dots, 6$, where $a_1 = (1, 0)^T$ and $a_i = R_6^{i-1}a_1$ where R_6 denotes a rotation through angle $\pi/3$. At a point $\xi \in \Omega \subseteq \Lambda$, we define the set of outward-pointing nearest neighbour bonds in Ω to be

$$\mathcal{R}_\xi^\Omega := \{(\xi, \eta) \mid \eta \in \Omega, |\xi - \eta| = 1\},$$

and furthermore the set of all bonds between nearest neighbours in Ω to be the union

$$\mathcal{B}^\Omega := \bigcup_{\xi \in \Omega} \mathcal{R}_\xi^\Omega = \{(\xi, \eta) \in \Lambda^2 \mid |\xi - \eta| = 1\}.$$

For any bond $b = (\xi, \xi + a_i)$, we denote the reverse bond by $-b := (\xi + a_i, \xi)$. In the particular case where $\Omega = \Lambda$, we will write $\mathcal{B}$ for $\mathcal{B}^\Lambda$, and $\mathcal{R}_\xi$ for $\mathcal{R}_\xi^\Lambda$.

For $y \in \mathscr{W}(\Omega)$ and $b = (\xi, \eta) \in \mathcal{B}^\Omega$ we define the difference operator

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

Moreover, we set $Dy := (Dy_b)_{b \in \mathcal{B}^\Omega}$. We also note that $Dy_{-b} = -Dy_b$.

With this notation, we can now define two important discrete function spaces. Due to the homogeneity of the lattice, we may assume without loss of generality that the point $\xi_0 = (0, \frac{\sqrt{3}}{3})^T \in \Omega$, and thus we define

$$\begin{aligned}\mathscr{W}_0(\Omega) &:= \{v \in \mathscr{W}(\Omega) \mid v(\xi_0) = 0 \text{ and } \text{supp}(Dv) \text{ is bounded}\}, \quad \text{and} \\ \mathscr{W}^{1,2}(\Omega) &:= \{v \in \mathscr{W}(\Omega) \mid v(\xi_0) = 0 \text{ and } Dv \in \ell^2(\mathcal{B}^\Omega)\}.\end{aligned}$$

It is shown in Proposition 9 of [OS12] that $\mathscr{W}^{1,2}(\Lambda)$, equipped with the inner product

$$\langle u, v \rangle := \sum_{b \in \mathcal{B}} Du_b Dv_b$$

is a Hilbert space and $\mathscr{W}_0(\Lambda) \subset \mathscr{W}^{1,2}(\Lambda)$ is dense. It may easily be seen that the same is true when Λ is replaced by $\Omega \subset \Lambda$.

We now introduce a crucial concept required to define the notion of a dislocation. We denote the set of *bond length 1-forms* by

$$[Dy] := \{\alpha : \mathcal{B}^\Omega \rightarrow [-1/2, 1/2] \mid \alpha_{-b} = -\alpha_b \text{ and } Dy_b - \alpha_b \in \mathbb{Z} \text{ for all } b \in \mathcal{B}^\Omega\}. \quad (3.1)$$

We note that, if $Dy_b \notin \frac{1}{2} + \mathbb{Z}$ for all $b \in \mathcal{B}^\Omega$, then $\alpha \in [Dy]$ is unique, but in general there is ambiguity in the definition of α . This non-uniqueness is an issue which we will return to in §3.1.6.

The motivation behind this definition is that α_b defines the ‘shortest bond length’ between the two lines of nuclei represented by the 2D lattice sites ξ, ξ' , where $b = (\xi, \xi')$, in that

$$\min_{\substack{\eta, \eta' \in \mathcal{L} \\ \Pi_\nu \eta = \xi, \Pi_\nu \eta' = \xi'}} |y(\eta) - y(\eta')| = \sqrt{1 + \alpha_b^2};$$

see also Figure 3.1b for an illustration.

The importance of the concept of bond length stems from the fact that due to the invariance of the lattice under the addition of integer ‘shifts’, the energy of the lattice can only depend on α_b , but not on Dy_b directly.

3.1.3 The lattice complex

We now review some terminology of discrete algebraic topology which is convenient for our analysis. We follow the language described in [AO05], where further details and applications to the study of dislocations can be found. For further details on the definition of a CW complex and other aspects of algebraic topology, see for example [Hat02].

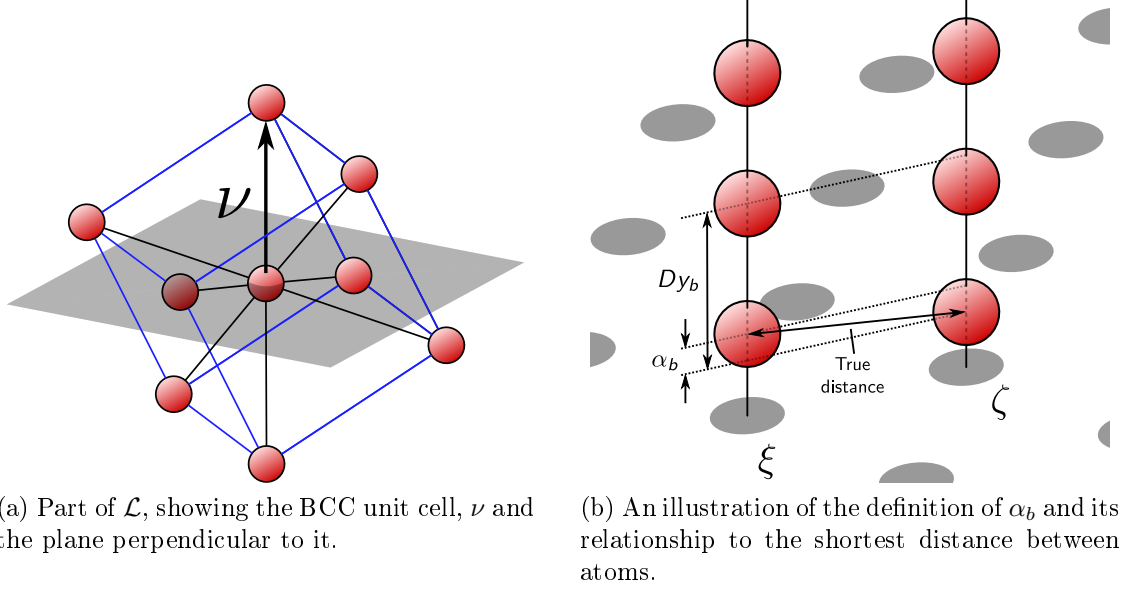


Figure 3.1: The lattice geometry.

Repeating the definitions of $\Lambda, \mathcal{B}$, we define a lattice complex as in §2.3.3 of [AO05] to be a CW complex with

$$\begin{aligned}\Lambda &:= \left\{ \xi \in \mathbb{R}^2 \mid \xi \in \Pi_\nu \mathcal{L} + \left(\frac{1}{2}, \frac{\sqrt{3}}{6}\right)^T \right\}, \\ \mathcal{B} &:= \left\{ (\xi, \zeta) \in \Lambda^2 \mid |\xi - \zeta| = 1 \right\}, \quad \text{and} \\ \mathcal{C} &:= \left\{ (\xi, \zeta, \eta) \in \Lambda^3 \mid (\xi, \zeta), (\zeta, \eta), (\eta, \xi) \in \mathcal{B} \right\}\end{aligned}$$

denoting the sets of 0-cells, 1-cells and 2-cells of the lattice complex respectively (see Figure 3.2 for an illustration). From now on, we will not explicitly use the terms p -cell, p -chain and p -cochain as defined in §2.2 of [AO05], preferring instead the more evocative terminology ‘lattice points’ for elements of Λ , ‘bonds’ for elements of $\mathcal{B}$, and ‘cells’ for elements of $\mathcal{C}$. We note the additive structure that may be defined on these objects, and write $a \in A$ to mean that a is an elementary p -cell contained in the p -chain A . We also frequently use the boundary operator ∂ , which maps p -chains to their boundaries, assigning orientations in the usual way.

We then follow §3 of [AO05] in defining p -forms and integration on the lattice, writing

$$\int_U F := \sum_{e \in U} F(e),$$

where U is a p -chain, e are p -cells, and F is a p -form (i.e. a real-valued function on

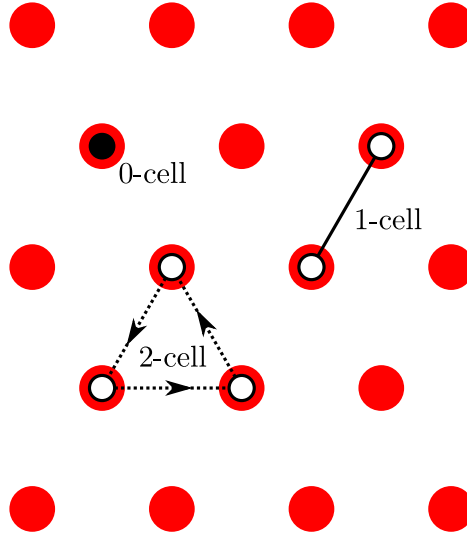


Figure 3.2: An illustration of 0-, 1- and 2-cells in the triangular lattice. The arrows show the orientation of the positively-oriented 2-cell. Note that orientation only makes sense for 1- and 2-cells.

p -cells). We note that this definition is linear in F and U , in the sense that

$$\begin{aligned} \int_{U+V} \lambda F + G &= \lambda \sum_{e \in U} F(e) + \lambda \sum_{e \in V} F(e) + \sum_{e \in U} G(e) + \sum_{e \in V} G(e), \\ &= \lambda \int_U F + \int_U G + \lambda \int_V F + \int_V G, \end{aligned}$$

for any $\lambda \in \mathbb{R}$, p -chains U and V , and p -forms F and G .

For $\Omega \subset \Lambda$, we define the corresponding sets of cells to be

$$\mathcal{C}^\Omega := \{(\xi, \zeta, \eta) \in \mathcal{C} \mid \xi, \zeta, \eta \in \Omega\}.$$

It is straightforward to check that Ω , $\mathcal{B}^\Omega$ and $\mathcal{C}^\Omega$ together satisfy the definition of a CW subcomplex of the full lattice complex presented above, and so we may make use of the same definitions of integration and p -forms restricted to this subcomplex.

We remark here that with the definition of the complexes above, ‘bond length 1-forms’ α as defined in §3.1.2 are true 1-forms in the sense defined in §3.1 of [AO05].

We will also use the notion of lattice paths, which we define in the natural way as 1-chains

$$\Gamma := \sum_{k=1}^L (\xi_k, \xi_{k+1}),$$

where $(\xi_k, \xi_{k+1}) \in \mathcal{B}$ for each k . We denote the length of a path Γ by $|\Gamma| := L$.

3.1.4 Measures of lattice distance

Since we will make use of more than simply the algebraic structure that a lattice complex entails, we will occasionally abuse the notation given above by identifying bonds and cells with their closed convex hulls; that is, we write

$$\begin{aligned} x \in b = (\xi, \zeta) & \quad \text{to mean} \quad x \in \text{conv}\{\xi, \zeta\}, & \text{and} \\ x \in C = (\xi, \zeta, \eta) & \quad \text{to mean} \quad x \in \text{conv}\{\xi, \zeta, \eta\}, \end{aligned}$$

where $\text{conv}(\Omega)$ denotes the closed convex hull of a set $\Omega \subset \mathbb{R}^2$; it will be clear from the context whether we are referring to spatial points or subchains. Since we frequently refer to them, we define x^C to be the barycentre of a cell C , and C_0 the cell for which $x^{C_0} = 0$.

One form of distance between elements in the complex that we employ is the usual notion of Euclidean distance of sets,

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

In Chapter 4, we will frequently refer to the distance of cells from the origin, and so to keep notation concise, we set

$$d_\xi := \text{dist}(0, \xi), \quad d_b := \text{dist}(0, b), \quad \text{and} \quad d_C := \text{dist}(0, C).$$

Furthermore, it will also be convenient to employ a graph theoretic notion of distance. Since Λ can be identified with a planar graph with edges $b \in \mathcal{B}$, we can further identify cells with nodes in the dual graph, and bonds as edges in this graph (see §4.6 of [Die10]). This allows us to define the *hopping distance*, $\text{hop}_2(C, C')$ as the length of the shortest path in the dual graph between the cells $C, C' \in \mathcal{C}$, as in §1.3 of [Die10]. We note that since the dual graph is connected, this distance is always finite, and we have the following ‘triangle inequality’ for any dual lattice points A, B and C :

$$\text{hop}_2(A, C) \leq \text{hop}_2(A, B) + \text{hop}_2(B, C). \quad (3.2)$$

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

$$\begin{aligned} G^C(x) &:= R_6^i(x - x^C) = 0 \quad \text{where } i \in \{0, 1\} \text{ is such that } G^C(\Lambda) = \Lambda, \quad \text{and} \\ H^C(x) &:= (G^C)^{-1}(x) = R_6^{-i}x + x^C, \end{aligned}$$

noting 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

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

3.1.6 The Burgers vector

We now define the *Burgers vector* as used in this model. This is the fundamental geometric concept describing the nature of a dislocation [HL82].

We call a path $\Gamma = \sum_{k=1}^L (\xi_k, \xi_{k+1})$ as defined in §3.1.3 a *Burgers loop* (or simply a *loop*) if $\Gamma = \partial A$, where A is a sum of positively-oriented cells in $\mathcal{C}^\Omega$. If Γ is a loop, $y \in \mathcal{W}(\Omega)$, and $\alpha \in [Dy]$ is an associated bond length 1-form, then

$$\int_{\Gamma} \alpha = \sum_{b \in \Gamma} Dy_b + \sum_{b \in \Gamma} (\alpha_b - Dy_b) = 0 + N \in \mathbb{Z}.$$

We call the integer N the Burgers vector of the bond length 1-form α around the loop Γ .

Definition 3.1.1 (Dislocation core). A *dislocation core* of a bond length 1-form α is a positively oriented 2-cell $C \in \mathcal{C}^\Omega$ such that $\int_{\partial C} \alpha \neq 0$.

We will refer to cores as being ‘contained in’ α . For future reference, we remark that

$$\left| \int_{\partial C} \alpha \right| \leq \frac{|\partial C|}{2} = \frac{3}{2}. \quad (3.3)$$

It follows that the Burgers vector around a single 2-cell can only be $-1, 0$ or 1 , and hence we define the sets of dislocation cores

$$\begin{aligned} \mathcal{C}^+[\alpha] &:= \left\{ C \in \mathcal{C}^\Omega \mid C \text{ positively oriented, } \int_{\partial C} \alpha = +1 \right\}, \\ \mathcal{C}^-[\alpha] &:= \left\{ C \in \mathcal{C}^\Omega \mid C \text{ positively oriented, } \int_{\partial C} \alpha = -1 \right\}, \\ \mathcal{C}^\pm[\alpha] &:= \mathcal{C}^+[\alpha] \cup \mathcal{C}^-[\alpha]. \end{aligned}$$

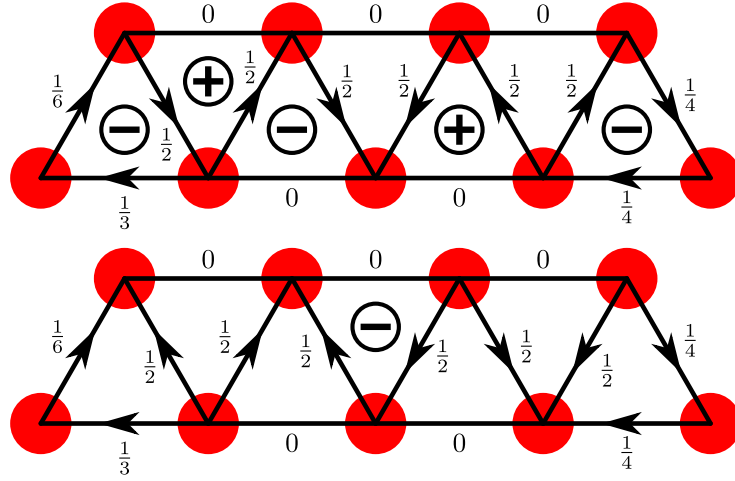


Figure 3.3: Two examples of bond length 1-forms corresponding to the same deformation. The numbers are the value of the 1-form on the relevant bond, and arrows indicate the bond direction in which it is positive. Note that both the number and the positions of the dislocation cores present change, but the sum of the Burgers vectors does not.

Remark 3.1.1. It is interesting to note that if $\alpha, \alpha' \in [Dy]$, then they need not have the same number of cores; see Figure 3.3 for an illustration of this fact.

The only point at which this ambiguity is an issue is if α has $C, C' \in \mathcal{C}^\pm[\alpha]$ which are adjacent. In that case, it may be checked that the $b \in \partial C$ such that $-b \in \partial C'$ must have $\alpha_b \in \{-1/2, 0, 1/2\}$. In the case where $\alpha_b = \pm 1/2$, redefining $\alpha_b = \mp 1/2$ removes these cores and α remains a bond length 1-form in $[Dy]$, so we will always assume that minimising sequences have $\alpha_b = 0$ for any bond b shared by 2 adjacent cores.

For a deformation of the infinite lattice, the *net Burgers vector* is obtained by summing the signs of the cores, or equivalently, by computing the Burgers vector on a sufficiently large loop enclosing all cores. Since $\alpha \in [Dy]$ is not necessarily unique for a given y , we ensure that such a concept can be defined unambiguously.

For our purposes it will be enough to consider displacements with some prescribed far-field behaviour.

Proposition 3.1.1. *Let $y \in \mathcal{W}(\Lambda)$ and $\alpha \in [Dy]$ such that $\alpha_b \rightarrow 0$ as $d_b \rightarrow \infty$. Then, for any $\alpha' \in [Dy]$, $\mathcal{C}^\pm[\alpha']$ is finite and*

$$\sum_{C \in \mathcal{C}^\pm[\alpha']} \int_{\partial C} \alpha' = \sum_{C \in \mathcal{C}^\pm[\alpha]} \int_{\partial C} \alpha = \int_{\Gamma} \alpha, \quad (3.4)$$

where Γ is any loop that encloses all cores in α .

Proof. If $\alpha_b \rightarrow 0$ as $d_b \rightarrow \infty$ then

$$\int_{\partial C} \alpha \rightarrow 0 \quad \text{as} \quad d_C \rightarrow \infty.$$

Since $\int_{\partial C} \alpha \in \mathbb{Z}$ it follows that $\int_{\partial C} \alpha = 0$ for d_C sufficiently large, and hence the number of dislocation cores present in α is finite.

Moreover, since $\alpha_b \in (-1/2, 1/2)$ for d_b sufficiently large, it follows that $\alpha_b = \alpha'_b$ for all $\alpha' \in [Dy]$ and d_b sufficiently large. In particular, $\mathcal{C}^\pm[\alpha']$ is also finite.

To prove (3.4), let Γ be a loop that encloses all the cores in α for which $\Gamma = \partial A$. Then

$$\int_{\Gamma} \alpha = \sum_{C \in A} \int_{\partial C} \alpha = \sum_{C \in \mathcal{C}^\pm[\alpha]} \int_{\partial C} \alpha.$$

Taking Γ such that $\alpha_b = \alpha'_b$ for all $b \in \Gamma$ we obtain the first identity in (3.4) as well. $\square$

The other case in which we need to ensure we have a well-defined net Burgers vector is that of a finite set Ω . In this case, we need to further restrict the bond-length 1-forms in order to ensure the net Burgers vector is unique. Let $\Omega \subset \Lambda$ be finite, and let $\mathcal{C}_+^\Omega$ be

$$\mathcal{C}_+^\Omega := \sum \{C \in \mathcal{C}^\Omega \mid C \text{ positively oriented}\}.$$

If $y \in \mathcal{W}(\Omega)$ and $\alpha \in [Dy]$, we call α *well-oriented* if $\alpha_b \in (-\frac{1}{2}, \frac{1}{2}]$ for all $b \in \partial \mathcal{C}_+^\Omega$. It is clear that for any $y \in \mathcal{W}(\Omega)$ there always exists a well-oriented bond-length 1-form $\alpha \in [Dy]$. We now show that the net Burgers vector can be defined unambiguously for such α .

Proposition 3.1.2. *Suppose that $\Omega \subset \Lambda$ is finite, $y \in \mathcal{W}(\Omega)$, and $\alpha, \alpha' \in [Dy]$ are well-oriented. Then*

$$\sum_{C \in \mathcal{C}^\pm[\alpha']} \int_{\partial C} \alpha' = \sum_{C \in \mathcal{C}^\pm[\alpha]} \int_{\partial C} \alpha = \int_{\mathcal{B}_+^{\partial \Omega}} \alpha.$$

Proof. By definition, $\alpha'_b = \alpha_b$ for all $b \in \partial \mathcal{C}_+^\Omega$, and hence

$$\sum_{C \in \mathcal{C}^\pm[\alpha']} \int_{\partial C} \alpha' = \sum_{C \in \mathcal{C}_+^\Omega} \int_{\partial C} \alpha' = \int_{\partial \mathcal{C}_+^\Omega} \alpha' = \int_{\partial \mathcal{C}_+^\Omega} \alpha = \sum_{C \in \mathcal{C}_+^\Omega} \int_{\partial C} \alpha = \sum_{C \in \mathcal{C}^\pm[\alpha]} \int_{\partial C} \alpha. \quad \square$$

These two results permit us to define the *net Burgers vector*.

Definition 3.1.2 (Net Burgers vector). Suppose $\Omega \subseteq \Lambda$, $y \in \mathcal{W}(\Omega)$ and either (i) $\Omega = \Lambda$ and $\alpha_b \rightarrow 0$ as $d_b \rightarrow \infty$ for some $\alpha \in [Dy]$; or (ii) Ω is finite; then we define the *net Burgers vector* of y to be

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

where if (i) holds, $\alpha \in [Dy]$ is arbitrary, and if (ii) holds, $\alpha \in [Dy]$ is well-oriented.

The quantity $B[y]$ can be experimentally observed from outside the system, by determining the strain at ‘infinity’, or at the boundary of the crystal. For example, if $B[y] = 1$, then this tells the observer that there must be at least one dislocation in the system, but nothing about the total number.

3.1.7 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

$$(C, s) \in \mathcal{D} \quad \text{implies that} \quad (C, -s) \notin \mathcal{D}. \quad (3.5)$$

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

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

and in the case where Ω is finite, we define the minimum separation between the dislocations and the boundary to be

$$S_{\mathcal{D}} := \inf \{ \text{dist}(C, b) \mid b \in \partial \mathcal{C}_+^\Omega \}.$$

3.2 Convex lattice polygons

We now make precise the class of finite $\Omega \subset \Lambda$ that we will consider in Chapter 5.

We say that $\Omega \subset \Lambda$ is a *convex lattice polygon* if

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

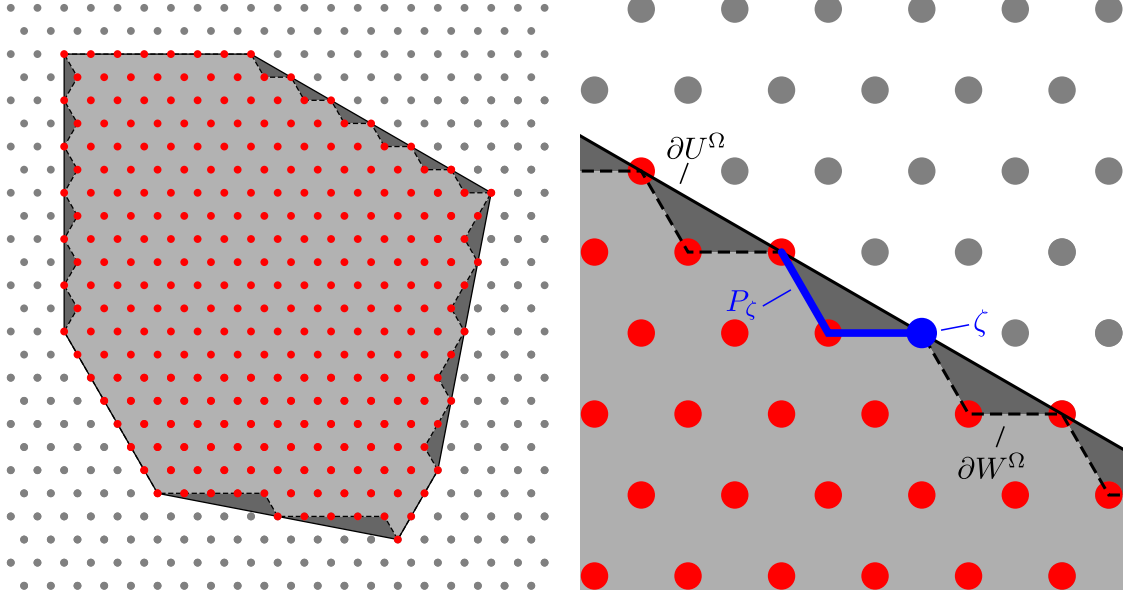


Figure 3.4: The figure on the left shows an example of a convex lattice polygon. Here, Ω is the set of red points, W^Ω is the light grey region and the dark grey region corresponds to $U^\Omega \setminus W^\Omega$. The boundaries of U^Ω and W^Ω are denoted by dashed and plain lines respectively. The figure on the right illustrates the definition of P_ζ , clearly showing the periodic structure of ∂W^Ω .

For a convex lattice polygon, we define corresponding ‘continuum’ domains

$$U^\Omega := \text{conv}(\Omega) \quad \text{and} \quad W^\Omega := \text{clos}(\mathcal{C}_+^\Omega).$$

We note that $\Omega \subset W^\Omega \subseteq U^\Omega$. To quantify the size of Ω , we define the ρ_Ω to be

$$\rho_\Omega := \sup_{x, x' \in U^\Omega} \text{dist}(x, x').$$

The positively-oriented boundary ∂W^Ω may be expressed as the union

$$\partial W^\Omega = \partial \mathcal{C}_+^\Omega \cup \{\xi \in \partial b \mid b \in \partial \mathcal{C}_+^\Omega\},$$

i.e. the set of bonds which follow the positively-oriented boundary of the entire subcomplex within the full lattice and the set of lattice points connected by such bonds. Since we will sum over this set of lattice points later, for notational convenience we write $\xi \in \partial W^\Omega$ to mean $\xi \in \partial W^\Omega \cap \Omega$.

It may be readily checked that ∂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 $\kappa_0 := \kappa_M$.

We define $\Gamma_m := (\kappa_{m-1}, \kappa_m) \subset \mathbb{R}^2$ to be the straight segments of the boundary. It is clear that $\kappa_m \in \Omega$ for all m .

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

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

Define the *lattice tangent vector* to Γ_m to be

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

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

$$\partial W^\Omega = \bigcup_{m=1}^M \bigcup_{j=0}^{J_m} P_{\kappa_m + j \tau_m} \quad \text{where} \quad P_\zeta := \{x \in \partial W^\Omega \mid (x - \zeta) \cdot \tau_m \in [0, |\tau_m|^2]\}. \quad (3.6)$$

An illustration of the definition of P_ζ may be found on the right-hand side of Figure 3.4. Denoting the 1-dimensional Hausdorff measure by $\mathcal{H}^1$, we define the *index* of Γ_m and of ∂W^Ω respectively, to be

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

3.3 Energy difference functional

We now introduce another key concept in the formulation of the main results of the two following chapters: the energy difference function. We assume that lattice sites (corresponding to lines of atoms in the BCC crystal) interact via a nearest-neighbour pair potential $\psi : \mathbb{R} \rightarrow \mathbb{R}$, which satisfies the following properties:

Assumptions on the potential ψ .

($\psi 0$) $\psi \in C(\mathbb{R}) \cap C^4(\mathbb{R} \setminus (\mathbb{Z} + 1/2))$;

($\psi 1$) ψ is 1-periodic;

($\psi 2$) ψ is even;

($\psi 3$) $\psi(r) = 0$ if and only if $r \in \mathbb{Z}$;

($\psi 4$) $\psi''(0) = \mu > 0$.

These latter assumptions are quite general, and are natural in the physical context: $(\psi 1)$ and $(\psi 2)$ encode lattice symmetries, and $(\psi 3)$ and $(\psi 4)$ state that the system has a stable crystalline ground state.

Assumption $(\psi 0)$ is simply the minimal regularity required for the proofs of subsequent chapters: it may be possible to weaken this regularity assumption further, but this would add little, at the expense of readability. We note that the results of Chapter 5 will require the slightly stronger assumption that $\psi \in C^4(\mathbb{R})$.

We further note that additional technical assumptions on ψ will be required in Chapters 4 and 5, but these are discussed in the relevant context, and are not required for the derivation of the model presented here. The prototypical example of a potential satisfying all of the assumptions here is $\psi(r) = \psi^{\text{lin}}(r) := \frac{1}{2} \text{dist}(r, \mathbb{Z})^2$.

Let $\Omega \subseteq \Lambda$. For two displacements $y, \tilde{y} \in \mathcal{W}(\Omega)$ we define the energy difference functional, formally for the moment, as

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

If Ω is finite, it is immediate that $E^\Omega(y; \tilde{y})$ is well-defined, since it is simply a finite sum. Similarly, if $\Omega = \Lambda$ and $y - \tilde{y} \in \mathcal{W}_0(\Lambda)$, then $E^\Lambda(y; \tilde{y})$ is also well-defined since the sum is effectively finite.

For arbitrary displacements $y, \tilde{y} \in \mathcal{W}(\Lambda)$, $E^\Lambda(y; \tilde{y})$ need not be well-defined. However, we next show that under certain conditions, E^Λ can be extended by continuity to relative displacements $y - \tilde{y} \in \dot{\mathcal{W}}^{1,2}(\Lambda)$.

3.3.1 Extension of the energy difference functional

Fix a displacement $\hat{y} \in \mathcal{W}(\Lambda)$ and define the functional $\mathcal{E}(u) := E^\Lambda(\hat{y} + u; \hat{y})$, which is always well-defined for $u \in \mathcal{W}_0(\Lambda)$. If $D\hat{y}_b \in \mathbb{R} \setminus (\mathbb{Z} + (\frac{1}{2} - \epsilon, \frac{1}{2} + \epsilon))$ for all $b \in \mathcal{B}$, and for some $\epsilon > 0$, then the first and second variations (in the sense of directional derivatives) are also well-defined, and given by

$$\langle \delta \mathcal{E}(0), v \rangle = \sum_{b \in \mathcal{B}} \psi'(D\hat{y}_b) \cdot Dv_b, \quad \text{for } v \in \mathcal{W}_0(\Lambda), \quad \text{and} \quad (3.7)$$

$$\langle \delta^2 \mathcal{E}(0) v, w \rangle = \sum_{b \in \mathcal{B}} \psi''(D\hat{y}_b) \cdot Dv_b Dw_b \quad \text{for } v, w \in \mathcal{W}_0(\Lambda). \quad (3.8)$$

The assumptions on ψ imply that $\psi''(D\hat{y}_b)$ is uniformly bounded, so $\delta^2 \mathcal{E}(0)$ can clearly be extended by continuity to $v, w \in \dot{\mathcal{W}}^{1,2}(\Lambda)$, but this is less obvious for $\delta \mathcal{E}(0)$ or for $\mathcal{E}$ itself. We first state a general result.

Lemma 3.3.1. *Let $\hat{y} \in \mathcal{W}(\Lambda)$ satisfy $D\hat{y}_b \in \mathbb{R} \setminus (\mathbb{Z} + (\frac{1}{2} - \epsilon, \frac{1}{2} + \epsilon))$ for some $\epsilon > 0$ and suppose that $\delta\mathcal{E}(0)$ is a bounded linear functional ($\langle \delta\mathcal{E}(0), v \rangle \leq C\|Dv\|_2$ for all $v \in \mathcal{W}_0(\Lambda)$). Then, $\mathcal{E} : \mathcal{W}_0(\Lambda) \rightarrow \mathbb{R}$ is continuous with respect to the norm $\|D \cdot\|_2$; hence, there exists a unique continuous extension of $\mathcal{E}$ to $\dot{\mathcal{W}}^{1,2}(\Lambda)$.*

Proof. The proof of this result is analogous to the proof of Theorem 2.8 (ii) in [OT13]. For convenience we give a brief outline.

For $u \in \mathcal{W}_0(\Lambda)$ it is easy to see that

$$\mathcal{E}(u) = \sum_{b \in \mathcal{B}} [\psi(D\hat{y}_b + Du_b) - \psi(D\hat{y}_b) - \psi'(D\hat{y}_b)Du_b] + \sum_{b \in \mathcal{B}} \psi'(D\hat{y}_b)Du_b.$$

Since we assume that $\delta\mathcal{E}(0)$ is a bounded functional, the second term on the right-hand side is continuous. Using the fact that $\|Dw\|_\infty \leq \|Dw\|_2$, the smoothness of ψ , and the fact that each summand in the first group is effectively quadratic in Du_b , it is easy to show that the first term on the right-hand side is continuous as well. $\square$

For future reference, we now derive a simple condition on $\hat{y}$ under which $\delta\mathcal{E}(0)$ is a bounded functional. Applying summation by parts to (3.7) we obtain

$$\langle \delta\mathcal{E}(0), v \rangle = \sum_{\xi \in \Lambda} f(\xi) \cdot v(\xi), \quad \text{where} \quad f(\xi) := \sum_{b \in \mathcal{R}_\xi} \psi'(D\hat{y}_b) \quad (3.9)$$

is the force acting on atom ξ under the displacement $\hat{y}$. The following result states that, if $\hat{y}$ is sufficiently close to equilibrium in the far-field, then $\delta\mathcal{E}(0)$ is a bounded linear functional.

Lemma 3.3.2. *Suppose that a displacement $\hat{y} \in \mathcal{W}(\Lambda)$ has associated forces $f(\xi)$ satisfying the bound $|f(\xi)| \leq C_1(1 + |\xi|)^{-t}$ for some $t > 2$ and for all $\xi \in \Lambda$, then $\langle \delta\mathcal{E}(0), v \rangle \leq C_2\|Dv\|_2$ for all $v \in \mathcal{W}_0(\Lambda)$.*

Proof. Proposition 12 in [OS12] immediately implies that

$$\left\| \frac{v}{\log(|\xi|+2)} \right\|_\infty \leq C\|Dv\|_2, \quad (3.10)$$

for some constant $C > 0$. (This inequality is essentially a consequence of the embedding $\|v\|_{\text{BMO}} \leq C\|\nabla v\|_{L^2}$ for $v \in C^1(\mathbb{R}^2)$.)

We can therefore estimate

$$|\langle \delta\mathcal{E}(0), v \rangle| \leq \sum_{\xi \in \Lambda} |f(\xi)| |v(\xi)| \leq \|\log(|\xi|+2)f\|_1 \left\| \frac{v}{\log(|\xi|+2)} \right\|_\infty.$$

The assumption $|f(\xi)| \leq C|\xi|^{-t}$ with $t > 2$ implies that $\|\log(|\xi|+2)f\|_1$ is finite. $\square$

We now note that more generally, for any $y, \tilde{y} \in \mathcal{W}(\Omega)$ for which $E^\Omega(y, \tilde{y})$ is defined, where $Dy_b \in \mathbb{R} \setminus (\mathbb{Z} + (\frac{1}{2} - \epsilon, \frac{1}{2} + \epsilon))$ for all $b \in \mathcal{B}^\Omega$, Gateaux derivatives of E^Ω (in $\mathcal{W}_0(\Omega)$ directions) in its first argument exist up to fourth-order, and do not depend on the second argument. These derivatives are denoted $\delta^j E^\Omega(y)$, so that for $v, w \in \mathcal{W}_0(\Omega)$,

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

In particular we note that $\delta \mathcal{E}(0) = \delta E(\hat{y})$ and $\delta^2 \mathcal{E}(0) = \delta^2 E(\hat{y})$.

3.3.2 Stable equilibria

Using the terminology of energy differences, we now define what we mean by a stable equilibrium displacement. Intuitively, the definition entails that finite energy perturbations cannot lower the energy.

Definition 3.3.1 (Stable equilibrium). (i) A displacement $y \in \mathcal{W}(\Omega)$ is a *locally stable equilibrium* if there exists $\epsilon > 0$ such that $E^\Omega(y + u; y) \geq 0$ for all $u \in \mathcal{W}_0(\Omega)$ with $\|Du\|_2 \leq \epsilon$.

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

$$\langle \delta^2 E^\Omega(y)v, v \rangle \geq \lambda \|Dv\|_{\ell^2}^2 \quad \forall v \in \mathcal{W}_0(\Omega). \quad (3.11)$$

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

These notions of equilibrium will be the focus of the results in the following chapters.

3.4 Discussion

As remarked in §1.2, the model analysed here is similar to those in [Pon07] and [ADGP13], although the underlying lattice considered is the square lattice rather than the triangular lattice. The earliest formulation of a similar model to study $\frac{1}{2}[111]$ screw dislocations in BCC crystals appears to be in [VPB70]: more recent results concerning the computation of the core structure of this class of dislocations using related methods are to be found in [CGD⁺09], [GD10] and [IKY12].

Chapter 4

Globally stable equilibria with unit net Burgers vector

This chapter is devoted to the proof of Theorem 4.1.1, which states that there exist globally stable equilibria in the full lattice which have unit net Burgers vector. In §4.1, we describe the additional assumption on ψ to those stated in §3.3 used here, before stating Theorem 4.1.1 and providing an outline of its proof. In §4.2, this result is reformulated in Theorem 4.2.1 as a statement about the existence of a global minimiser for a variational problem on $\mathcal{W}^{1,2}(\Lambda)$, and §4.3 is then devoted to the proof of Theorem 4.2.1. The results of this chapter may also be found in [HO14b].

4.1 Main result

4.1.1 Key assumption

In addition to the assumptions on ψ stated in §3.3, throughout this chapter we will also assume that ψ satisfies the following growth assumption.

Growth assumption near $\mathbb{Z}$.

$$(\psi 5) \quad \psi(x) \geq \frac{1}{2}\psi''(0)x^2 \text{ for all } x \in [-\frac{1}{2}, \frac{1}{2}].$$

The reason for this ‘technical’ assumption will become apparent in §4.3.1, where we use it to establish an *a priori* bound on the number of dislocation dipoles in finite energy configurations. It may be possible to replace $(\psi 5)$ by a weaker variant, although a stability assumption in some form will always be necessary to prevent the lattice itself from becoming unstable.

4.1.2 Statement of the main result

Recalling Definition 3.1.2 and Definition 3.3.1, the existence of a screw dislocation can be formulated as follows.

Theorem 4.1.1. *There exists a globally stable equilibrium displacement $y \in \mathcal{W}(\Lambda)$ with net Burgers vector $B[y] = 1$.*

The notion of global stability described in Definition 3.3.1 is equivalent to the statement that a displacement is stable if any finite energy perturbation increases the energy of the system. Describing a dislocation configuration as the minimiser of an energy difference functional gives us access to the Direct Method of the Calculus of Variations.

We refer to this result as the existence of a ‘geometrically necessary’ dislocation since we do not prescribe the absolute number of dislocation cores, only the net Burgers vector.

Outline of the proof of Theorem 4.1.1.

1. We define a reference configuration $\hat{y}(\xi) = \frac{1}{2\pi} \arctan\left(\frac{\xi_2}{\xi_1}\right)$ (the continuum linear elasticity solution for a dislocation), with the aim of minimising the energy difference functional $\mathcal{E}(u) := E(\hat{y} + u; \hat{y})$ over a suitable class of functions u .

Using the results of Lemma 3.3.1 and Lemma 3.3.2, we verify that $\mathcal{E}$ may be continuously extended to a functional over $\dot{\mathcal{W}}^{1,2}(\Lambda)$.

2. In order to use the Direct Method to establish the existence of a minimiser to $\mathcal{E}$, the crucial step is to obtain a global lower bound on the energy. This is the main step in the proof, and requires careful geometric estimates based on the number of dislocation cores and the distance between them. We prove that $\mathcal{E}(u) \gtrsim \|\beta\|_2^2 - 1$, where β can be thought of as belonging to $[Du]$ (however, see (4.9) for the precise definition).
3. In particular, this lower bound guarantees that the number of dislocation cores is bounded along a minimising sequence as well as weak compactness of a minimising sequence u^n .
4. The final step is to ensure that $\lim u^n$ has unit net-Burgers vector. In our present context it is possible, by introducing a dislocation dipole, to effectively translate the geometrically necessary core to infinity, and thus obtain a limiting displacement with zero net Burgers vector. We shift the minimising sequence and employ a concentration compactness argument to prevent this. $\square$

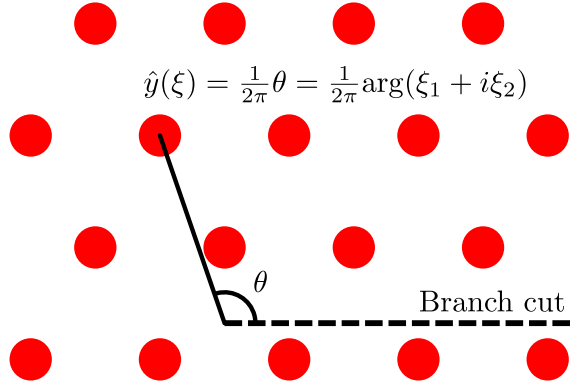


Figure 4.1: An illustration of the chosen coordinate system and the definition of reference displacement, $\hat{y}$.

4.2 Variational formulation

4.2.1 The reference displacement

We now specify the reference displacement $\hat{y}$ used in the definition of $\mathcal{E}$ in §3.3.1. It is best to think of $\hat{y}$ as prescribing a far-field boundary condition $y(\xi) \sim \hat{y}(\xi)$ as $|\xi| \rightarrow \infty$. We wish to choose $\hat{y}$ in such a way that it enforces a geometrically necessary dislocation, and at the same time satisfies the condition of Lemma 3.3.2.

A natural choice is the dislocation displacement field from linear elasticity theory. Since it is instructive (though not essential to our proofs) we give a brief motivation of this construction. In the far-field, we expect that continuum linearised elasticity theory is a good approximation to the atomistic equilibrium condition $\delta\mathcal{E}(0) = 0$. This can be formalised by first deriving the Cauchy–Born approximation and then linearising it. Due to the hexagonal symmetry of Λ one finds that the linearised continuum approximation is simply Laplace’s equation, $\Delta\hat{y}(x) = 0$; see §10 in [LL59].

Hence, following Section 3-2 in Hirth & Lothe [HL82], we define $\hat{y}$ as follows:

$$\hat{y}(x) := \frac{1}{2\pi} \arg(x) = \frac{1}{2\pi} \arctan\left(\frac{x_2}{x_1}\right), \quad (4.1)$$

where we identify $x \in \mathbb{R}^2$ with the point $x_1 + ix_2 \in \mathbb{C}$, and the branch cut is taken along the positive ξ_1 -axis, as shown in Figure 4.1.

The gradient (away from the branch cut) is given by

$$\nabla\hat{y}(x) = \left(\frac{-x_2}{2\pi r^2}, \frac{x_1}{2\pi r^2}\right)^T, \quad (4.2)$$

where $r := |x|$. This function can be extended to a function in $C^\infty(\mathbb{R}^2 \setminus \{0\})$, which we take as the *definition* of $\nabla\hat{y}$ from now on. Moreover, we can check that indeed $\Delta\hat{y}(x) = \operatorname{div}(\nabla\hat{y}(x)) = 0$, in the pointwise sense, for $x \neq 0$.

Let $\hat{\alpha} = (\hat{\alpha}_b)_{b \in \mathcal{B}}$ be a bond-length 1-form associated with $\hat{y}$; we claim that this is unique, and the following lemma provides a convenient formula for $\hat{\alpha}_b$ in terms of $\nabla \hat{y}$.

Lemma 4.2.1. *Let $\hat{\alpha} \in [D\hat{y}]$; then, for any bond $b = (\xi, \xi + a_i) \in \mathcal{B}$, we have*

$$\hat{\alpha}_b = \int_0^1 \nabla \hat{y}(\xi + ta_i) \cdot a_i dt. \quad (4.3)$$

Proof. By definition, $\nabla \hat{y}$ is independent of the choice of branch cut. Moreover, if the branch cut is chosen differently, then the displacement at each site is only changed by an integer, which means $\hat{\alpha}$ does not change; hence, $\hat{\alpha}$ is also independent of the branch cut.

Now fix $b = (\xi, \xi + a_i) \in \mathcal{B}$. Since the origin lies at the centre of a cell we can redefine $\hat{y}$ with a branch cut that does not intersect b . The Fundamental Theorem of Calculus gives

$$\int_0^1 \nabla \hat{y}(\xi + ta_i) \cdot a_i dt = \hat{y}(\xi + a_i) - \hat{y}(\xi) = \frac{1}{2\pi} (\arg(\xi + a_i) - \arg(\xi)), \quad (4.4)$$

and since we have assumed that b is a nearest neighbour bond, it has length 1. The term on the right-hand side is $1/2\pi$ times the angle formed by the points ξ , 0 and $\xi + a_i$, which is maximised by making ξ and $\xi + a_i$ as close to the origin as possible — that is, when ξ and $\xi + a_i$ are on the boundary of C_0 . It follows that the angle can be no larger than $\frac{2\pi}{3}$, and hence $\hat{\alpha}_b = \hat{y}(\xi + a_i) - \hat{y}(\xi) \in [-\frac{1}{3}, \frac{1}{3}]$. This implies that $\hat{\alpha}$ is unique, since $D\hat{y}_b \neq \pm \frac{1}{2}$ for all $b \in \mathcal{B}$. $\square$

As an immediate corollary of Lemma 4.2.1, we obtain the following bound on $\hat{\alpha}_b$:

$$|\hat{\alpha}_b| \leq \frac{1}{2\pi d_b} \quad \forall b \in \mathcal{B}. \quad (4.5)$$

To conclude our analysis of $\hat{y}$, we show that it satisfies the conditions of Lemma 3.3.2.

Lemma 4.2.2. *Let $\hat{y}$ be defined by (4.1), and let $f(\xi), \xi \in \Lambda$, be the associated forces as in (3.9), then $\hat{\alpha} \in [D\hat{y}]$ satisfies $\hat{\alpha}_b \in [-1/3, 1/3]$ and*

$$|f(\xi)| \lesssim |\xi|^{-3} \quad \forall \xi \in \Lambda.$$

In particular $\hat{y}$ satisfies all conditions of Lemma 3.3.2.

Proof. Recall from (3.9) that

$$f(\xi) = \sum_{b \in \mathcal{R}_\xi} \psi'(D_b \hat{y}) = \sum_{b \in \mathcal{R}_\xi} \psi'(\hat{\alpha}_b).$$

Taylor expanding ψ'_b to third order, using the fact that $\psi'(0) = \psi'''(0) = 0$ (since ψ is even about 0), gives

$$f(\xi) = \sum_{b \in \mathcal{R}_\xi} \left[\psi''(0) \hat{\alpha}_b + \frac{1}{6} \psi^{(4)}(s_b) (\hat{\alpha}_b)^3 \right],$$

for some $s_b \in \text{conv}\{0, \hat{\alpha}_b\}$. Applying (4.5) we obtain

$$f(\xi) = \sum_{b \in \mathcal{R}_\xi} \psi''(0) \hat{\alpha}_b + O(d_b^{-3}). \quad (4.6)$$

We now inspect the sum on the right-hand side of (4.6) in more detail. Applying (4.3) we rewrite this sum as

$$\sum_{b \in \mathcal{R}_\xi} \psi''(0) \hat{\alpha}_b = \sum_{i=1}^6 \psi''(0) \int_0^1 \nabla \hat{y}(\xi + ta_i) \cdot a_i dt.$$

Taylor expanding $\nabla \hat{y}(\xi + ta_i)$ and using the fact that $|\nabla^4 \hat{y}(x)| \lesssim |x|^{-4}$, we obtain

$$\int_0^1 \nabla \hat{y}(\xi + ta_i) \cdot a_i dt = \nabla \hat{y}(\xi) \cdot a_i + \frac{1}{2} \nabla^2 \hat{y}(\xi) [a_i, a_i] + \frac{1}{6} \nabla^3 \hat{y}(\xi) [a_i, a_i, a_i] + O(|\xi|^{-4}).$$

Summing over $i = 1, \dots, 6$ the first and third terms cancel since $a_{i+3} = -a_i$, hence we obtain

$$\sum_{b \in \mathcal{R}_\xi} \psi''(0) \hat{\alpha}_b = \frac{1}{2} \sum_{i=1}^6 a_i^T \nabla^2 \hat{y}(\xi) a_i + O(|\xi|^{-4}). \quad (4.7)$$

We now observe that

$$\frac{1}{2} \sum_{i=1}^6 a_i^T \nabla^2 \hat{y}(\xi) a_i = -\frac{3}{2} \Delta \hat{y}(\xi) = 0.$$

Inserting the last identity into (4.7) and combining the resulting estimate with (4.6) we obtain the stated estimate on $|f(\xi)|$. $\square$

4.2.2 The variational problem in $\mathcal{W}^{1,2}(\Lambda)$

Combining Lemma 4.2.2 with Lemma 3.3.1 and Lemma 3.3.2, we deduce that $\mathcal{E}(u) := E(\hat{y} + u; \hat{y})$ is a well-defined and continuous functional on $\mathcal{W}^{1,2}(\Lambda)$, where $\hat{y}$ is the reference configuration defined in (4.1). It will later be convenient to recall from the proof of Lemma 3.3.1 that the explicit definition of the extension is

$$\mathcal{E}(u) = \sum_{b \in \mathcal{B}} [\psi(\hat{\alpha}_b + Du_b) - \psi(\hat{\alpha}_b) - \psi'(\hat{\alpha}_b) Du_b] + \langle \delta \mathcal{E}(0), u \rangle. \quad (4.8)$$

In the next section, §4.3, we will prove the following result.

Theorem 4.2.1. *There exists $u \in \dot{\mathcal{W}}^{1,2}(\Lambda)$ such that $\mathcal{E}(u) \leq \mathcal{E}(v)$ for all $v \in \dot{\mathcal{W}}^{1,2}(\Lambda)$.*

As an immediate corollary we can now prove Theorem 4.1.1.

Proof of Theorem 4.1.1. Let $y := \hat{y} + u$, where u is a minimiser of $\mathcal{E}$ in $\dot{\mathcal{W}}^{1,2}(\Lambda)$. Since $Du \in \ell^2(\mathcal{B})$ it follows that $|Du_b| \rightarrow 0$ uniformly as $d_b \rightarrow \infty$. Using also the fact that $|\hat{\alpha}_b| \rightarrow 0$ uniformly (cf. (4.5)), we conclude that $\alpha_b = \hat{\alpha}_b + Du_b + z_b$, where z_b is a compactly supported, integer-valued 1-form. From the definition of the net Burgers vector and from (3.4), it now follows immediately that $B[y] = B[\hat{y}] = 1$. Moreover, minimality of u implies that y is a globally stable equilibrium in the sense of Definition 3.3.1. $\square$

Theorem 4.2.1 is interesting in its own right: it shows that atomistic configurations containing dislocations can be obtained as global minimisers of a variational problem formulated over Λ . This is particularly useful for further study of dislocations in this model.

We also remark that any local minimiser u of $\mathcal{E}$ in $\dot{\mathcal{W}}^{1,2}(\Lambda)$ would give rise to a locally stable equilibrium with net Burgers vector $B(\hat{y} + u) = 1$. The advantage of local minimisers is that they can be computed numerically.

4.3 Proof of Theorem 4.2.1

As currently formulated, it is not obvious that the energy $\mathcal{E}$ is bounded below, and it is even less clear whether $\mathcal{E}$ is coercive in a sense which would allow us to invoke the Direct Method. This is due in large part to the fact that the reference configuration is nonlinear and ψ is periodic, so the integrand has infinitely many energy wells.

The periodicity of ψ allows the creation of dislocation dipoles ‘cheaply’. If dipoles are well separated, then each dipole gives a positive contribution to the energy which is proportional to the logarithm of the dipole length (the separation distance between the two cores of the dipole). However, for generic configurations of dipoles the sign of the energy contribution is difficult to determine, since it depends strongly upon the relative orientations of the dipoles. In essence, this is a geometric nonlinearity of the system, and most of the effort expended in what follows will be to control the number of dipoles that can form.

From a technical point of view the issue arises as follows: in §3.1.2 we introduced $\alpha \in [Dy]$, since the energy of the displacement y only depends on α due to the periodicity of the potential ψ . Consequently, if we have a sequence u^n with $\mathcal{E}(u^n)$

uniformly bounded, then this will bound only $\|\beta^n\|_2$ for $\beta^n \in [Du^n]$, and not $\|Du^n\|_2$. In particular, generic minimising sequences cannot be weakly compact.

By exploiting the vertical shift invariance (§4.3.2) and the horizontal translation invariance (§4.3.3) of the energy $\mathcal{E}$, we will *construct* a weakly compact minimising sequence. Having made this special choice of minimising sequence, we use a *profile decomposition* in §4.3.6. We show that each profile obtained in this way has net Burgers vector zero, leading to the conclusion that the net Burgers vector of the limit remains 1, and proving the existence of a minimiser with the required properties.

4.3.1 An elementary lower bound

Our eventual goal is to establish a coercivity result for $\mathcal{E}$. We begin with an elementary lower bound that will motivate subsequent constructions.

Let $y = \hat{y} + u$, $u \in \mathcal{W}^{1,2}(\Lambda)$, be a trial displacement, $\alpha \in [Dy]$, and recall that $\hat{\alpha} = [D\hat{y}]$ is unique. Since $u \in \mathcal{W}^{1,2}(\Lambda)$, and hence $Du_b \rightarrow 0$ as $d_b \rightarrow \infty$, it follows that y has a well-defined net Burgers vector in the sense of Definition 3.1.2, and $B[y] = B[\hat{y}] = 1$.

Let

$$\beta := \alpha - \hat{\alpha}; \tag{4.9}$$

this 1-form satisfies the property that

$$\int_{\partial C} \beta \neq 0 \quad \text{if and only if} \quad \int_{\partial C} \alpha \neq \int_{\partial C} \hat{\alpha},$$

that is, dislocation cores present in β are those that are introduced by the addition of u to $\hat{y}$.

Remark 4.3.1. We note that β_b does not necessarily belong to $[-1/2, 1/2]$, and hence is not a bond length 1-form, so the definitions of §3.1.6 do not strictly apply; however, it remains a 1-form in the sense defined in §3.1 of [AO05]. As $\int_{\partial C} \beta \in \{0, 1, -1\}$ for all $C \in \mathcal{C}$, we therefore slightly abuse our notation and refer to dislocation cores in β as the cells $C \in \mathcal{C}$ for which

$$\int_{\partial C} \beta = \pm 1.$$

We also define $\mathcal{C}^+[\beta]$, $\mathcal{C}^-[\beta]$ and $\mathcal{C}^\pm[\beta]$ in the obvious way.

Next, we define $z : \mathcal{B} \rightarrow \mathbb{Z}$ via

$$Du = \beta + z, \tag{4.10}$$

which is compactly supported since $\beta, Du \in \ell^2(\mathcal{B})$. We shall see in §4.3.2 that the support of z can be thought of as a union of branch cuts connecting dislocation dipoles.

With this notation, we obtain the following result, which relies crucially upon assumption $(\psi 5)$.

Lemma 4.3.1. *For any $u \in \mathcal{W}^{1,2}(\Lambda)$ with $Du = \beta + z$ as in (4.10) and for any $\epsilon > 0$, we have*

$$\mathcal{E}(u) \geq \left(\frac{1}{2}\psi''(0) - \epsilon\right)\|\beta\|_{\ell^2}^2 - \sum_{b \in \mathcal{B}} \psi'(\hat{\alpha}_b)z_b + \langle \delta \mathcal{E}(0), u \rangle - C_\epsilon, \quad (4.11)$$

where $C_\epsilon > 0$ is a constant that is independent of u .

Proof. This estimate arises from the expression (4.8); using the periodicity of the potential ψ , we can write

$$\mathcal{E}(u) = \sum_{b \in \mathcal{B}} (\psi(\hat{\alpha}_b + \beta_b) - \psi(\hat{\alpha}_b) - \psi'(\hat{\alpha}_b)\beta_b) - \sum_{b \in \mathcal{B}} \psi'(\hat{\alpha}_b)z_b + \langle \delta \mathcal{E}(0), u \rangle.$$

Define the function

$$g(s, t) := \begin{cases} \frac{\psi(t+s) - \psi(t) - \psi'(t)s}{s^2} & s \neq 0, \\ \frac{1}{2}\psi''(t) & s = 0. \end{cases}$$

By assumption $(\psi 5)$ in §4.1.1, $g(s, 0) \geq \frac{1}{2}\psi''(0)$ for any $|s| \leq 1/2$.

Since g is uniformly continuous on $[-1/2, 1/2] \times [-\tau, \tau]$ for some $\tau > 0$, it follows that for each $\epsilon > 0$ there exists $\delta(\epsilon) > 0$ such that

$$g(s, t) \geq \frac{1}{2}\psi''(0) - \epsilon \quad \text{for } |s| \leq \frac{1}{2} + \delta(\epsilon) \text{ and } |t| \leq \delta(\epsilon).$$

Next, we note that (4.5) implies

$$|\hat{\alpha}_b| \leq \frac{1}{2\pi d_b} \quad \text{and} \quad |\beta_b| = |\alpha_b - \hat{\alpha}_b| \leq \frac{1}{2} + \frac{1}{2\pi d_b}.$$

Hence there exists $R_0 > 0$ such that, for $d_b \geq R_0$,

$$g(\beta_b, \hat{\alpha}_b) \geq \frac{1}{2}\psi''(0) - \epsilon,$$

which can equivalently be stated as

$$\psi(\hat{\alpha}_b + \beta_b) - \psi(\hat{\alpha}_b) - \psi'(\hat{\alpha}_b)\beta_b \geq \left(\frac{1}{2}\psi''(0) - \epsilon\right)|\beta_b|^2 \quad \text{for } d_b \geq R_0. \quad (4.12)$$

It may be checked that

$$\#\{b \mid d_b < R_0\} \lesssim R_0^2,$$

and since ψ , ψ' and β are uniformly bounded, it therefore follows that

$$\sum_{b \in \mathcal{B}} \left(\psi(\hat{\alpha}_b + \beta_b) - \psi(\hat{\alpha}_b) - \psi'(\hat{\alpha}_b)\beta_b \right) \geq \left(\frac{1}{2}\psi''(0) - \epsilon \right) \sum_{b \in \mathcal{B}} |\beta_b|^2 - CR_0^2.$$

□

We can think of $\|\beta\|_2^2$ as estimating elastic stored energy. In the following sections we will establish several results on $z = Du - \beta$, which will eventually allow us to bound the remaining terms $\langle \delta\mathcal{E}(0), u \rangle$ and $\sum_b \psi'(\hat{\alpha}_b)z_b$ in (4.11).

4.3.2 Dipoles & branchcuts

Let $y = \hat{y} + u$, $u \in \mathcal{W}^{1,2}(\Lambda)$, be a trial displacement, $\alpha \in [Dy]$, and let β, z be defined by (4.10). While α and hence β are uniquely defined (except in borderline cases when $\alpha_b \in \{\pm 1/2\}$), one can exploit the vertical shift invariance of the lattice (encoded in assumption $(\psi 1)$, periodicity of ψ) to construct equivalent displacements $\tilde{u} \in \mathcal{W}^{1,2}(\Lambda)$,

$$\tilde{u} := u + U \tag{4.13}$$

where $U : \Lambda \rightarrow \mathbb{Z}$ and $U \in \mathcal{W}_0(\Lambda)$, and hence modify the z component.

If we let $\tilde{y} := \hat{y} + \tilde{u}$, then clearly, $\alpha \in [D\tilde{y}]$ and this leads to the same definition of β . Crucially, though, $D\tilde{u} - \beta \neq Du - \beta$. We can therefore ask how to choose U in an ‘optimal’ way. It turns out that minimising the total length of the branch cuts is a useful choice, which amounts to minimising $\|Du + DU - \beta\|_1 = \|z + DU\|_1$. Since z has compact support, a minimiser clearly exists, but it need not be unique; see Figure 4.2. We may therefore assume, without loss of generality, that u satisfies the following property.

Definition 4.3.1 (DMCP). A function $u \in \mathcal{W}^{1,2}(\Lambda)$ satisfies the *discrete minimal connection property (DMCP)* if

$$\|Du - \beta\|_1 = \|z\|_1 = \min_{Z: \Lambda \rightarrow \mathbb{Z}} \|Du + DZ - \beta\|_1. \tag{4.14}$$

This minimality condition is similar to the idea of *minimal connections* introduced in [BCL86].

We will now establish various properties of the structure of z defined in (4.10). In particular, we will show that z can be decomposed into a sum $\sum z^m$ and that the support of each z^m is analogous to a branch cut for a dipole.

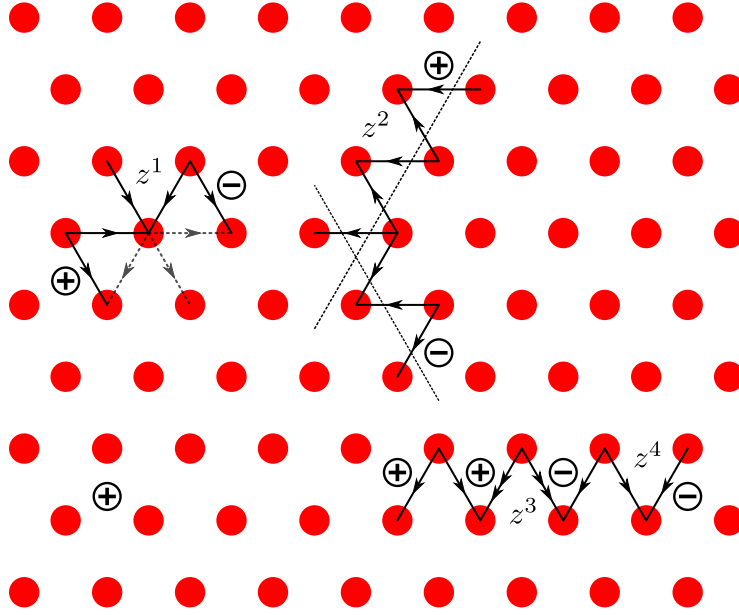


Figure 4.2: A typical example of the support of a minimal z and its decomposition into z^m for a given distribution of dipoles. A single arrow means that $z_b = 1$ on the bond pointing in the direction of the arrow, and a double arrow means $z_b = 2$. The grey dashed bonds on the left of the diagram show an alternative definition of z with the same minimal norm, and the black dashed lines show two lines which show that z^2 can be decomposed into 2 straight cuts.

Lemma 4.3.2. *Let $u \in \mathcal{W}^{1,2}(\Lambda)$ satisfy the DMCP (4.14) and suppose $Du = \beta + z$ as in (4.10). Then we can write*

$$z = \sum_{m=1}^M z^m, \quad (4.15)$$

where $M = \#\mathcal{C}^+[\beta]$ is the number of dipoles contained in β and $z^m : \mathcal{B} \rightarrow \{-1, 0, +1\}$, $m = 1, \dots, M$, satisfy the following properties:

1. $z_{b_i}^m = 1$ on a sequence of bonds $(b_i)_{i=0}^n$ such that
 - (a) ∂b_i and ∂b_{i+1} share a common 0-cell for each $i = 0, \dots, n-1$,
 - (b) $b_0 \in \partial C_m^-$ and $-b_n \in \partial C_m^+$ where $C_m^+ \in \mathcal{C}^+[\beta]$ and $C_m^- \in \mathcal{C}^-[\beta]$.
2. $z_b^m = 0$ for bonds outside the set $\{\pm b_i \mid i = 0, \dots, n\}$.

Proof. The result is geometrically intuitive; see Figure 4.2. We therefore postpone a complete proof to Appendix A.1. $\square$

We will say that z^m connects the dislocation cores C_m^+ and C_m^- . Moreover, we obtain the following corollary.

Corollary 4.3.1. *Each 1-form z^m in the decomposition (4.15) can be identified with a shortest path in the dual lattice between $C_m^+ \in \mathcal{C}^+[\alpha]$ and $C_m^- \in \mathcal{C}^-[\alpha]$, and further*

$$\|z^m\|_1 = \text{hop}_2(C_m^+, C_m^-).$$

Proof. First, we observe that, due to the **DMCP** (4.14) and the decomposition proven in Lemma 4.3.2,

$$\|z\|_1 = \sum_{m=1}^M \|z^m\|_1. \quad (4.16)$$

That is, if $z_b^m, z_b^{m'} \neq 0$, then $z_b^m, z_b^{m'}$ have the same sign.

The construction employed in the proof of Lemma 4.3.2 identifies a sequence of bonds b_i and cells $C_{m,i}$ such that $b_i, -b_{i+1} \in \partial C_{m,i}$, $z_{b_i}^m = 1$. Using the natural identification of cells with points in the dual lattice, this implies that $C_{m,i}$ are adjacent in the dual lattice, and furthermore that b_i can be identified with edges connecting these cells; this leads to the fact that

$$\|z^m\|_1 \geq \text{hop}_2(C_m^+, C_m^-).$$

To prove the converse, we take the path in the dual lattice corresponding to z^m , adjoin a shortest path between C_m^+ and C_m^- in the dual lattice, and thus obtain a closed dual lattice path. We construct a polygonal closed path in $\mathbb{R}^2$ by connecting the barycentres of the cells along the path and define U to be the characteristic function of the bounded interior of this loop in $\mathbb{R}^2$.

It is now straightforward to check that by defining $\tilde{z}^m := z^m + DU$ and $\tilde{z} := z - z^m + \tilde{z}^m$

$$\|\tilde{z}\|_1 \leq \sum_{m'=1}^M \|z^{m'}\|_1 - \|z^m\|_1 + \|\tilde{z}^m\|_1.$$

Since U is a compactly supported integer shift as in (4.13), the discrete minimal connection property (4.14) implies that $\|z^m\|_1 \leq \|\tilde{z}^m\|_1 = \text{hop}_2(C_m^+, C_m^-)$, completing the proof. $\square$

Later on it will be convenient to assume that each cut z^m is made up of at most two *straight cuts*: straight cuts are defined to be 1-forms $z : \mathcal{B} \rightarrow \{-1, 0, 1\}$ for which there exists a line $L := \{x^C + ta_i \mid t \in \mathbb{R}\}$, where x^C is the barycentre of some $C \in \mathcal{C}$ and a_i a nearest neighbour direction, such that $z_b \neq 0$ when the bond satisfies $b \cap L \neq \emptyset$,

$$\text{clos}\{x \in \mathbb{R}^2 \mid x \in b \in \mathcal{B}, z_b \neq 0\}$$

is a connected set, and $z_b > 0$ either exclusively on bonds in the directions a_{i+1} and a_{i+2} or in the directions a_{i-1} and a_{i-2} . We will say that a straight cut *lies in the direction* a_j whenever $a_i = \pm a_j$ in the definition of the corresponding L . See the cut depicted in the centre of Figure 4.2 for a visualisation of the definition.

In the next lemma, we show that we can always choose the decomposition (4.15) such that each z^m is composed of at most 2 straight cuts. We will refer to any u as in the conclusion of Lemma 4.3.3 as satisfying the *straight cuts property*.

Lemma 4.3.3. *Let $u \in \mathcal{W}^{1,2}(\Lambda)$, and $Du = \beta + z$ as in (4.10). Then there exists $\tilde{u} \in \mathcal{W}^{1,2}(\Lambda)$ satisfying the **DMCP** (4.14) as well as $D\tilde{u} = \beta + \sum_{m=1}^{\#C^+[\beta]} z^m$ where each z^m is the sum of at most 2 straight cuts.*

Proof. The idea is to show that we may always find a shortest path in the dual lattice between any pair of cells which is made up of 2 straight segments. It is intuitively clear from Figure 4.2 that this can always be done.

A complete proof is postponed until Appendix A.2. □

4.3.3 Shifting the Origin

Suppose that $y = \hat{y} + u$, where $u \in \mathcal{W}^{1,2}(\Lambda)$ satisfies the **DMCP** (4.14). Recall the definition of H^C from §3.1.5 as a lattice automorphism which maps C_0 onto C . Let

$$u^C := u \circ H^C + \hat{y} \circ H^C - \hat{y}. \quad (4.17)$$

It follows that $\hat{y}(\xi) + u^C(\xi) = \hat{y}(H^C\xi) + u(H^C\xi)$ for all lattice points $\xi \in \Lambda$, so that there are corresponding bond length 1-forms $\alpha^C \in [D\hat{y} + Du^C]$ satisfying

$$\alpha^C = \alpha \circ H^C.$$

As before, define $\beta^C := \alpha^C - \hat{\alpha}$. According to these definitions,

$$\hat{y}(H^C\xi) - \hat{y}(\xi) := \frac{1}{2\pi} (\arg(\xi + x^C) - \arg(\xi));$$

if we make this function single-valued by introducing a compact polygonal branch cut passing through the barycentres of a shortest dual lattice path between C_0 and C , then it is a straightforward exercise to show that

$$|D(\hat{y} \circ H^C)_b - D\hat{y}_b| \lesssim d_b^{-2};$$

therefore $u^C \in \dot{\mathcal{W}}^{1,2}(\Lambda)$, and

$$\begin{aligned}\mathcal{E}(u^C) &= E(\hat{y} + u^C; \hat{y}) \\ &= E(\hat{y} \circ H^C + u \circ H^C; \hat{y}) \\ &= E(\hat{y} \circ H^C + u \circ H^C; \hat{y} \circ H^C) + E(\hat{y} \circ H^C; \hat{y}) \\ &= \mathcal{E}(u),\end{aligned}$$

noting that the first term on the third line is simply a resummation of $\mathcal{E}(u)$, and the second term vanishes.

For each $C \in \mathcal{C}^+[\alpha]$, we can replace u^C with $\tilde{u}^C = u^C + U$ for some $U : \Lambda \rightarrow \mathbb{Z}$, such that $\|Du^C + DU - \beta^C\|_1$ is minimal, i.e. $\tilde{u}^C$ satisfies the **DMCP** (4.14). We obtain that

$$\mathcal{E}(\tilde{u}^C) = \mathcal{E}(u^C) = \mathcal{E}(u).$$

To summarise, we have constructed a corrector displacement $\tilde{u}^C \in \dot{\mathcal{W}}^{1,2}(\Lambda)$ with the same energy as u , but for which $C \in \mathcal{C}^+[\alpha]$ has been shifted to the origin. Upon minimising $\|D\tilde{u}^C - \beta^C\|_1$ amongst all choices $C \in \mathcal{C}^+[\alpha]$, we obtain the following result.

Lemma 4.3.4. *Let $v \in \dot{\mathcal{W}}^{1,2}(\Lambda)$, then there exists $u \in \dot{\mathcal{W}}^{1,2}(\Lambda)$ such that $\mathcal{E}(u) = \mathcal{E}(v)$ and such that the discrete optimal connection property (**DOCP**) holds:*

Definition 4.3.2 (DOCP). There exists $\alpha \in [D(\hat{y} + u)]$ such that

$$\|Du - \beta\|_1 = \min_{C \in \mathcal{C}^+[\alpha]} \min_{U: \Lambda \rightarrow \mathbb{Z}} \|Du^C + DU - \beta^C\|_1, \quad (4.18)$$

where $\beta = \alpha - \hat{\alpha}$, u^C is defined by (4.17) and $\beta^C = \alpha \circ H^C - \hat{\alpha}$.

The crucial property that we obtain from the **DOCP** (4.18) is a bound on the distance between the necessary core at C_0 and all negative cores.

Lemma 4.3.5. *Suppose $u \in \dot{\mathcal{W}}^{1,2}(\Lambda)$ satisfies the **DOCP** and let $z = \sum_{m=1}^M z^m$ according to (4.15). Then,*

$$\text{hop}_2(C_0, C_m^-) \geq \text{hop}_2(C_m^+, C_m^-), \quad \text{for } m = 1, \dots, M, \quad (4.19)$$

where we recall that z^m connects the cores $C_m^+ \in \mathcal{C}^+[\alpha]$ and $C_m^- \in \mathcal{C}^-[\alpha]$.

Proof. Suppose the converse for contradiction. Then there exists m and a dual lattice path connecting C_0 to C_m^- which is strictly shorter than $\text{hop}_2(C_m^+, C_m^-)$. Letting $H := H^{C_m^+}$ and $v := u^{C_m^+}$,

$$Dv - \beta \circ H = z \circ H + \tilde{z} = \sum_m z^m \circ H + \tilde{z},$$

where $\tilde{z}$ is the contribution coming from the branch cut in $\hat{y} \circ H - \hat{y}$. Consider the closed curve passing from $HC_m^+ = C_0$ to HC_0 along the branch cut, then along a shortest lattice path between HC_0 and HC_m^- , and then back to HC_m^+ along the support of $z^m \circ H$. By a similar argument to that in Corollary 4.3.1, we can define $w \in \mathcal{W}_0(\Lambda)$ as $w(\xi) = 1$ for $\xi \in \Lambda$ inside the curve, and 0 outside. It can then be checked that $v + w$ has a corresponding $\bar{z}$ which satisfies

$$\|\bar{z}\|_1 = \|z \circ H\| - \|z^m \circ H\| + \text{hop}_2(C_0, C_m^-) = \sum_{i \neq m} \|z^i\|_1 + \text{hop}_2(C_0, C_m^-) < \|z\|_1,$$

the required contradiction. $\square$

As a corollary we obtain the following stronger property.

Corollary 4.3.2. *Suppose $u \in \mathcal{W}^{1,2}(\Lambda)$ satisfies the **DOCP** (4.18) and let $z = \sum_{m=1}^M z^m$ according to (4.15). Then, for any $m \in \{1, \dots, M\}$ and for any cell $C \in \mathcal{C}$ such that $z_b^m \neq 0$ for some $b \in \partial C$,*

$$\text{hop}_2(C_0, C) \geq \text{hop}_2(C_m^+, C). \quad (4.20)$$

Proof. Lemma 4.3.5 states that, if $C^- \in \mathcal{C}^-[\alpha]$ and $C^+ \in \mathcal{C}^+[\alpha]$ are connected by z^m , then

$$\text{hop}_2(C_0, C^-) \geq \text{hop}_2(C^+, C^-).$$

It is clear that any subpath of a shortest path in a graph is also a shortest path. By the construction of z^m , C lies on a shortest path between C^+ and C^- , and therefore

$$\text{hop}_2(C^+, C^-) = \text{hop}_2(C^+, C) + \text{hop}_2(C, C^-).$$

The triangle inequality for paths (3.2) now directly implies

$$\text{hop}_2(C_0, C) \geq \text{hop}_2(C^+, C). \quad \square$$

4.3.4 Estimating $\langle \delta\mathcal{E}(0), u \rangle$

In §4.3.2 and §4.3.3, we showed that for any $u \in \mathcal{W}^{1,2}(\Lambda)$, we can find $\tilde{u} \in \mathcal{W}^{1,2}(\Lambda)$ such that $\mathcal{E}(u) = \mathcal{E}(\tilde{u})$, and for which the corresponding branch cuts z satisfy the **DOCP** (4.18). We are now in a position to exploit the chosen structure of z to derive compactness for minimising sequences.

Our first step is to provide a stronger bound on $\delta\mathcal{E}(0)$. We have already shown that $|\langle \delta\mathcal{E}(0), u \rangle| \lesssim \|Du\|_{\ell^2}$, but this will not be sufficient since our estimates so far only provide a bound on β , and not on Du itself. Therefore we need to estimate $|\langle \delta\mathcal{E}(0), u \rangle|$ only in terms of $\|\beta\|_2$.

Lemma 4.3.6. *For each $u \in \mathcal{W}^{1,2}(\Lambda)$, let $\beta_u := \beta$ be defined through (4.9). There exists a constant $C > 0$ such that*

$$\langle \delta\mathcal{E}(0), u \rangle \leq C \|\beta_u\|_2 \quad \forall u \in \mathcal{W}^{1,2}(\Lambda) \quad \text{satisfying the DOCP (4.18)}. \quad (4.21)$$

We provide the proof of this fundamental estimate throughout the remainder of this section.

Recall the definition of ξ_0 from §3.1.2. For any $\xi \in \Lambda$, it is always possible to express the difference $\xi - \xi_0$ as

$$\xi - \xi_0 = na_i + ma_{i+1},$$

for some nearest neighbour lattice direction a_i and some $n, m \in \mathbb{N} \cup \{0\}$ with $n \neq 0$ unless $\xi = \xi_0$. We then define the path Γ_ξ to be

$$\Gamma_\xi := \sum_{j=0}^{n-1} (\xi_0 + ja_i, \xi_0 + (j+1)a_i) + \sum_{j=0}^{m-1} (\xi_0 + na_i + ja_{i+1}, \xi_0 + na_i + (j+1)a_{i+1});$$

cf. Figure 4.3. Integrating Du_b along Γ_ξ , we obtain

$$\begin{aligned} |u(\xi)| &= \left| \int_{\Gamma_\xi} Du \right| = \left| \int_{\Gamma_\xi} \beta + z \right| \\ &\leq |\Gamma_\xi|^{1/2} \left(\sum_{b \in \Gamma_\xi} |\beta_b|^2 \right)^{1/2} + \left| \int_{\Gamma_\xi} z \right| \\ &\lesssim |\xi|^{1/2} \|\beta\|_2 + \left| \int_{\Gamma_\xi} z \right|, \end{aligned} \quad (4.22)$$

using the Cauchy-Schwarz inequality. We now bound the final term in (4.22).

Lemma 4.3.7. *Suppose $u \in \mathcal{W}^{1,2}(\Lambda)$ satisfies the **DOCP** (4.18) and the straight cuts property (cf. Lemma 4.3.3); then*

$$\left| \int_{\Gamma_\xi} z \right| \lesssim \min \{ |\xi|^2, \#\mathcal{C}^+[\alpha] \}.$$

Proof. First, we note that for any straight cut z' ,

$$\left| \int_{\Gamma_\xi} z' \right| \leq 1.$$

This follows from the fact that all $b \in \mathcal{B}$ for which $z'_b = 1$ can be written as

$$(\xi + na_j, \xi + na_j + a_{j+1}) \quad \text{or} \quad (\xi + na_j, \xi + na_j + a_{j+2})$$

for some $\xi \in \Lambda$, $n \in \mathbb{N}$ and some nearest neighbour lattice direction a_j , and the definition of Γ_ξ . Using the straight cuts property, we find that

$$\left| \int_{\Gamma_\xi} z \right| \leq \sum_m \left| \int_{\Gamma_\xi} z^m \right| \leq 2 \#\mathcal{C}^+[\alpha].$$

To prove the second bound, enumerate the bonds $b_j \in \Gamma_\xi$, beginning with the bond $b_1 = (\xi_0, \xi_0 + a_i)$. Each $b_j \in \partial C^{b_j}$ for some $C^{b_j} \in \mathcal{C}$. Since u satisfies the **DOCP**, Corollary 4.3.2 applies, and $z_{b_j}^m \neq 0$ implies that if z^m connects to $C^+ \in \mathcal{C}^+[\alpha]$, then

$$\text{hop}_2(C^+, C^{b_j}) \leq \text{hop}_2(C_0, C^{b_j}) \leq \text{hop}_2(C_0, C^{b_0}) + 2j,$$

where we have repeatedly applied the triangle inequality (3.2). This will entail a bound on the number of z^m whose support could intersect Γ_ξ . Further application of the triangle inequality implies that

$$\#\{C \in \mathcal{C} \mid \text{hop}_2(C, C^{b_j}) \leq \text{hop}_2(C_0, C^{b_0}) + 2j\} \lesssim j^2.$$

Since by (3.3) each cell can contain at most one dislocation core, we must therefore have

$$\left| \int_{\Gamma_\xi} z \right| \lesssim |\Gamma_\xi|^2 \lesssim |\xi|^2. \quad \square$$

Next, we show that the number of cores can be bounded in terms of β . This is intuitive, since as discussed in [Pon07], each core stores a positive amount of elastic energy. Let $C \in \mathcal{C}^\pm[\beta]$, then Jensen's inequality implies

$$\int_{\partial C} |\beta|^2 \geq \frac{1}{3} \left| \int_{\partial C} \beta \right|^2 = \frac{1}{3}. \quad (4.23)$$

Hence, we obtain

$$\#\mathcal{C}^\pm[\beta] \leq 3 \|\beta\|_2^2. \quad (4.24)$$

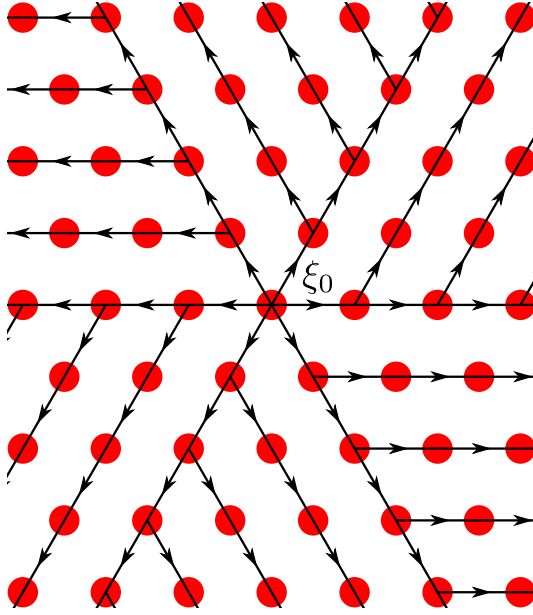


Figure 4.3: The definition of the paths Γ_ξ .

Proof of Lemma 4.3.6. We now combine Lemma 4.3.7, Lemma 4.2.2 and (4.24) to estimate

$$\begin{aligned} |\langle \delta \mathcal{E}(0), u \rangle| &\leq \sum_{\xi \in \Lambda} |f(\xi)| |u(\xi)|, \\ &\lesssim \sum_{\xi \in \Lambda} \left\{ \|\beta\|_2 |\xi|^{-5/2} + \min(\|\beta\|_2^2, |\xi|^2) |\xi|^{-3} \right\}. \end{aligned}$$

We note that the $|\xi|^{-5/2} \in \ell^1(\Lambda)$, so that the first term is bounded above by $C\|\beta\|_2$. The second term splits into

$$\sum_{\xi \in \Lambda} \min(\|\beta\|_2^2, |\xi|^2) |\xi|^{-3} \leq \sum_{|\xi| \leq \|\beta\|_2} |\xi|^{-1} + \|\beta\|_2^2 \sum_{|\xi| > \|\beta\|_2} |\xi|^{-3}.$$

Straightforward radial estimates yield the bounds

$$\sum_{|\xi| \leq \|\beta\|_2} |\xi|^{-1} \lesssim \|\beta\|_2 \quad \text{and} \quad \sum_{|\xi| > \|\beta\|_2} |\xi|^{-3} \lesssim \|\beta\|_2^{-1}.$$

Combining the previous estimates, we obtain the stated result. $\square$

4.3.5 Estimating $\sum_{b \in \mathcal{B}} z_b \psi'(\hat{\alpha}_b)$

In this section, we estimate the second group in (4.11). Here, we must resort to careful quantitative bounds which use the structure of the lattice and the form of $\hat{\alpha}$.

Lemma 4.3.8. *Suppose that $u \in \mathcal{W}^{1,2}(\Lambda)$ satisfies the **DOCP** (4.18), then for any cut z^m connecting to a dipole $C^+ \in \mathcal{C}^+[\alpha]$ to $C^- \in \mathcal{C}^-[\alpha]$, we have the lower bound:*

$$\sum_{b \in \mathcal{B}} z_b^m \psi'(\hat{\alpha}_b) \geq -\psi''(0) \frac{\operatorname{arcsinh}(2/\sqrt{3})}{\pi} - c_0 \operatorname{hop}_2(C_0, C^-)^{-1}, \quad (4.25)$$

where $c_0 > 0$ is independent of u .

Remark 4.3.2. The explicit constant in (4.25) is strongly related to the structure of the lattice, and is crucial to the proof of Theorem 4.3.3. To generalise this analysis to models based on other lattices, similar careful estimates would be required to obtain the correct value.

The complete proof of Lemma 4.3.8 is given in Appendix A, but since this is a crucial part of the analysis in this chapter, we provide a brief sketch.

Sketch of the proof of Lemma 4.3.8. A crucial consequence of the **DOCP** is (4.20), as this inequality says that the dipoles described by each z^m satisfy

$$\begin{aligned} \text{either: } & \operatorname{hop}_2(C_0, C^+) \leq \operatorname{hop}_2(C_0, C^-); \\ \text{or: } & \operatorname{hop}_2(C_0, C^-) < \operatorname{hop}_2(C_0, C^+), \quad \text{but} \quad \operatorname{hop}_2(C^+, C^-) \leq \operatorname{hop}_2(C_0, C^-). \end{aligned}$$

Since there is a positive dislocation core present in C_0 , dipoles in the first category give a positive contribution to the sum, since the repulsive force between C^+ and C_0 dominates.

In the second case, the attractive forces between C_0 and C^- dominate, hence these dipoles give a negative contribution to the energy. Requiring the straight cuts property derived in Lemma 4.3.3 allows us to obtain estimates on the terms in the sums

$$\sum_{b \in \mathcal{B}} \psi'(\hat{\alpha}_b) z_b^m$$

using (4.5), and estimating sums in terms of integrals that can be evaluated explicitly. Thus, we obtain explicit bounds for various different cases in terms of $\operatorname{hop}_2(C_0, C^-)$ and $\operatorname{hop}_2(C^+, C^-)$. These estimates are logarithmic, and hence turn out to essentially depend upon the ratio

$$\frac{\operatorname{hop}_2(C^+, C^-)}{\operatorname{hop}_2(C_0, C^-)} \leq 1;$$

the final result is the bound stated in (4.25). $\square$

We have now collected all estimates required to obtain a coercivity result. Although we state the result for general $u \in \mathcal{W}^{1,2}(\Lambda)$, we will only require it later for u satisfying the **DOCP**.

Theorem 4.3.3. *Let $u \in \mathcal{W}^{1,2}(\Lambda)$, then there exists $\alpha \in [D\hat{y} + Du]$ and $\beta = \alpha - \hat{\alpha}$, such that*

$$\mathcal{E}(u) \geq c_1 \|\beta\|_2^2 + c_2 \#\mathcal{C}^\pm[\beta] - c_3, \quad (4.26)$$

where $c_i > 0$ are independent of u .

We note that since we will show $\|\beta\|_2^2 \gtrsim \#\mathcal{C}^\pm[\beta]$, we could write (4.26) more concisely as

$$\mathcal{E}(u) \geq c_1 \|\beta\|_2^2 - c_3.$$

Proof. The bound is clearly invariant under the vertical shift and horizontal shift and rotation transformations we applied in §4.3.2 and §4.3.3. Without loss of generality, we may therefore assume that u satisfies the **DOCP** (4.18). Moreover, according to Remark 3.1.1 we can choose $\alpha \in [D\hat{y} + Du]$ in such a way that $\alpha_b = 0$ on *any* bond that lies on the intersection between two cores.

Summing (4.25) over m , we find that

$$\sum_{b \in \mathcal{B}} z_b \psi'(\hat{\alpha}_b) \geq -\psi''(0) \frac{\operatorname{arcsinh}(2/\sqrt{3})}{2\pi} \#\mathcal{C}^\pm[\beta] - c_0 \sum_{C \in \mathcal{C}^-[\beta]} \operatorname{hop}_2(C, C_0)^{-1}. \quad (4.27)$$

for some $c_0 > 0$.

The second group in (4.27) can be estimated using the fact that each cell can contain no more than 1 dislocation core, so that for any $\delta > 0$, there is a constant C_δ such that

$$\sum_{C \in \mathcal{C}^-[\beta]} \operatorname{hop}_2(C, C_0)^{-1} \geq -\delta \#\mathcal{C}^\pm[\beta] - C_\delta.$$

Bringing together (4.11), (4.21) and (4.27), we have that for arbitrary $\epsilon > 0$ and $\delta > 0$

$$\mathcal{E}(u) \geq \left(\frac{1}{2}\psi''(0) - \epsilon\right)\|\beta\|_2^2 - \left(\psi''(0) \frac{\operatorname{arcsinh}(2/\sqrt{3})}{2\pi} + \delta\right)\#\mathcal{C}^\pm[\beta] - C_{\epsilon,\delta}.$$

Since we assumed that $\alpha_b = 0$ on any bond that is adjacent to two cores (cf. Remark 3.1.1), we obtain from (4.23) that

$$\|\beta\|_2^2 \geq \frac{1}{3}\#\mathcal{C}^\pm[\beta].$$

Since

$$\frac{1}{3} > \frac{\operatorname{arcsinh}(2/\sqrt{3})}{\pi} \approx 0.314,$$

the result follows by taking ϵ and δ small enough. $\square$

4.3.6 Existence of minimisers of $\mathcal{E}$

With the coercivity result of Theorem 4.3.3 in place, we are now in a position to apply the Direct Method and establish existence of a minimiser of $\mathcal{E}$ in $\mathcal{W}^{1,2}(\Lambda)$.

Take a sequence $u^n \in \mathcal{W}^{1,2}(\Lambda)$ such that

$$\mathcal{E}(u^n) \rightarrow \inf_{u \in \mathcal{W}^{1,2}(\Lambda)} \mathcal{E}(u).$$

Referring back to §4.3.3, we may assume that u^n satisfies the **DOCP**. Let $\alpha^n \in [D\hat{y} + Du^n]$ satisfy the condition of Theorem 4.3.3, and $\beta^n := \alpha^n - \hat{\alpha}$. Theorem 4.3.3 then implies that β^n has a weakly convergent subsequence in $\ell^2(\mathcal{B})$. In the next lemma, we also obtain convergence of Du^n .

Lemma 4.3.9. *Suppose $u^n \in \mathcal{W}^{1,2}(\Lambda)$ is a minimising sequence for which each u^n satisfies the **DOCP** (4.18). Then there exists a subsequence which converges weakly in $\mathcal{W}^{1,2}(\Lambda)$, and the corresponding z^n converges weakly in any $\ell^p(\mathcal{B})$ with $1 < p < 2$.*

Proof. Theorem 4.3.3 implies that, selecting a subsequence of u^n (not relabelled), we may assume that $\beta^n \rightharpoonup \beta$ weakly in $\ell^2(\mathcal{B})$ and that $M := \#\mathcal{C}^+[\beta^n]$ is constant along the sequence.

Let $Du^n = \beta^n + z^n$. Lemma 4.3.2 implies that each z^n can be decomposed into

$$z^n = \sum_{m=1}^M z^{n,m}.$$

Let B be any finite sum of positively-oriented cells. Since weak convergence in $\ell^2(\mathcal{B})$ implies pointwise convergence, it follows that

$$\int_{\partial B} \beta^n = - \int_{\partial B} z^n \rightarrow N \in \mathbb{Z} \quad \text{as } n \rightarrow \infty.$$

We enumerate the cores $C^{n,m} \in \mathcal{C}^\pm[\alpha^n]$, $n \in \mathbb{N}$, $m = 1, \dots, 2M+1$. Let $\mathcal{M}_{\text{bdd}}$ be the set of indices of cores that remain at a bounded distance from the origin, that is,

$$\mathcal{M}_{\text{bdd}} := \left\{ m \in \{1, \dots, 2M+1\} \mid \sup_{n \in \mathbb{N}} d_{C^{n,m}} < +\infty \right\}.$$

Since the core centres $x^{C^{n,m}}$ with $m \in \mathcal{M}_{\text{bdd}}$ can only take a finite number of positions, we can extract a further subsequence (not relabelled) so that they are constant.

We therefore observe that

$$A := \sum \mathcal{C}^\pm[\beta] = \sum_{m \in \mathcal{M}_{\text{bdd}}} C^{n,m}, \quad \text{for all } n.$$

Then, for any finite sum of cells B , $B \supset A$, we have

$$\lim_{n \rightarrow \infty} \int_{\partial B} \beta^n = \lim_{n \rightarrow \infty} \int_{\partial A} \beta^n = \int_{\partial A} \beta =: N \in \mathbb{Z}.$$

We aim to show that $N = 0$. For all n sufficiently large, applying Jensen's inequality implies

$$\int_{\partial A} |\beta^n|^2 \geq \frac{1}{|\partial A|} \left| \int_{\partial A} \beta^n \right|^2 = \frac{N^2}{|\partial A|}.$$

Let $B_0^0 \supset A$ be a finite sum of cells that form a convex lattice polygon, and let

$$B_k^0 = B_{k-1}^0 \cup \{C : \overline{\partial C} \cap B_{k-1}^0 \neq \emptyset\},$$

for $k \in \mathbb{N}$. By considering all possible corners for a convex lattice polygon it is straightforward to show that $|\partial B_k^0| = |\partial B_{k-1}^0| + 6$. Since $\lim_{n \rightarrow \infty} \int_{\partial B_k^0} \beta^n = N \in \mathbb{Z}$, there exist n_k such that $\int_{\partial B_i^0} \beta^{n_k} = N$ for $i = 1, \dots, k$, and hence,

$$\|\beta^{n_k}\|_2^2 \geq \sum_{i=0}^k \int_{\partial B_i^0} |\beta^{n_k}|^2 \geq \sum_{i=0}^k \frac{N^2}{|\partial B_k^0|} \gtrsim N^2 \log(k).$$

Since $\|\beta^{n_k}\|_2$ is bounded, we obtain that $N = 0$. We can therefore conclude that, for any finite sum of positively oriented cells b , $B \supset A$,

$$\int_{\partial B} z^n \rightarrow 0 \quad \text{as } n \rightarrow \infty.$$

Using a concentration compactness argument, we now show that we can ‘group’ those cores which diverge into sums of cells with net Burgers vector zero.

To that end, define the lattice translation operators $H_m^n := H^{C_m^n}$, where $C_m^n \in \mathcal{C}^+[\beta^n]$ and $\beta_m^n := \beta^n \circ H_m^n$. Note that

$$\|\beta_m^n\|_2 = \|\beta^n\|_2,$$

so β_m^n is a bounded sequence for each m , and we can select a subsequence such that $\beta_m^n \rightharpoonup \beta_m$ for some β_m in $\ell^2(\mathcal{B})$ and for each $m = 1, \dots, M$. As above, it follows that there exists a finite sum of positively-oriented cells A^m which contains C_0 and all dislocation cores of β_m , and is such that for any sum of positively-oriented cells B containing A^m as a subsum,

$$-\int_{\partial B} z^n \circ H_m^n = \int_{\partial B} \beta_m^n = 0 \quad \text{for } n \text{ sufficiently large.} \quad (4.28)$$

Let $A_m^n := (H_m^n)^{-1}A^m$, then we have shown that, for all n sufficiently large, all dislocation cores in β^n lie within the set

$$S^n := \bigcup_{m=1}^M A_m^n.$$

We are now ready to establish that $\|z^n\|_1$ is bounded. Since each z^n satisfies the **DMCP**, $\|z^n\|_\infty \leq M$. We therefore simply need to rule out the possibility that $\#\text{supp}\{z^n\} \rightarrow \infty$ as $n \rightarrow \infty$ (i.e., that the branch cut lengths diverge).

Fix some $m \in \{1, \dots, M\}$ and suppose that the core $C_m^n \in \mathcal{C}^+[\beta^n]$ is connected to $K_1^n \in \mathcal{C}^-[\beta^n]$ by $z^{n,m}$. We claim that $K_1^n \in A^{n,m}$.

If this were false and $K_1^n \in A_{\ell_1}^n$ where $\ell_1 \neq m$, then there must be $L_1^n \in \mathcal{C}^+[\beta^n]$, $L_1^n \in A_{\ell_1}^n$, which is connected to another core $K_2^n \in \mathcal{C}^-[\beta^n]$ outside of $A_{\ell_1}^n$ and outside A_m^n . Upon iterating this construction, we find a series of cores $K_1^n, L_1^n, K_2^n, L_2^n, \dots$, which must eventually repeat.

Let $L_0^n := C_m^n$. We know, by construction of the groups A_ℓ^n that $\text{hop}_2(L_i^n, K_{i+1}^n) \rightarrow \infty$ but $\text{hop}_2(K_i^n, L_i^n)$ is bounded as $n \rightarrow \infty$ for each i . This clearly contradicts the **DMCP** and hence the **DOCP**.

Hence, the claim that $K_1^n \in A^{n,m}$ follows, and this immediately implies that $\|z^n\|_1$ is bounded.

Since $\|z_n\|_1$ is bounded and ℓ^1 compactly embeds into ℓ^p for any $p > 1$, it follows that we may extract a further subsequence which weakly converges in some $\ell^p(\mathcal{B})$ with $p \in (1, \infty)$. Choosing such a subsequence for $p \in (1, 2)$, this further implies that both z^n and β^n converge weakly in $\ell^2(\mathcal{B})$, and in particular that u^n converges weakly in $\dot{\mathcal{W}}^{1,2}(\Lambda)$, as required. $\square$

We now complete the proof of our main result.

Proof of Theorem 4.2.1. Invoking the result of Lemma 4.3.9, suppose that the minimising sequence $u^n \rightharpoonup u$ in $\dot{\mathcal{W}}^{1,2}(\Lambda)$, which is a candidate minimiser for $\mathcal{E}$, and furthermore that the corresponding z^n converges weakly in $\ell^p(\mathcal{B})$ with $1 < p < 2$. It remains to show that $\liminf \mathcal{E}(u^n) \geq \mathcal{E}(u)$. Recall from (4.8) that

$$\mathcal{E}(u) = \sum_{b \in \mathcal{B}} [\psi(\hat{\alpha}_b + Du_b) - \psi(\hat{\alpha}_b) - \psi'(\hat{\alpha}_b)Du_b] + \langle \delta \mathcal{E}(0), u \rangle.$$

Since the second term is a bounded linear functional, it is weakly continuous. Using (4.5), it may be shown that the linear functional L defined to be

$$L(z) := \sum_{b \in \mathcal{B}} \psi'(\hat{\alpha}_b)z_b$$

is in $(\ell^p(\mathcal{B}))^*$ for all $p < 2$, and is therefore also weakly continuous along the sequence. From (4.12) we obtain that there exists $R_0, \lambda > 0$ such that, for $d_b \geq R_0$,

$$\psi(\hat{\alpha}_b + Du_b^n) - \psi(\hat{\alpha}_b) - \psi'(\hat{\alpha}_b)\beta_b^n \geq \lambda|\beta_b^n|^2 \geq 0.$$

We can therefore apply Fatou's lemma to obtain

$$\liminf_{n \rightarrow \infty} \sum_{b \in \mathcal{B}} \psi(\hat{\alpha}_b + Du_b^n) - \psi(\hat{\alpha}_b) - \psi'(\hat{\alpha}_b)\beta_b^n \geq \sum_{b \in \mathcal{B}} \psi(\hat{\alpha}_b + Du_b) - \psi(\hat{\alpha}_b) - \psi'(\hat{\alpha}_b)\beta_b,$$

and thus, in combination with the weak continuity of L and $\delta\mathcal{E}(0)$ along the minimising sequence,

$$\inf_{v \in \mathcal{W}^{1,2}(\Lambda)} \mathcal{E}(v) = \liminf_{n \rightarrow \infty} \mathcal{E}(u^n) \geq \mathcal{E}(u) \geq \inf_{v \in \mathcal{W}^{1,2}(\Lambda)} \mathcal{E}(v),$$

completing the proof of Theorem 4.2.1. □

4.4 Discussion

The main result of this chapter was Theorem 4.1.1, which appears to be the first result showing that a dislocation exists as the ground state of a variational problem. In the following chapter, we will show that this behaviour is far from generic, but the present result is an important basis for developing this model to better understand more general situations.

It should be pointed out here that the analysis carried out in this chapter relies crucially upon $(\psi 5)$, and that a similar (but weaker) assumption is required for some of the results of [ADGP13]. It is however unclear that this should be necessary in general: it would therefore be of significant interest to better understand this assumption in future.

Chapter 5

Locally stable equilibria with arbitrary net Burgers vector

In this chapter, we present the statement and proof of Theorem 5.1.1, which is the second main result concerning the model for screw dislocations in the BCC lattice presented in Chapter 3. This result states that if Ω is either the full lattice or a convex lattice polygon, we may find locally stable equilibria which contain dislocations of arbitrary net Burgers vector, as long as the dislocation cores are suitably far apart and, in the polygonal case, are suitably distant from the boundary of the crystal.

In §5.1, we state Theorem 5.1.1 and present the key assumption under which this result is proved. In §5.2, we prove some auxiliary results, and §5.3 and §5.4 make up the proof of the theorem in the cases where $\Omega = \Lambda$ and Ω is a convex lattice polygon respectively. The results of this chapter are also to be found in [HO14a].

5.1 Main result

5.1.1 Strong stability assumption

In this chapter, we make slightly different assumptions on ψ to those of Chapter 4. We continue to assume $(\psi 1)$ to $(\psi 4)$ as given in §3.3, but since we need to ensure that the energy difference functional has directional derivatives at all possible $y \in \mathcal{W}(\Omega)$, $(\psi 0)$ is slightly strengthened to:

Regularity assumption.

$(\psi 0') \quad \psi \in C^4(\mathbb{R}).$

It is again possible that this regularity assumption could be relaxed with additional work, but this would provide little gain whilst adding further technicalities to the proofs below.

Since the focus here is on multiple dislocation cores, we remove the technical assumption ($\psi 5$) made in Chapter 4, instead directly assuming the existence of a single stable core. Our key assumption here is therefore the following statement.

Strong stability assumption.

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

Throughout the rest of the chapter, u is fixed to satisfy **STAB**, and we denote $\lambda_d := \lambda$, the stability constant from (3.11) with $y = \hat{y} + u$. In addition, we fix a finite collection of cells, A , such that $\mathcal{C}^\pm[\alpha] \subset A$ for any $\alpha \in [D\hat{y} + Du]$.

As we will see in §5.2.1, **STAB** in fact implies ($\psi 4$). In general, it is difficult to say anything further about the relationship between ($\psi 5$) and **STAB**, but to demonstrate that our assumptions hold for a non-trivial class of potentials, we prove the following lemma.

Lemma 5.1.1. *Let $\psi_{\text{lin}}(r) := \frac{1}{2}\lambda \text{dist}(r, \mathbb{Z})^2$ and suppose $\psi \in C^4(\mathbb{R})$ satisfies*

$$|\psi^{(j)}(r) - \psi_{\text{lin}}^{(j)}(r)| \leq \epsilon |r|^{p-j} \quad \text{for } |r| \leq 1/2 - \epsilon_0 \quad \text{and } j = 1, 2, \quad (5.1)$$

where $p > 2$, $\epsilon_0 > 0$ is a fixed constant depending on ψ_{lin} , and ϵ is sufficiently small. Then there exists $w \in \dot{\mathcal{W}}^{1,2}(\Lambda)$ such that $\hat{y} + w$ is a strongly stable equilibrium.

Proof. Let E_{lin} denote the energy difference functional with potential ψ_{lin} , and E be the energy difference functional with potential ψ .

The potential ψ_{lin} satisfies the assumptions of Theorem 4.1.1, hence there exists $u \in \dot{\mathcal{W}}^{1,2}(\Lambda)$ such that $y = \hat{y} + u$ is a globally stable equilibrium of E_{lin} . Suppose that $Dy_b \in \frac{1}{2} + \mathbb{Z}$ for some $b = (\eta, \zeta) \in \mathcal{B}$, and let

$$z_t(\xi) := y(\xi) + \begin{cases} t & \xi = \eta, \\ 0 & \text{otherwise.} \end{cases}$$

A direct calculation similar to that undertaken in Lemma 5.1 in [ADGP13] demonstrates that there exists $\epsilon_0 > 0$ such that $E(z_t; y) < 0$ for all $|t| \leq \epsilon_0$. It follows that $\text{dist}(Dy_b, \frac{1}{2} + \mathbb{Z}) > \epsilon_0$, and hence

$$\langle \delta^2 E_{\text{lin}}(y + u)v, v \rangle = \sum_{b \in \mathcal{B}} \psi_{\text{lin}}''(Dy_b) Dv_b^2 = \lambda \|Dv\|_2^2.$$

Applying the growth conditions assumed in (5.1),

$$\begin{aligned} |\langle \delta E(y), v \rangle - \langle \delta E_{\text{lin}}(y), v \rangle| &\lesssim \epsilon \|Dv\|_2 && \text{for any } v \in \mathcal{W}^{1,2}(\Omega), \\ |\langle \delta^2 E(y)v, v \rangle - \langle \delta^2 E_{\text{lin}}(y)v, v \rangle| &\lesssim \epsilon \|Dv\|_2^2 && \text{for any } v \in \mathcal{W}^{1,2}(\Omega), \end{aligned}$$

so when ϵ is small enough, an application of the Inverse Function Theorem as stated below in Lemma 5.2.6 implies there exists $w - u \in \mathcal{W}^{1,2}(\Lambda)$ such that $\|Dw - Du\|_2 \lesssim \epsilon$, and $\hat{y} + w = y + w - u$ is a strongly stable equilibrium for E . $\square$

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 [EOS13].

5.1.2 Statement of the main result

We state the existence result for stable dislocation configurations in the infinite lattice and in convex lattice polygons. For this purpose, we recall the definitions of a dislocation core configuration, $\mathcal{D}$, and the separation distances $L_{\mathcal{D}}$ and $S_{\mathcal{D}}$ from §3.1.7, as well as the definitions of the lattice automorphisms G^C and H^C from §3.1.5.

Since we state the result for both types of domain together, we denote $S_{\mathcal{D}} := +\infty$ for the case $\Omega = \Lambda$. We note 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 $\text{index}(\partial W^\Omega)$, but otherwise not on the size or shape of the domain.

Theorem 5.1.1. *Suppose that **STAB** holds and either $\Omega = \Lambda$ or Ω is a convex lattice polygon.*

(1) *For each $N \in \mathbb{N}$ there are constants $L_0 = L_0(N)$ and $S_0 = S_0(\text{index}(\partial W^\Omega), N)$ 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 $z \in \mathcal{W}(\Omega)$, and for any $\alpha \in [Dz]$,*

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

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 with 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 $w \in \mathcal{W}^{1,2}(\Omega)$ 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 $\text{index}(\partial W^\Omega)$.

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

5.1.3 Strategy of the proof

In both cases, the overall strategy of proof is similar:

- For a given dislocation configuration $\mathcal{D}$, we construct an approximate equilibrium z using the linear elasticity solution for the dislocation configuration, and a truncated version of the core corrector u , whose existence we assumed in **STAB**.
- We obtain bounds which demonstrate that for these approximate equilibria, $\delta E^\Omega(z)$ decays to zero as $L_{\mathcal{D}} \rightarrow \infty$ or $S_{\mathcal{D}} \rightarrow \infty$.
- We show that for any $\epsilon > 0$, $\delta^2 E^\Omega(z) \geq \lambda_d - \epsilon$ as $L_{\mathcal{D}}, S_{\mathcal{D}} \rightarrow \infty$.
- We apply the Inverse Function Theorem to demonstrate the existence of a ‘corrector’ $w \in \mathcal{W}^{1,2}(\Omega)$ such that $z + w$ is a strongly stable equilibrium. Using the bounds on $\delta E^\Omega(z)$, we show that $\|Dw\|_{\ell^2}$ can be made arbitrarily small by making more stringent requirements on $\mathcal{D}$, and hence it may be demonstrated that the condition on the core position holds. This then completes the proof of parts (1) and (2) of the statement.
- Part (3) of the statement is proved via the construction of explicit counterexamples.

5.2 Auxiliary results

Before proceeding to the main proof of Theorem 5.1.1, we deduce several auxiliary results.

5.2.1 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 amongst all $y \in \mathcal{W}(\Lambda)$, and demonstrates that **STAB** implies $(\psi 4)$.

Lemma 5.2.1. *Suppose that **STAB** holds, then the deformation $y \equiv 0$ is a strongly stable equilibrium for any $\Omega \subset \Lambda$. Precisely,*

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

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

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

and since $\text{dist}(Dy_b, \mathbb{Z}) \rightarrow 0$ as $\text{dist}(b, 0) \rightarrow \infty$, 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. $\square$

5.2.2 The linear elasticity residual

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

Lemma 5.2.2. *Let $\mathcal{D}$ be a dislocation configuration in Λ and $z := \sum_{(C,s) \in \mathcal{D}} \hat{y} \circ H^C$ (as a function on $\mathbb{R}^2$), then for $L_{\mathcal{D}}$ sufficiently large, there exists $g : \mathcal{B} \rightarrow \mathbb{R}$ such that*

$$\langle \delta E(z), v \rangle = \sum_{b \in \mathcal{B}} g_b Dv_b \quad \text{and} \quad |g_b| \leq c \sum_{(C,s) \in \mathcal{D}} \text{dist}(b, C)^{-3}. \quad (5.2)$$

Proof. The canonical form for $\delta E(z)$ given in §3.3.1 is $\langle \delta E(z), v \rangle = \sum \psi'(\alpha_b) Dv_b$, where $\alpha \in [Dz]$. When $L_{\mathcal{D}}$ is sufficiently large, arguing as in Lemma 4.2.1, it follows that $\alpha_b \in (-\frac{1}{2}, \frac{1}{2})$, hence is unique, and furthermore $\alpha_{(\xi, \xi + a_i)} = \int_0^1 \nabla z(\xi + ta_i) \cdot a_i dt$. Here and throughout this chapter, $\nabla^j z$ means the extension of the relevant derivative of z to a function in $C^\infty(\mathbb{R}^2 \setminus \bigcup_{(C,s) \in \mathcal{D}} \{x^C\})$, or $C^\infty(U^\Omega \setminus \bigcup_{(C,s) \in \mathcal{D}} \{x^C\})$ in the convex lattice polygon case.

In particular we note that $|\psi'(\alpha_b)| \lesssim \sum \text{dist}(b, C)^{-1}$ only, necessitating the removal of a ‘divergence-free component’. To this end, let $\omega_b := \bigcup \{C' \in \mathcal{C} \mid \pm b \in \partial C'\}$ 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

$$h_b := \frac{\psi''(0)}{V} \lim_{\epsilon \rightarrow 0} \int_{\omega_b \setminus \bar{C}_\epsilon} \nabla z \cdot a_i dx \quad \text{and} \quad g_b := \psi'(\alpha_b) - h_b.$$

It is fairly straightforward to show that the limit exists (i.e. h_b and g_b are well-defined) and that

$$\sum_{b \in \mathcal{B}} h_b Dv_b = \lim_{\epsilon \rightarrow 0} \frac{\psi''(0)}{V} \int_{\mathbb{R}^2 \setminus \bar{C}_\epsilon} \nabla z \cdot \nabla I v dx = 0$$

for all $v \in \mathcal{W}_0(\Lambda)$, 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

$$\psi'(\alpha_b) - h_b = \psi'(0) + \psi''(0) \left(\alpha_b - \frac{1}{V} \lim_{\epsilon \rightarrow 0} \int_{\omega_b \setminus \bar{C}_\epsilon} \nabla z \cdot a_i \, dx \right) + \frac{1}{2} \psi'''(0) |\alpha_b|^2 + O(|\alpha_b|^3).$$

The first and third terms vanish by the evenness of ψ , and in the second term, we write $\alpha_b = \frac{1}{V} \int_{\omega_b} \nabla z \cdot a_i \, dx$, where a_i is the direction of the bond b . We then estimate this same term by Taylor expanding about m , the midpoint of b : using the symmetry of b and ω_b to eliminate the term involving $\nabla^2 z$, we obtain

$$\frac{1}{V} \int_{\omega_b} \nabla z \cdot a_i \, dx - \frac{1}{V} \lim_{\epsilon \rightarrow 0} \int_{\omega_b \setminus \bar{C}_\epsilon} \nabla z \cdot a_i \, dx = O(|\nabla^3 z|).$$

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

5.2.3 Regularity of the corrector

We now slightly refine the general regularity result of Theorem 3.1 in [EOS13], exploiting the evenness of the potential ψ .

Lemma 5.2.3. *Let u be the core corrector whose existence was postulated in **STAB**: then there exists a constant C_{reg} such that*

$$|Du_b| \leq C_{\text{reg}} \text{dist}(b, C)^{-2} \quad \text{for all } b \in \mathcal{B} \text{ and } (C, s) \in \mathcal{D}.$$

Proof. Our setting satisfies all assumptions of the $d = 2, m = 1$ (anti-plane) case described in §2.1 of [EOS13] with $\mathcal{N}_\xi = \{a_i \mid i = 1, \dots, 6\}$ for all $\xi \in \Lambda$, and the complete set of assumptions summarised in **(pD)** in §2.4.5 of [EOS13]. Using Lemma 5.2.2, we may apply Lemma 3.4 of [EOS13] with $p = 3$, implying $|Du_b| \lesssim \text{dist}(b, C)^{-2}$. $\square$

5.2.4 Approximation by truncation

Following [EOS13] we define a family of truncation operators Π_R^C , which we will apply to $u \in \dot{\mathcal{W}}^{1,2}(\Omega)$. Let $\eta \in C^1(\mathbb{R}^2)$ 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 of $\mathbb{R}^2$ given by $\mathcal{C}$. For $R > 2$ let $A_R := B_R \setminus B_{R/2+1}$, an annulus over which $\eta(x/R)$ is not constant. Define $\Pi_R^C : \mathcal{W}^{1,2} \rightarrow \mathcal{W}_0$ by

$$\Pi_R^C u(\xi) := \eta\left(\frac{\xi - x^C}{R}\right) (u(\xi) - a_R^C), \quad \text{where} \quad a_R^C := \oint_{x^C + A_R} Iu(x) dx.$$

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

The following result concerns the approximation property of the family of truncation operators Π_R^C , and follows from results in [EOS13].

Lemma 5.2.4. *Let $v \in \mathcal{W}^{1,2}(\Lambda)$ and $C \in \mathcal{C}$, then*

$$\|D\Pi_R^C v - Dv\|_{\ell^2(\mathcal{B})} \leq \gamma_1 \|Dv\|_{\ell^2(\mathcal{B} \setminus B_{R/2}(x^C))}, \quad (5.3)$$

where γ_1 is independent of R, v and C .

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

$$\|D\Pi_R^C(u \circ G^C) - D(u \circ G^C)\|_{\ell^2(\mathcal{B})} \leq \gamma_2 R^{-1}, \quad (5.4)$$

where γ_2 is independent of R and C .

Proof. Since $\|\cdot\|_{\ell^2(\mathcal{B})}$ is invariant under the transformation induced by composing functions with lattice automorphisms, we may assume without loss of generality that $C = C_0$, whence the estimate (5.3) is simply a restatement of Lemma 4.3 in [EOS13]; the second estimate (5.4) then follows immediately from Lemma 5.2.3. $\square$

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

Lemma 5.2.5. *There exist constants $\lambda_{d,R}$ such that*

$$\langle \delta^2 E^\Lambda(\hat{y} + \Pi_R u)v, v \rangle \geq \lambda_{d,R} \|Dv\|_2^2 \quad \text{for all } v \in \mathcal{W}_0, \quad (5.5)$$

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

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

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

where $\epsilon_R \lesssim R^{-1}$ as $R \rightarrow \infty$ by the result of Lemma 5.2.4. $\square$

5.2.5 Inverse Function Theorem

To conclude this collection of auxiliary results, we review a quantitative version of the Inverse Function Theorem, adapted from Lemma B.1 in [LO13].

Lemma 5.2.6. *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*

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

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

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

5.3 Proof for the infinite lattice

Before considering the case of finite lattice domains, we first set out to prove Theorem 5.1.1 in the case when $\Omega = \Lambda$. Here we are able to give a substantially simplified argument concerning only the interaction between dislocations, avoiding the additional difficulty of the interaction of dislocations with the boundary present in the other case.

5.3.1 Analysis of the predictor

Suppose that $\mathcal{D}$ is a dislocation configuration in Λ : we define an *approximate solution* or *predictor* with truncation radius R to be

$$z := \sum_{(C,s) \in \mathcal{D}} s (\hat{y} + \Pi_R u) \circ G^C. \quad (5.6)$$

The following result provides the first ingredient required for us to apply Lemma 5.2.6: a bound on the residual of such approximate solutions.

Lemma 5.3.1. *Suppose z is the approximate solution for a dislocation configuration $\mathcal{D}$ in Λ , defined in (5.6), 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 $L_{\mathcal{D}} > L_0$,*

$$\|\delta E(z)\|_{\mathcal{H}^{1,2}(\Lambda)^*} \leq cL_{\mathcal{D}}^{-1}.$$

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

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

The statement of Lemma 5.2.4 implies that $\|Dv^i\|_2 \lesssim \|Dv\|_2$ for $i = 0, \dots, N$.

Since $\delta E(\hat{y} + u) = 0$, we decompose the residual as

$$\begin{aligned} \langle \delta E(z), v \rangle &= \sum_{i=0}^N \langle \delta E(z), v^i \rangle, \\ &= \langle \delta E(z), v^0 \rangle + \sum_{i \neq 0} \langle \delta E(z) - \delta E(y^i), v^i \rangle \\ &\quad + \sum_{i \neq 0} \langle \delta E(y^i) - \delta E(\hat{y}^i + u \circ G^i), v^i \rangle \\ &=: T_1 + T_2 + T_3, \end{aligned} \tag{5.7}$$

and analyse T_1 , T_2 and T_3 separately.

The term T_1 : Employing Lemma 5.2.2 and using the fact that $z = \sum_{i=1}^N \hat{y}^i$ in $\text{supp}(v^0)$, we obtain that

$$\begin{aligned} |T_1| &= |\langle \delta E(z), v^0 \rangle| \leq \sum_{b \in \mathcal{B}} |g_b| |Dv_b^0| \\ &\lesssim \sum_{b \in \mathcal{B}} \sum_{i=1}^N \text{dist}(b, C^i)^{-3} |Dv_b^0| \\ &\lesssim \sum_{i=1}^N \left(\sum_{\substack{b \in \mathcal{B} \\ \text{dist}(b, C^i) \geq r/2-1}} \text{dist}(b, C^i)^{-6} \right)^{1/2} \|Dv^0\|_2 \\ &\lesssim r^{-2} \|Dv\|_2. \end{aligned} \tag{5.8}$$

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

$$\begin{aligned} \langle \delta E(z) - \delta E(y^i), v^i \rangle &= \sum_{b \in \mathcal{B}} \psi''(s_b) \sum_{j \neq i} D\hat{y}_b^j Dv_b^i \\ &= \psi''(0) \sum_{j \neq i} \sum_{b \in \mathcal{B}} D\hat{y}_b^j Dv_b^i + \sum_{b \in \mathcal{B}} h_b Dv_b^i, \end{aligned} \tag{5.9}$$

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

$$|h_b| = \left| (\psi''(s_b) - \psi''(0)) \sum_{j \neq i} D\hat{y}_b^j \right| \lesssim (1 + \text{dist}(b, C^i))^{-2} L_{\mathcal{D}}^{-1},$$

where we have Taylor expanded and used the evenness of ψ to arrive at the estimate on the right. The first group on the right-hand side of (5.9) can be estimated as in (5.8) to obtain $|\sum_{b \in \mathcal{B}} D\hat{y}_b^j Dv_b^i| \lesssim L_{\mathcal{D}}^{-2} \|Dv\|_2$ for all $j \neq i$. For the second group, we have

$$\left| \sum_{b \in \mathcal{B}} h_b Dv_b^i \right| \lesssim L_{\mathcal{D}}^{-1} \left(\sum_{\substack{b \in \mathcal{B} \\ \text{dist}(b, C^i) \leq r+1}} (1 + \text{dist}(b, C^i))^{-4} \right)^{1/2} \|Dv^i\|_2 \lesssim L_{\mathcal{D}}^{-1} \|Dv\|_2.$$

The term T_3 : The final term is straightforward to estimate using the truncation result of Lemma 5.2.4;

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

Conclusion: Inserting the estimates for T_1, T_2 and T_3 into (5.7), we obtain

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

5.3.2 Stability of the predictor

We next prove that $\delta^2 E(z)$ is positive, where z is the predictor constructed in (5.6). This result employs ideas similar to those in the proof of Theorem 4.8 in [EOS13], modified in this context to an aperiodic setting and to cover multiple defect cores.

Lemma 5.3.2. *Let z be given by (5.6). There exist positive constants $R_0 = R_0(N)$ and $L_0 = L_0(N)$ such that if $R \geq R_0$ and $L_{\mathcal{D}} \geq L_0$, then there exists $\lambda_{L,R} \geq \lambda_d/2$ so that*

$$\langle \delta^2 E(z)v, v \rangle \geq \lambda_{L,R} \|Dv\|_2^2 \quad \forall v \in \dot{\mathcal{W}}^{1,2}(\Lambda).$$

Proof. Lemma 5.2.5 implies the existence of R_0 such that $\lambda_{d,R} \geq 3\lambda_d/4 > 0$ for all $R \geq R_0$, thus we fix a truncation radius $R \geq R_0$, and hence assume $L_{\mathcal{D}} \geq 2R$. We now argue by contradiction. Suppose that there exists no L_0 which satisfies the statement. It follows that there exists a sequence of dislocation configurations, denoted $\mathcal{D}^n$, such that

1. $N := |\mathcal{D}^n|$, $|\{(C, +1) \in \mathcal{D}^n\}|$ and $|\{(C, -1) \in \mathcal{D}^n\}|$ are constant,
2. $L^n := L_{\mathcal{D}^n} \rightarrow \infty$ as $n \rightarrow \infty$, and

3. $\delta^2 E(z^n) < \lambda_d/2$ for all n , where z^n are the approximate solutions corresponding to $\mathcal{D}^n$ with truncation radius R .

The second and third conditions comprise the negation of the statement, and the first condition may be assumed without loss of generality by taking subsequences. Enumerate the elements $(C^{n,i}, s^{n,i}) \in \mathcal{D}^n$, and write $G^{n,i} := G^{C^{n,i}}$ and $H^{n,i} := H^{C^{n,i}}$. By the invariance of the energy difference under lattice automorphisms 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 ,

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

exists since $\delta^2 E(z)$ is a bounded bilinear form on $\dot{\mathcal{W}}^{1,2}(\Lambda)$ for any $z \in \mathcal{W}(\Lambda)$. Let $v^n \in \mathcal{W}_0(\Lambda)$ 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 $\dot{\mathcal{W}}^{1,2}(\Lambda)$, 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 Lemma 4.9 in [EOS13] which states that there exists a sequence of radii, $r^n \rightarrow \infty$, for which we may also assume $r^n \leq L^n/3$, such that for each i , $w^{n,i} := \Pi_{r^n}^{C^{n,i}} v^n$ satisfies

$$w^{n,i} \circ H^{n,i} \rightarrow \bar{w}^i \quad \text{and} \quad (v^n - w^{n,i}) \circ H^{n,i} \rightharpoonup 0 \quad \text{in } \dot{\mathcal{W}}^{1,2}(\Lambda). \quad (5.10)$$

We write $\bar{w}^{n,i} := w^{n,i} \circ H^{n,i}$, and define $w^{n,0} := v^n - \sum_{i=1}^N w^{n,i}$, so

$$\begin{aligned} \langle \delta^2 E(z^n) v^n, v^n \rangle &= \sum_{i,j} \langle \delta^2 E(z^n) w^{n,i}, w^{n,j} \rangle \\ &= \sum_i \langle \delta^2 E(z^n) w^{n,i}, w^{n,i} \rangle + 2 \sum_{i \neq 0} \langle \delta^2 E(z^n) w^{n,0}, w^{n,i} \rangle, \end{aligned}$$

where $r^n \leq L^n/3$ implies that $\text{supp}\{w^{n,i}\}$ for $i \neq 0$ only overlaps with $\text{supp}\{w^{n,0}\}$. When $i = 1, \dots, N$,

$$\begin{aligned} \langle \delta^2 E(z^n) w^{n,i}, w^{n,i} \rangle &= \langle [\delta^2 E(z^n \circ H^{n,i}) - \delta^2 E(\hat{y} + \Pi_R u)] \bar{w}^{n,i}, \bar{w}^{n,i} \rangle \\ &\quad + \langle \delta^2 E(\hat{y} + \Pi_R u) \bar{w}^{n,i}, \bar{w}^{n,i} \rangle, \\ &\geq \left(\lambda_{d,R} - \frac{N \|\psi'''\|_\infty}{2L^n/3} \right) \|Dw^{n,i}\|_2^2. \end{aligned} \quad (5.11)$$

For the $i = 0$ term, we can write:

$$\begin{aligned}\langle \delta^2 E(z^n) w^{n,0}, w^{n,0} \rangle &= \langle [\delta^2 E(z^n) - \delta^2 E(0)] w^{n,0}, w^{n,0} \rangle + \langle \delta^2 E(0) w^{n,0}, w^{n,0} \rangle, \\ &\geq \left(\psi''(0) - \frac{N \|\psi'''\|_\infty}{r^n} \right) \|Dw^{n,0}\|_2^2.\end{aligned}\quad (5.12)$$

Next, we consider 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 can therefore write

$$\begin{aligned}\langle \delta^2 E(z^n) w^{n,0}, w^{n,i} \rangle &= \langle [\delta^2 E(z^n \circ H^{n,i}) - \delta^2 E(\hat{y} + \Pi_R u)] (\bar{v}^{n,i} - \bar{w}^{n,i}), \bar{w}^{n,i} \rangle \\ &\quad + \langle \delta^2 E(\hat{y} + \Pi_R u) (\bar{v}^{n,i} - \bar{w}^{n,i}), \bar{w}^{n,i} - \bar{w}^i \rangle \\ &\quad + \langle \delta^2 E(\hat{y} + \Pi_R u) (\bar{v}^{n,i} - \bar{w}^{n,i}), \bar{w}^i \rangle, \\ &=: T_1 + T_2 + T_3.\end{aligned}$$

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

$$\begin{aligned}T_1 &\leq \frac{N \|\psi'''\|_\infty}{2L^{n/3}} \left(\|Dv^{n,i}\|_2 + \|Dw^{n,i}\|_2 \right) \|Dw^{n,i}\|_2 \leq \frac{N \|\psi'''\|_\infty}{L^{n/3}} \quad \text{and} \\ T_2 &\leq \|\psi''\|_\infty \left(\|Dv^{n,i}\|_2 + \|Dw^{n,i}\|_2 \right) \|D\bar{w}^{n,i} - D\bar{w}^i\|_2,\end{aligned}$$

both of which converge to 0 as $n \rightarrow \infty$ due to (5.10). Since (5.10) also implies that $\bar{v}^{n,i} - \bar{w}^{n,i} \rightarrow 0$ as $n \rightarrow \infty$, $T_3 \rightarrow 0$ as well, and hence

$$\langle \delta^2 E(z^n) w^{n,0}, w^{n,i} \rangle \rightarrow 0 \quad (5.13)$$

as $n \rightarrow \infty$ for each i . Putting (5.13) and the result of Lemma 5.2.1 together with the estimates (5.11) and (5.12), we obtain

$$\langle \delta^2 E(z^n) v^n, v^n \rangle \geq (\lambda_{d,R} - \epsilon^n) \sum_{i=1}^N \|Dw^{n,i}\|_2^2 + \epsilon^n, \quad (5.14)$$

where $\epsilon^n \rightarrow 0$ as $n \rightarrow \infty$.

To complete the proof of the statement, we now check that

$$\liminf_{n \rightarrow \infty} \left(\sum_{i=0}^N \|Dw^{n,i}\|_2^2 - \|Dv^n\|_2^2 \right) \geq 0. \quad (5.15)$$

By definition, $\sum_{i=0}^N |Dw_b^{n,i}|^2 \neq |Dv_b^n|^2$ only when $b \in \text{supp}\{Dw^{n,i}\} \cap \text{supp}\{Dw^{n,0}\}$ for some $i \neq 0$. In this case

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

Therefore, consider

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

Since $w^{n,0} \circ H^{n,i} \rightharpoonup 0$ and $\bar{w}^{n,i} \rightarrow \bar{w}^i$, it follows that $\delta^{n,i} \rightarrow 0$, and thus (5.15) holds. Further,

$$\lambda_n + n^{-1} \geq \langle \delta^2 E(z^n) v^n, v^n \rangle \geq (\lambda_{d,R} - \epsilon^n) \left(1 - \sum_{i=0}^N \delta^{n,i}\right) + \epsilon^n,$$

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

5.3.3 Conclusion of the proof

We now conclude the proof of Theorem 5.1.1 by proving each of the three statements in turn.

Proof of (2). Lemma 5.3.1 and Lemma 5.3.2 enable us to state that there exists L_0 and R_0 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 ,

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

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 5.2.6, since $\frac{2Mr}{\mu^2} \leq \frac{1}{2} < 1$. This implies that there exists $w \in \mathcal{W}^{1,2}(\Lambda)$ with $\|Dw\|_2 \leq c' L_{\mathcal{D}}^{-1}$ such that

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

and it follows that $z+w$ is a local equilibrium. The constant c' depends only on the number of dislocations, establishing item (2) of Theorem 5.1.1.

Proof of (1). First, we increase R_0 if necessary, so that $\frac{|\mathcal{D}|}{2\pi R_0} \leq \frac{1}{4}$. Let z be the predictor corresponding to a dislocation configuration $\mathcal{D}$ satisfying all the hypotheses

required to prove statement (2) above, as well as this additional condition. If $\alpha \in [Dz]$, any $b \in \mathbb{R}^2 \setminus B_R(x^C)$ for all $(C, s) \in \mathcal{D}$ must satisfy $\alpha_b \in [-\frac{1}{4}, \frac{1}{4}]$, and furthermore

$$\alpha_b = \sum_{(C,s) \in \mathcal{D}} s(\hat{\alpha} \circ G^C)_b.$$

Taking $L_{\mathcal{D}} > 4c'$ in the proof of statement (2) above, there exists $w \in \dot{\mathcal{W}}^{1,2}(\Lambda)$ such that $z + w$ is a strongly stable local equilibrium, and $\|Dw\|_{\infty} \leq \|Dw\|_2 < \frac{1}{4}$. This choice entails that $\alpha'_b = \alpha_b + Dw_b$ for any $\alpha' \in [Dz + Dw]$ and any $b \in \mathbb{R}^2 \setminus B_R(x^C)$ for all $(C, s) \in \mathcal{D}$.

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

$$\begin{aligned} \int_{\partial A^{C'}} \alpha' &= \int_{\partial A^{C'}} \sum_{(C,s) \in \mathcal{D}} s(\hat{\alpha} \circ G^C) + Dw = s' \quad \text{for any } (C', s') \in \mathcal{D}, \quad \text{and} \\ \int_{\partial C} \alpha' &= 0 \quad \text{for any } C \notin \bigcup_{(C,s) \in \mathcal{D}} A^C, \quad \text{implying } \mathcal{C}^{\pm}[\alpha'] \subset \bigcup_{(C,s) \in \mathcal{D}} H^C(A). \end{aligned}$$

Proof of (3). We divide the proof of (3) into two cases: $B[z] = 0$, and $|B[z]| > 1$. We note that we may exclude $B[z] = \pm 1$, since Theorem 4.1.1 implies the existence of a globally stable equilibrium in this case.

Suppose z is a strongly stable equilibrium such that $B[z] = 0$, arising from (2) in Theorem 5.1.1. We note that Dz will in general not be in $\dot{\mathcal{W}}^{1,2}(\Lambda)$, since it contains a superposition of translated copies of $\hat{y}$, each of which has an infinitely long branchcut on which $|D\hat{y}_b| \rightarrow 1$ as $b \rightarrow \infty$. Nevertheless, we show it is possible to find a non-zero deformation $v \in \dot{\mathcal{W}}^{1,2}(\Lambda)$ such that $Dz_b - Dv_b \in \mathbb{Z}$ for all $b \in \mathcal{B}$, and hence, by using the periodicity of the potential, $E(z - v; z) = E(0; v) < 0$.

$B[z] = 0$ implies that $\#\{(C, 1) \in \mathcal{D}\} = \#\{(C, -1) \in \mathcal{D}\}$, so enumerating $(C_+^i, 1), (C_-^i, -1) \in \mathcal{D}$ for $i = 1, \dots, \#\mathcal{D}/2$, we define

$$\begin{aligned} v^i(x) &:= \frac{1}{2\pi} \left[\arg(x - x^{C_+^i}) - \arg(x - x^{C_-^i}) \right], \\ \text{and} \quad v &:= \sum_{i=1}^{\#\mathcal{D}/2} v^i + \left(z - \sum_{(C,s) \in \mathcal{D}} s(\hat{y} \circ G^C) \right), \end{aligned} \tag{5.16}$$

where v^i is defined with a branch cut of finite length between $x^{C_+^i}$ and $x^{C_-^i}$. By similar arguments to those used in Lemma 5.2.2, we may extend ∇v^i to a function which is $C^\infty(\mathbb{R}^2 \setminus \{x^{C_+^i}, x^{C_-^i}\}; \mathbb{R}^2)$, and it may be directly verified that $|\nabla v^i(x)| \lesssim |x|^{-2}$ for $|x|$ suitably large. When v^i is restricted to Λ , it clear that $v^i \in \dot{\mathcal{W}}^{1,2}(\Lambda)$. Furthermore,

the characterisation of z given in statement (2) of Theorem 5.1.1 and the fact that $v^i \in \dot{\mathcal{W}}^{1,2}(\Lambda)$ imply that $v \in \dot{\mathcal{W}}^{1,2}(\Lambda)$.

Using the definition of v and fact that $\frac{1}{2\pi} \arg(x)$ is defined up to an integer depending upon the choice of branch cut, $z(\xi) - v(\xi) \in \mathbb{Z}$ for all $\xi \in \Lambda$, and hence $Dz_b - Dv_b \in \mathbb{Z}$ for all $b \in \mathcal{B}$. Using the periodicity and evenness of ψ , we therefore obtain

$$\begin{aligned} E(z - v; z) &= \sum_{b \in \mathcal{B}} \psi(Dz_b - Dv_b) - \psi(Dz_b - Dv_b + Dv_b) \\ &= \sum_{b \in \mathcal{B}} \psi(0) - \psi(Dv_b) = -E(v; 0) < 0, \end{aligned}$$

as Lemma 5.2.1 implies that $0 = \operatorname{argmin}\{E(u; 0) \mid u \in \dot{\mathcal{W}}^{1,2}(\Omega)\}$. It follows that z cannot be a globally stable equilibrium in this case.

If $|B[z]| > 1$, then by applying the evenness of the potential, we may suppose without loss of generality that $B[z] > 1$. Here, we consider only the case where $B[z] = 2$; the general case follows along the same lines, but with the estimates constructed in the latter part of the proof simply requiring $B[z] - 1$ cores to be kept close to the origin while varying the position of the final core.

Suppose that $\#\mathcal{D} = 2 + 2m$, where $m \in \mathbb{N} \cup \{0\}$. If $m > 0$, then by properties of the Burgers vector, there exist cores $(C_-^i, -1) \in \mathcal{D}$ for $i = 1, \dots, m$. We choose to enumerate m distinct positive cores of the form $(C_+^i, +1) \in \mathcal{D}$, and define v^i as in (5.16) with branch cuts of finite length. Let

$$v := \sum_{i=1}^m v^i + \left(z - \sum_{i=1}^m (\hat{y} \circ G^{C_+^i} - \hat{y} \circ G^{C_-^i}) \right).$$

Since $v^i \in \dot{\mathcal{W}}^{1,2}(\Lambda)$, it is clear that v takes the form

$$v = \hat{y} \circ G^C + \hat{y} \circ G^{C'} + w \quad \text{where } w \in \dot{\mathcal{W}}^{1,2}(\Lambda),$$

with $(C, +1), (C', +1) \in \mathcal{D}$ distinct and satisfying $C, C' \neq C_+^i$ for all $i = 1, \dots, m$. Once more, $Dv_b - Dz_b \in \mathbb{Z}$ for all $b \in \mathcal{B}$.

Consider a deformation w^0 , taking the form

$$w^0(\xi) = \frac{1}{2\pi} (\arg(\xi) + \arg(\xi - ka_1)), \quad (5.17)$$

recalling from §3.1.5 that ka_1 is the barycentre of a cell, and where $\arg(x)$ and $\arg(x - x^{C^0})$ have been defined via branch cuts coinciding respectively with those of $\hat{y} \circ G^C$

and $\hat{y} \circ G^{C'}$ except on a set of finite 1-dimensional Hausdorff measure. With this choice, $w^0 - \hat{y} \circ G^C - \hat{y} \circ G^{C'} \in \mathcal{W}^{1,2}(\Lambda)$, and hence $w^0 - v \in \mathcal{W}^{1,2}(\Lambda)$.

We now construct a deformation which has an arbitrarily negative energy difference when compared with y , and hence also when compared with z . This demonstrates that z cannot be a globally stable equilibrium.

Define

$$u^l(\xi) := \frac{1}{2\pi} (\arg(\xi - (k+l)a_1) - \arg(\xi - ka_1)), \quad \text{and} \quad w^l(\xi) := w^0(\xi) + u^l(\xi),$$

where u^l is defined with a branch cut which lies on the x_1 -axis between l and $k+l$. Note that $u^l \in \mathcal{W}^{1,2}(\Lambda)$, and hence $w^l - y, w^l - v \in \mathcal{W}^{1,2}(\Lambda)$.

We suppose that k is sufficiently large such that $\alpha^0 \in [Dy]$ is unique, which also implies that $\alpha^l \in [Dw^l]$ are unique. Let $\beta_b^l := \alpha_b^l - \alpha_b^0$, and set $Z_b^l := Du_b^l - \beta_b^l$. Z^l is supported only on bonds b which intersect the branch cut between k and $k+l$ on the x_1 -axis.

Consider the energy difference

$$E(w^0; w^l) = E(w^l - u^l; w^l) = \sum_{b \in \mathcal{B}} \psi(\alpha_b^l - \beta_b^l) - \psi(\alpha_b^l) + \psi'(\alpha_b^l) Du_b^l - \langle \delta E(w^l), u^l \rangle,$$

where we have used the periodicity of the potential ψ . Taylor expanding as in Lemma 4.3.1, we have the lower bound

$$E(y; w^l) \geq \sum_{b \in \mathcal{B}} \frac{1}{2} (\psi''(0) - \epsilon) |\beta_b^l|^2 + \psi'(\alpha_b^l) Z_b^l - \langle \delta E(w^l), u^l \rangle - C_\epsilon, \quad (5.18)$$

where $\epsilon > 0$ is arbitrary, and C_ϵ is a positive constant which blows up as $\epsilon \rightarrow 0$.

By possibly increasing k so that Lemma 5.2.2 applies, we find that we may write

$$-\langle \delta E(w^l), u^l \rangle + \sum_{b \in \mathcal{B}} \psi'(\alpha_b^l) Z_b^l = \sum_{b \in \mathcal{B}} -g_b^l Du_b^l + \psi'(\alpha_b^l) Z_b^l = \sum_{b \in \mathcal{B}} -g_b^l \beta_b^l + h_b^l Z_b^l.$$

Here, $g_b^l := \psi'(\alpha_b^l) - h_b^l$, where as in the proof of Lemma 5.2.2,

$$h_b^l = \frac{\psi''(0)}{V} \lim_{\epsilon \rightarrow 0} \int_{\omega_b \setminus \bar{C}_\epsilon} \nabla w^l \cdot a_i dx.$$

By using the explicit expression for ∇u^l and the decay properties of g^l , we have

$$\sum_{b \in \mathcal{B}} g_b^l \beta_b^l \lesssim \sum_{b \in \mathcal{B}} \left(\frac{1}{\text{dist}(b, 0)^3} + \frac{1}{\text{dist}(b, ka_1)^3} \right) \left(\frac{1}{\text{dist}(b, ka_1)} + \frac{1}{\text{dist}(b, (k+l)a_1)} \right), \quad (5.19)$$

which is uniformly bounded independently of the choice of l : this may be seen by repeated use of Young's inequality with $p = 4/3$.

It can be shown that $Z_b^l = 1$ for bonds of the form

$$b = (\xi_0 + (k+i)a_1 + a_2, \xi_0 + (k+i)a_1) \quad \text{or} \quad b = (\xi_0 + (k+i-1)a_1 + a_2, \xi_0 + (k+i)a_1)$$

for $i = 0, \dots, l-1$. Using the definition of h_b^l , and letting C^k and C^{k+l} be the cells with barycentres ka_1 and $(k+l)a_1$ respectively, we can write

$$\begin{aligned} \sum_{b \in \mathcal{B}} h_b^l Z_b^l &= \frac{\psi''(0)}{V} \int_{C^k} \nabla w^l \cdot (a_1 - a_2) dx + \frac{\psi''(0)}{V} \lim_{\epsilon \rightarrow 0} \int_{C^{k+l} \setminus B_\epsilon((k+l)a_1)} \nabla w^l \cdot a_2 dx \\ &\quad + \frac{\sqrt{3}\psi''(0)}{2\pi V} \int_{-\sqrt{3}/6}^{\sqrt{3}/3} \int_{k+\frac{1}{3}+\frac{y}{\sqrt{3}}}^{k+l+\frac{y}{\sqrt{3}}-\frac{1}{3}} \frac{x}{x^2 + y^2} + \frac{x - k - l}{(x - k - l)^2 + y^2} dx dy, \\ &=: T_1 + T_2 + T_3. \end{aligned}$$

It is straightforward to show that T_1 and T_2 are uniformly bounded independent of k and l . Evaluating the inner integral in T_3 directly, noting $V = 2/\sqrt{3}$, and performing some straightforward algebraic manipulation, we obtain

$$\begin{aligned} T_3 &= \frac{\psi''(0)}{2\pi} \int_{-\sqrt{3}/6}^{\sqrt{3}/3} \log \left(\frac{((k+l+y/\sqrt{3}-1/3)^2 + y^2)((y/\sqrt{3}-1/3)^2 + y^2)}{((k+1/3+y/\sqrt{3})^2 + y^2)((l-y/\sqrt{3}-1/3)^2 + y^2)} \right) dy \\ &\geq \frac{\sqrt{3}\psi''(0)}{4\pi} \log \left(\frac{(k+l-1/2)^2/12}{((k+2/3)^2 + 1/3)((l-1/2)^2 + 1/3)} \right), \end{aligned} \quad (5.20)$$

where on the second line, we have minimised the numerator and maximised the denominator of the fraction inside the logarithm for $y \in [-\sqrt{3}/6, \sqrt{3}/3]$ and then integrated. We note that for fixed k , this function is uniformly bounded for $l \in \mathbb{N}$.

Combining (5.18), (5.19) and (5.20), we have now established the lower bound

$$E(y; w^l) \geq c_0 \|\beta^l\|_{\ell^2}^2 - c_1, \quad (5.21)$$

where c_0 and c_1 are positive constants independent of l .

To estimate $\|\beta^l\|_{\ell^2}^2$ below, we define a series of volumes K_i . Let $K_1 = C^{k+l}$, and inductively define

$$K_i = \left(\bigcup \{C \in \mathcal{C} \mid C \text{ positively-oriented, } \text{clos}(C) \cap \text{clos}(K_{i-1}) \neq \emptyset\} \cup K_{i-1} \right)$$

for $i = 2, \dots, l$. By construction, $\int_{\partial K_i} \beta^l = 1$, and it may be verified that $\#\partial K_i = 6i - 3$. Applying Jensen's inequality, we have

$$\|\beta^l\|_{\ell^2}^2 \geq \sum_{i=1}^l \int_{\partial K_i} |\beta_b^l|^2 \geq \sum_{i=1}^l \frac{1}{6i-3} \left| \int_{\partial K_i} \beta_b^n \right|^2 \geq \sum_{i=1}^l \frac{1}{6i-3} \geq \frac{\log(2l+1)}{6}. \quad (5.22)$$

Combining (5.21) and (5.22), we have shown that $E(w^l; y) \lesssim -c'_0 \log(l) + c_1$ for l sufficiently large, where c'_0 and c'_1 are positive constants independent of l .

Recalling the construction of v , y and w^l , we have

$$E(w^l - v + z; z) = E(w^l; z) = E(w^l; y) + E(y; v) \leq -c'_0 \log(l) + c'_1 + E(y; v)$$

and hence letting $l \rightarrow \infty$, we see that z cannot be a globally stable equilibrium. $\square$

5.4 Proof for the convex lattice polygons

As in §5.3, we construct approximate solutions and then prove estimates on the derivative and Hessian of the energy difference so that we may apply Lemma 5.2.6. The two main differences between this and the preceding analysis are (i) $\hat{y}$ does *not* satisfy the natural boundary conditions of Laplace's equation, and (ii) we must estimate residual force contributions at the boundary, which cannot be achieved by a simple truncation argument as in §5.2.4: 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*, $\bar{y} \in C^1(U^\Omega) \cap C^2(\text{int}(U^\Omega))$, chosen to satisfy

$$-\Delta \bar{y} = 0 \quad \text{in } U^\Omega, \quad \nabla \bar{y} \cdot \nu = - \sum_{(C,s) \in \mathcal{D}} s \nabla(\hat{y} \circ G^C) \cdot \nu \quad \text{on } \partial U^\Omega, \quad (5.23)$$

where ν is the outward unit normal on ∂U^Ω . We shall demonstrate in §5.4.1 that $\bar{y}$ exists and satisfies the stated regularity.

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

$$z := \sum_{(C,s) \in \mathcal{D}} s (\hat{y} + \Pi_R u) \circ G^C + \bar{y}. \quad (5.24)$$

5.4.1 The continuum boundary corrector

Here, 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 [Gri11] to obtain regularity of solutions to (5.23).

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

$$-\Delta \bar{y} = 0 \quad \text{in } U^\Omega, \quad \nabla \bar{y} \cdot \nu = g_m \quad \text{on } \Gamma_m, \quad (5.25)$$

where as in §3.2, Γ_m are the straight segments of ∂U^Ω between corners (κ_{m-1}, κ_m) , ν is the outward unit normal, and

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

Since ν is constant along Γ_m , it follows that $g_m \in C^\infty(\Gamma_m)$, and so applying Corollary 4.4.3.8 in [Gri11], it may be seen that this problem has a solution in $H^2(U^\Omega)$ 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 (5.25) in terms of $\text{dist}(x', \partial U^\Omega)$, 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 5.4.1. *Suppose the U^Ω is a convex lattice polygon, and $\bar{y}$ solves (5.25). Then there exist constants c_1 and c_2 which are independent of the domain such that*

$$|\nabla \bar{y}(x)| \leq c_1 \text{dist}(x, x')^{-1} \quad \text{for any } x \in U^\Omega, \quad \|\nabla \bar{y}\|_\infty \leq c_1 \text{dist}(x', \partial U^\Omega)^{-1}, \quad (5.26)$$

$$\text{and} \quad \|\nabla^2 \bar{y}\|_{L^2(U^\Omega)} \leq c_3 \frac{\log(\text{dist}(x', \partial U^\Omega))}{\text{dist}(x', \partial U^\Omega)}. \quad (5.27)$$

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

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

By virtue of Corollary 4.4.3.8 in [Gri11], there exists a unique $\Psi \in H^2(U^\Omega)$ 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

$$\nabla \Psi^*(x) = R_4^T \nabla \Psi(x) \quad \text{for all } x \in U^\Omega, \quad (5.28)$$

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

$$\frac{\partial \Psi^*}{\partial \nu} = \frac{\partial \Psi}{\partial \tau} = \frac{(x - x')}{2\pi|x - x'|^2} \cdot R_4 \nu = -\nabla \hat{y}(x - x') \cdot \nu \quad \text{on } \partial U^\Omega, \quad \text{and} \quad -\Delta \Psi^* = 0 \quad \text{in } U^\Omega,$$

where τ is the unit tangent vector to ∂U^Ω with the positive orientation. By uniqueness of solutions for (5.25), it follows that $\Psi^* = \bar{y}$ up to an additive constant, and hence $\bar{y}$ is a harmonic conjugate of Ψ . Furthermore, by differentiating (5.28),

$$\|\nabla^2 \Psi\|_{L^2(U^\Omega)} = \|\nabla^2 \bar{y}\|_{L^2(\Omega)}. \quad (5.29)$$

The identities (5.28) and (5.29) will allow us to use estimates on the derivatives of Ψ to directly deduce (5.26) and (5.27).

To prove (5.26), we rely upon Proposition 1 in [Fro93], which states that there exists a constant c_1 depending only on $\text{diam}(U^\Omega)$ such that

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

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 $\text{diam}(U^\Omega)$ and is therefore independent of the domain (as long as it remains convex). Taking the Euclidean norm of both sides in (5.28) now implies the pointwise bound in (5.26), and the L^∞ bound follows immediately as the partial derivatives of $\bar{y}$ satisfy the strong maximum principle.

To prove (5.27), 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

$$-\Delta(\Psi - \Phi) = \Delta\Phi \quad \text{in } U^\Omega, \quad \Psi - \Phi \in H^2(U^\Omega) \cap H_0^1(U^\Omega),$$

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

$$\begin{aligned} \Phi(x) &:= -\frac{1}{2\pi} \phi(|x - x'|/\text{dist}(x', \partial U^\Omega)) \log(|x - x'|), \\ \text{where } \phi &\in C^\infty([0, +\infty)) \quad \text{and} \quad \phi(r) = \begin{cases} 0 & r \in [0, \frac{1}{4}], \\ 1 & r \geq 1. \end{cases} \end{aligned}$$

By construction $\Phi \in C^\infty(U^\Omega)$, and $\nabla^2 \Phi \in L^2(\mathbb{R}^2)$. Thus $\Delta\Phi \in L^2(U^\Omega)$, and the existence of a unique solution $\Psi - \Phi \in H^2(U^\Omega) \cap H_0^1(U^\Omega)$ follows from Theorem 3.2.1.2 in [Gri11]). Furthermore, inspecting the proof of Theorem 4.3.1.4 in [Gri11], we see that

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

and thus a straightforward integral estimate yields

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

where c_2 is independent of the domain. □

5.4.2 Analysis of the predictor

We now prove that the predictor defined in (5.24) is indeed an approximate equilibrium. Our first step is to formulate the analogue of Lemma 5.2.2 in the polygonal case.

Lemma 5.4.2. *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 (5.23). 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 $g : \mathcal{B}^\Omega \rightarrow \mathbb{R}$ and $\Sigma : \{b \in \partial W^\Omega\} \rightarrow \mathbb{R}$ such that*

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

Furthermore,

$$|g_b| \leq c_1 \sum_{(C,s) \in \mathcal{D}} (1 + \text{dist}(b, C))^{-3} + c_1 \|\nabla^2 \bar{y}\|_{L^2(\omega_b)} \text{ for all } b \notin \partial W^\Omega, \quad (5.30)$$

and if $b \in P_\zeta \subset \partial W^\Omega$, then

$$|g_b + \Sigma_b| \leq c_2 \sum_{(C,s) \in \mathcal{D}} (1 + \text{dist}(P_\zeta, C))^{-1} + c_1 \|\nabla^2 \bar{y}\|_{L^2(\omega_b)}. \quad (5.31)$$

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

Proof. We begin by choosing L_0 and S_0 to ensure that $\alpha \in [Dz]$ is unique: since the constant in (5.26) 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 $\alpha_{(\xi, \xi+a_i)} = \int_0^1 \nabla z(\xi + ta_i) \cdot a_i dt$, where ∇z is to be understood as the extension of the gradient of z to a function in $C^\infty(U^\Omega \setminus \bigcup_{(C,s) \in \mathcal{D}} \{x^C\})$.

Let $\omega_b := \bigcup \{C \in \mathcal{C}^\Omega \mid \pm b \in \partial C, C \text{ positively oriented}\}$, the union of any cells in the boundary of which b lies. 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

$$h_b := \frac{\psi''(0)}{V} \lim_{\epsilon \rightarrow 0} \int_{\omega_b \setminus \bar{C}_\epsilon} \nabla z \cdot a_i dx \quad \text{and} \quad g_b := \psi'(\alpha_b) - h_b.$$

As in the proof of Lemma 5.2.2, an application of the divergence theorem demonstrates that the former (and hence the latter) definition makes sense. Let $v \in \mathcal{W}(\Omega)$,

and denote its piecewise linear interpolant Iv ; applying the divergence theorem once more,

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

Recalling the definition of P_ζ from (3.6), we find that

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

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

$$\int_{P_\zeta} Iv \nabla z \cdot \nu \, ds = Iv(\zeta + \tau) \int_{P_\zeta} \nabla z \cdot \nu \, ds - \int_{P_\zeta} Iv' \left(\int_{\gamma_\zeta^s} \nabla z \cdot \nu \, dt \right) ds,$$

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 3.4) 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 ∇Iv is constant along each bond,

$$\begin{aligned} \int_{P_\zeta} Iv \nabla z \cdot \nu \, ds &= - \sum_{b \in P_\zeta} \int_{b=(\xi, \xi+a_i)} \nabla Iv \cdot a_i \left(\int_{\gamma_\zeta^s} \nabla z \cdot \nu \, dt \right) ds, \\ &= \sum_{b \in P_\zeta} \Sigma_b Dv_b, \quad \text{where} \quad \Sigma_b := - \int_b \int_{\gamma_\zeta^s} \nabla z \cdot \nu \, dt \, ds. \end{aligned}$$

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

To obtain (5.30), we Taylor expand the potential to obtain

$$g_b = \psi''(0) \left(\int_b \nabla z \cdot a_i \, dx - \lim_{\epsilon \rightarrow 0} \frac{1}{V} \int_{\omega_b \setminus \bar{C}_\epsilon} \nabla z \cdot a_i \, dx \right) + O(|Dz_b|^3).$$

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 5.2.2 is to estimate the terms involving $\nabla \bar{y}$. As $\int_b \nabla \bar{y} \cdot a_i \, dx = \frac{1}{|\omega_b|} \int_{\omega_b} \nabla I\bar{y} \cdot a_i \, dx$, applying Jensen's inequality and standard interpolation error estimates (see for example §4.4 of [BS08]) gives

$$\begin{aligned} \int_b \nabla \bar{y} \cdot a_i \, dx - \frac{1}{V} \int_{\omega_b} \nabla \bar{y} \cdot a_i \, dx &= \frac{1}{V} \int_{\omega_b} (\nabla I\bar{y} - \nabla \bar{y}) \cdot a_i \, dx \\ &\leq \frac{1}{\sqrt{V}} \|\nabla I\bar{y} - \nabla \bar{y}\|_{L^2(\omega_b)} \\ &\leq c \|\nabla^2 \bar{y}\|_{L^2(\omega_b)} \end{aligned}$$

where $c > 0$ is a fixed constant. Applying Young's inequality and (5.26) to estimate $|Dz_b|^3$ now leads immediately to (5.30).

Estimate (5.31) 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

$$\begin{aligned} |g_b + \Sigma_b| &\leq \int_b \left| \frac{1}{2} \nabla z \cdot a_i - \int_{\gamma_\zeta^s} \nabla z \cdot \nu \, dt \right| ds + c \|\nabla^2 \bar{y}\|_{L^2(\omega_b)} \\ &\quad + \sum_{(C,s) \in \mathcal{D}} \|\nabla^2 \hat{y} \circ G^C\|_{L^\infty(\omega_b)} + O(|Dz_b|^3). \end{aligned}$$

Applying (5.26) to the first and last terms and using the decay of $\nabla \hat{y}$ now yields

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

Upon recalling the definition of $\text{index}(\partial W^\Omega)$ from §3.2, the proof is complete. $\square$

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

Lemma 5.4.3. *Suppose Ω is a convex lattice polygon, and z is the approximate solution corresponding to a dislocation configuration $\mathcal{D}$ in Ω defined in (5.24) with truncation radius $R = \min\{L_{\mathcal{D}}/5, S_{\mathcal{D}}^{1/2}\}$. Then there exist constants L_0 , S_0 and c depending only on $N = |\mathcal{D}|$ and $\text{index}(\partial W^\Omega)$ such that whenever $L_{\mathcal{D}} \geq L_0$ and $S_{\mathcal{D}} \geq S_0$,*

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

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 (5.25) with $x' = x^{C^i}$.

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

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

Lemma 5.2.4 implies there is a universal constant which is independent of Ω such that $\|Dv^i\|_2 \leq C\|Dv\|_2$ for any $i = 0, \dots, N$. Adding and subtracting terms, we write

$$\begin{aligned} \langle \delta E^\Omega(z), v \rangle &= \langle \delta E^\Omega(z), v^0 \rangle + \sum_i \langle [\delta E^\Omega(z) - \delta E^\Lambda(y^i)], v^i \rangle \\ &\quad + \sum_i \langle [\delta E^\Lambda(y^i) - \delta E^\Lambda(\hat{y}^i + u \circ G^i)], v^i \rangle, \\ &=: T_1 + T_2 + T_3. \end{aligned} \tag{5.32}$$

We estimate each of these terms in turn.

The term T_1 : Applying Lemma 5.4.2 and the fact that $z = \sum_{i=1}^N \hat{y}^i + \bar{y}^i$ in $\text{supp}(v^0)$, we make a similar estimate to that in Lemma 5.3.1:

$$\begin{aligned}
|T_1| &= \left| \sum_{b \in \mathcal{B}^\Omega} g_b Dv_b^0 + \sum_{b \in \partial W^\Omega} \Sigma_b Dv_b^0 \right| \\
&\leq c_1 \left(\left(\sum_{\substack{(C,s) \in \mathcal{D}, b \in \mathcal{B}^\Omega \\ \text{dist}(b,C) \geq r/2-1}} (1 + \text{dist}(b,C))^{-6} \right)^{1/2} + \|\nabla^2 \bar{y}\|_{L^2(W^\Omega)} \right) \|Dv^0\|_2 \\
&\quad + c_2 \left(\sum_{\zeta \in \partial W^\Omega \cap \partial U^\Omega} (1 + \text{dist}(P_\zeta, C^i))^{-2} \right)^{1/2} \|Dv^0\|_2, \\
&\leq c \left(r^{-2} + S_{\mathcal{D}}^{-1} \log(S_{\mathcal{D}}) + \text{index}(\partial W^\Omega)^{1/2} S_{\mathcal{D}}^{-1/2} \right) \|Dv^0\|_2. \tag{5.33}
\end{aligned}$$

To arrive at the final line we have used (5.27), 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 $z - y^i = \sum_{j \neq i} \hat{y}^j + \sum_j \bar{y}^j$ in the support of v^i . We expand as in Lemma 5.3.1 to obtain

$$\begin{aligned}
\langle \delta E^\Omega(z) - \delta E(y^i), v^i \rangle &= \sum_{b \in \mathcal{B}^\Omega} \psi''(s_b) \left(\sum_{j \neq i} D\hat{y}_b^j + \sum_{j=0}^N D\bar{y}_b^j \right) Dv_b^i, \\
&= \psi''(0) \sum_{b \in \mathcal{B}^\Omega} \left(\sum_{j \neq i} D\hat{y}_b^j + D\bar{y}_b^j \right) Dv_b^i + \psi''(0) \sum_{b \in \mathcal{B}^\Omega} D\bar{y}_b^i Dv_b^i + \sum_{b \in \mathcal{B}^\Omega} h_b Dv_b^i, \tag{5.34}
\end{aligned}$$

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

$$|h_b| = \left| (\psi''(s_b) - \psi''(0)) \left(\sum_{j \neq i} D\hat{y}_b^j + \sum_{j=0}^N D\bar{y}_b^j \right) \right| \lesssim |s_b|^2 r^{-1}.$$

Applying Lemma 5.4.2 to the first term in (5.34), a similar argument to that used to arrive at (5.33) gives

$$\sum_{b \in \mathcal{B}^\Omega} \left(\sum_{j \neq i} D\hat{y}_b^j + D\bar{y}_b^j \right) Dv_b^i \leq c \left(r^{-2} + S_{\mathcal{D}}^{-1} \log(S_{\mathcal{D}}) \right) \|Dv^i\|_2.$$

Applying the global form of (5.26) to the second term in (5.34),

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

and finally,

$$\begin{aligned} \sum_{b \in \mathcal{B}^\Omega} h_b Dv_b^i &\leq r^{-1} \left(\left(\sum_{\substack{b \in \mathcal{B}^\Omega, (C,s) \in \mathcal{D} \\ \text{dist}(b, C^i) \leq r+1}} (1 + \text{dist}(b, C))^{-4} \right)^{1/2} + r S_{\mathcal{D}}^{-2} \right) \|Dv^i\|_2 \\ &\leq c \left(r^{-1} + S_{\mathcal{D}}^{-2} \right) \|Dv^i\|_2. \end{aligned}$$

Combining these estimates gives

$$\langle \delta E^\Omega(z) - \delta E(y^i), v^i \rangle \leq c \left(r^{-1} + S_{\mathcal{D}}^{-1} \log(S_{\mathcal{D}}) + r S_{\mathcal{D}}^{-1} \right) \|Dv^i\|_2. \quad (5.35)$$

The term T_3 : The final group may be once more estimated using the truncation result of Lemma 5.2.4, giving

$$|\langle \delta E(y^i) - \delta E(\hat{y}^i + u \circ G^i), v^i \rangle| \lesssim R^{-1} \|Dv^i\|_2. \quad (5.36)$$

Conclusion: Inserting the estimates (5.33), (5.35) and (5.36) into (5.32), and using the fact that $\|Dv^i\|_2 \lesssim \|Dv\|_2$, we obtain the bound

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

5.4.3 Stability of the predictor

Next we prove the stability of the predictor configuration defined in (5.24).

Lemma 5.4.4. *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 (5.24), and furthermore:*

1. $\text{index}(\partial W^\Omega) \leq I_0$,
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

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

Proof. Fixing I_0 and N , we choose R_0 and L_0 such that the conclusion of Lemma 5.3.2 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. $\text{index}(\partial W^{\Omega^n}) = I_0$,
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. $S^n := S_{\mathcal{D}^n} \rightarrow \infty$ as $n \rightarrow \infty$ 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 (5.23) 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 $v^n \in \mathcal{W}^{1,2}(\Omega^n)$ such that $\|Dv^n\|_2 = 1$ and

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

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 , $\text{dist}(C^{n,i}, C^{n,j})$ either remains bounded or tends to infinity, and so define an equivalence relation $i \sim j$ if and only if $\text{dist}(C^{n,i}, C^{n,j})$ is uniformly bounded as $n \rightarrow \infty$.

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 ,

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

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 Lemma 4.9 in [EOS13], there exists a sequence $r^n \rightarrow \infty$ which we may also assume satisfies

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

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

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

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

$$\begin{aligned} \langle \delta^2 E^{\Omega^n}(z^n) v^n, v^n \rangle &= \sum_{[i]} \left(2 \langle \delta^2 E^{\Omega^n}(z^n) w^{n,[i]}, w^{n,0} \rangle + \langle \delta^2 E^{\Omega^n}(z^n) w^{n,[i]}, w^{n,[i]} \rangle \right) \\ &\quad + \langle \delta^2 E^{\Omega^n}(z^n) w^{n,0}, w^{n,0} \rangle. \end{aligned}$$

The definition of r^n and (5.26) imply that $\|\nabla \bar{y}^n\|_{L^\infty(U^{\Omega^n})} \leq c_1/r^n$, where c_1 is independent of n , so in a similar fashion to the proof of Lemma 5.3.2, we obtain:

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

where c represents a constant independent of n . Furthermore, the arguments of the proof of Lemma 5.3.2 imply that

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

and so we deduce that

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

for n sufficiently large, providing the required contradiction. $\square$

5.4.4 Conclusion of the proof

To conclude the proof of conclusions (1) and (2) of Theorem 5.1.1, we may apply small modifications of the arguments used in §5.3.3, and hence we omit these.

To prove conclusion (3), recall the result of Lemma 5.2.1, which states that $y \equiv 0$ is a globally stable equilibrium in any lattice domain. When Ω is a convex lattice polygon, $\mathcal{W}(\Omega) \subset \dot{\mathcal{W}}^{1,2}(\Omega)$, so if $z + w$ is the local equilibrium for E^Ω constructed in (1), then $-z - w \in \dot{\mathcal{W}}^{1,2}(\Omega)$, and furthermore

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

5.5 Discussion

In this chapter, we have demonstrated that configurations containing arbitrary numbers of screw dislocations exist as locally stable states in the model described in Chapter 3, and along the way we obtained a relatively precise characterisation of these states in terms of the continuum linear elasticity problem. This lends credence to the commonly held intuition that linear elasticity provides a good approximate description for the positions of all atoms in a crystal containing dislocations except those very close to the dislocation cores.

We briefly mention some extensions of this result which may be possible with some additional technical work.

A first possible extension would be to drop the requirement that ψ should be even, as would be the case if the body was under a mild 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 below, it appears that the analysis would be very similar to that contained here.

Secondly, it is straightforward to generalise the analysis carried out in §5.4 to ‘half-plane’ lattices, since the linear elastic corrector $\bar{y}$ may be constructed by 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 §5.4.1 in such domains.

Finally, it remains unclear whether the bounds obtained in Lemma 5.4.3 on the residual of approximate solutions represent a sharp decay rate in terms of $S_{\mathcal{D}}$ — it would be of interest to further understand this issue, which appears to be closely related to finding an improved linear elasticity predictor which takes into account surface stresses.

Chapter 6

Conclusions

This thesis has presented results concerning static models of point defects and screw dislocations in crystalline solids. As we saw in Chapter 1, this is far from being a complete catalogue of the possible defects, and it is of great relevance to go beyond the results here in order to better understand defect behaviour at non-zero temperature. In this concluding chapter, we therefore present and comment upon some questions which would seem to suggest themselves for additional study.

6.1 Defects as an equilibrium configurations

Chapter 4 proved that a screw dislocation exists as a globally stable equilibrium using an energy difference formulation, and as part of Chapter 2, we studied $\tilde{E}_\infty$, which may also be seen as an energy difference. A natural extension of this work would therefore be to better understand which other defects are globally stable in this manner.

Open problem. *Classify which crystalline defects exist as globally stable states using an energy difference formulation.*

The analysis undertaken here is not the first example of this approach to studying defect problems (see for example [CE11] and [BBH94]), but taken together, these results suggest that the technique may be widely applicable. This should allow further study of similar variational problems in infinite domains with prescribed boundary conditions ‘at infinity’ arising from some macroscopic problem.

As part of the study of the problem posed above, potentially the most difficult but arguably also the most interesting analysis would be that of a faceted crystal surface. It is well understood that the surfaces of crystals undergo a process known as surface reconstruction, where the atoms on the edge of the solid may experience perturbations of several interatomic spacings in order to accommodate the forces coming from the

bulk of the crystal. These perturbations are observed to be periodic along the surface of the solid, and decay into the bulk [OZL⁺03]. Solving the following problem would likely lead to an interesting insight into the nature of this process.

Open problem. *Prove that there exist equilibria corresponding to a stable crystal surface which are periodic tangent to the surface, and decay to the perfect crystal into the bulk.*

Qualitative properties of minimisers of such variational problems do not yet seem to have been studied in the mathematical literature, although some relevant work on surface energy is contained in [The11].

6.2 Dislocation dynamics from microscopic models

There are currently a large number of phenomenological dislocation dynamics models available, but there is still significant work to be done to rigorously derive these models from dynamics at the microscopic level. Given the current interest amongst the Materials Engineering community in accurate simulation of dislocation dynamics (see for example [BC06]), we pose the following problem.

Open problem. *Derive equations governing dislocation dynamics proceeding from a thermodynamical treatment of the Hamiltonian dynamics at the microscopic level, and furthermore describe the physical regime in which such equations are valid.*

As was remarked in §1.2, some work aiming at a better understanding of defect dynamics has already begun, notably in [ADGP13], [FIM12] and [EHIM09]. In each of these cases, the starting point is a quasistatic evolution at the microscopic level, rather than the Hamiltonian dynamics. In view of the description of equilibria of the potential energy presented here in Chapter 5 and in [ADGP13], it seems that a theory of dislocation dynamics based on approximating transition probabilities between these equilibrium states of the system might be possible in the near future.

6.3 Defining the dislocation core radius

As explained in §1.2.2, in the most common mesoscale approach to modelling dislocations, the elastic strain field due to a dislocation is truncated at a short distance away from the dislocation line. This distance is the *core radius* of the dislocation in such models. This procedure ensures that the field is non-singular at the dislocation,

and furthermore that the elastic energy of the body is finite. The truncation of the field is compensated by a core energy, which is generally left as a constant that is assumed to depend upon the Burgers vector.

An unsatisfactory feature of this approach is that it provides no means by which to assign the value of the core radius or core energy, and hence there can be no definitive elastic energy in the continuum model without further input from a microscopic theory. Furthermore, as mentioned in §5.5, the dislocation core radius is often stated to be a cut-off beyond which continuum linear elasticity accounts for the elastic strain, elastic forces, and elastic energy with a similar level of error.

In the analysis carried out in [EOS13] and Lemma 5.2.3 however, it can be seen that the additional strain beyond that predicted by linear elasticity due to the ‘discreteness’ of the lattice decays like $\text{dist}(b, C)^{-2}$, and is not compactly supported. Although this decay is faster than the principal contribution for the field predicted by linear elasticity, it will nevertheless have an important effect as dislocations come close to one another. Additionally, differences in the core symmetry of different forms of dislocation induce different rates of decay, and hence the interactions between dislocations of different types at short range may be quite different to those obtained using simply the field derived from linear elasticity.

A further important observation is that the perturbation to the energy density induced by the corrector field described above should behave approximately like $\text{dist}(b, C)^{-4}$, since the strain energy should be approximately quadratic near the perfect lattice. This suggests that a good definition for the dislocation core radius is likely to vary depending upon the particular physical observables under consideration. With all of these considerations in mind, we therefore pose the following problem.

Open problem. *Find clear criteria for assigning the core radius and core energy based on microscopic considerations of dislocations, and produce a good quantification of the error caused by taking such an approximation.*

Many attempts have been made to assign core radii based upon computational models for various materials, for example [Cha67] and [BS02]. With recent mathematical results obtained here and elsewhere on simple discrete models of dislocations, it may be hoped that a careful error analysis could balance the modelling and computational errors that arise when attempting to find a good definition of the core radius and core energy of a dislocation. This should help to clarify the definition of these concepts in a way which might be made more generally useful for computation in the future.

Appendix A

Analysis of branchcuts: proofs

In this appendix, we detail the proofs of the various geometrical lemmas from §4.3.

A.1 Proof of Lemma 4.3.2

We will prove this lemma algorithmically. First, if $z_b = 0$ everywhere, then the result is trivial. Next, we note that β contains an even number of dislocation cores, and $\#\mathcal{C}^+[\beta] = \#\mathcal{C}^-[\beta] < +\infty$ since $u \in \mathcal{W}^{1,2}$. We therefore enumerate $C_i^+ \in \mathcal{C}^+[\beta]$.

Put $C_{1,0} = C_1^+$. Since C_1^+ is a positive dislocation core and z_b is integer-valued, it follows that at least one bond $b_1 \in \partial C_1^+$ satisfies $z_b > 0$. Let $C_{1,1}$ be the cell such that $-b_1 \in C_{1,1}$. There are now 2 possibilities: either $C_{1,1} \in \mathcal{C}^-[\beta]$, in which case we stop, or we can find another bond $b_2 \in \partial C_{1,1}$ such that $z_b > 0$. Iterating, we obtain a (possibly infinite) sequence of cells $C_{1,j}$ and bonds b_j .

We now claim that no two bonds $b_j = b_k$ with $j \neq k$ in this sequence, and consequently the sequence terminates; suppose the converse for contradiction. Let j and k be indices such that $j < k$ and $k - j$ is minimal over all pairs of indices such that $b_j = b_k$. Define a polygonal curve P passing through the barycentres of the cells $x^{C_{1,j}}, \dots, x^{C_{1,k}}$. P is a simple continuous closed curve, since the cells $C_{1,j}, \dots, C_{1,k-1}$ are distinct by definition, and $C_{1,j} = C_{1,k}$. Hence, P partitions $\mathbb{R}^2$ into a bounded set Ω (the interior of P) and an unbounded set, $\mathbb{R}^2 \setminus \Omega$. Define $\tilde{u} = u \mp \mathbb{1}_\Omega$, taking the sign according to whether P traverses $\partial\Omega$ in an anticlockwise or clockwise direction respectively.

It is now straightforward to check that $D\tilde{u} = Du$ except on the bonds b_i . For each of the bonds b_i ,

$$D\tilde{u}_{b_i} = Du_{b_i} - 1 = \beta_{b_i} + z_{b_i} - 1,$$

but since $z_{b_i} \geq 1$, this contradicts the **DMCP**, (4.14). It follows that the sequence b_i contains no two identical bonds, and as z_b has compact support, the sequence must terminate at a negative dislocation core.

Define $z_b^1 = \pm 1$ if $\pm b \in \{b_1, \dots, b_n\}$, and $z_b^1 = 0$ otherwise, and then consider iterating the procedure described above starting at C_i^+ , but using the criterion at each step that each bond in the sequence must satisfy

$$z_b - \sum_{m=1}^{i-1} z_b^m > 0.$$

This leads to a sequence 1-forms, z^i ; the resulting 1-form

$$z_b - \sum_{i=1}^N z_b^i$$

must be identically zero. If not, then the same technique as used above shows that either the **DMCP** is violated, or else $\text{supp}\{z\}$ is infinite, and hence $u \notin \mathcal{W}^{1,2}$.

To complete the proof of Lemma 4.3.2, we simply need to show that for 2 adjacent bonds in the support of any z^m , $\partial b_i \cap \partial b_{i+1}$ is a single 0-cell. This is clear, since by definition $b_i, -b_{i+1} \in \partial C_{m,i}$, $b_i \neq b_{i+1}$ and $|\partial C_{m,i}| = 3$. $\square$

A.2 Proof of Lemma 4.3.3

We now show that we can always choose z^m to be made up of 2 straight cuts. Recall that Corollary 4.3.1 states that $\|z^m\|_1 = \text{hop}_2(C_m^+, C_m^-)$.

Next, define the 2-cell hop operators H_i for $i = 1, \dots, 6$ which act on 2-cells by taking a cell C to the first cell ‘in the direction a_i ’, that is, the positively-oriented cell which satisfies $C' \neq C$,

$$x^C + \frac{\sqrt{3}}{2} a_i \in C'.$$

It is straightforward to check this is well-defined; see Figure A.1. We can represent paths in the dual lattice by words taken from the alphabet of operators $\{H_1, \dots, H_6\}$. In general however, the representation is non-unique – to see this, it is clear that for C_2 in Figure A.1, $H_2 C_2 = H_1 C_2$. As with the vectors a_i , we define

$$H_{i+6m} := H_i$$

for any $m \in \mathbb{Z}$.

We note the following properties of the operators H_i , which may be easily checked:

1. The orbit of the group of operators generated by $\{H_1^2, \dots, H_6^2\}$ acting on any cell C is a lattice.
2. The operators H_i^2 and H_j commute for any i and j .
3. For any cell C and any i , one of the following is true: $H_i C = H_{i+1} C$ or $H_i C = H_{i-1} C$.
4. If $H_i C = H_j C$, then $H_i H_k^{2m} C = H_j H_k^{2m} C$, and if $H_i C \neq H_j C$, then $H_i H_k^{2m} C \neq H_j H_k^{2m} C$.
5. $H_{i+3} H_i = H_{i+3} H_i$ is the identity map for any i .
6. $H_i C \neq H_{i\pm 2} C$ for any cell C and for any i .

Setting $N := \|z^m\|_1$, we claim that for any pair of cells $C_m^\pm$, it is possible to write shortest paths in the dual lattice as a word of the form

$$H_{i+1}^{N-k} H_i^k \tag{A.1}$$

for some i and some $k \in \{1, \dots, N\}$. By the definition of the hopping operators, it is clear that such words represent a sequence of cells lying on the lines $x^{C_m^-} + ta_i$ and $x^{C_m^+} - ta_{i+1}$.

We now prove the claim: first, we show that any shortest path must be able to be written as a word made up of only 2 of the operators H_i and H_{i+1} . Suppose this is false, for contradiction. (6) implies that we may assume that it contains a segment which may be written as

$$H_{i+2} H_i^m H_{i-2} \quad \text{or} \quad H_{i-2} H_i^m H_{i+2}$$

for some i and some $m \in \mathbb{N}$. Since both cases are similar, we consider only the first. If C is the first cell in this subsequence, $H_{i-2} C \neq H_{i-3} C$, or else $H_i H_{i-2} C = H_i H_{i-3} C = C$ by (5), and there exists a shorter path. (3) therefore implies

$$H_{i-2} C = H_{i-1} C. \tag{A.2}$$

Invoking property (3) again, either

$$H_i H_{i-2} C = H_i H_{i-1} C = H_{i-1}^2 C \quad \text{or} \quad H_i H_{i-2} C = H_{i+1} H_{i-2} C = C. \tag{A.3}$$

Once more, the second case results in a contradiction; hence repeatedly using (2),

$$H_{i+2} H_i^{2k+1} H_{i-2} C = H_i^{2k} H_{i+2} H_i H_{i-2} C = H_i^{2k} H_{i+2} H_{i-1}^2 C = H_i^{2k} H_{i-1} C,$$

implying a contradiction in the case where m is odd. In the case that m is even, repeatedly using (2), (A.2) and (5), we have

$$H_{i+2}H_i^{2k}H_{i-2}C = H_i^{2k}H_{i+2}H_{i-2}C = H_i^{2k}H_{i+2}H_{i-1}C = H_i^{2k}C,$$

obtaining another contradiction; it follows that it is possible that every shortest path can be written as a word containing no more than 2 of the operators H_i .

We next show that if the two operators are H_i and H_{i+2} for some i , we may rewrite the word in terms of H_i and H_{i-1} , or H_{i+1} and H_i . In (A.3), we showed that for any cell C contained in a shortest path $H_iH_{i-2}C = H_{i-1}^2C$. Suppose that a shortest path is represented as a product of H_{i-2} and H_i . Then each pair H_iH_{i-2} may be replaced by H_{i-1}^2 , and using (2) to permute each of these pairs to the right, we eventually obtain one of

$$H_i^m H_{i-1}^{2n} \quad \text{or} \quad H_{i-2}^m H_i H_{i-1}^{2n}.$$

In the first case, the proof is complete. In the second case, it must be that $H_i H_{i-1}^{2n} = H_{i-1}^{2n+1}$ or else $m = 0$, since otherwise (3) implies

$$H_{i-2}^m H_i H_{i-1}^{2n} = H_{i-2}^m H_{i+1} H_{i-1}^{2n} = H_{i-2}^{m-1} H_{i-1}^{2n},$$

which is a contradiction. Hence we have proved the claim, and in fact since we have obtained a shortest path in the form (A.1), the lemma is proven for this particular case.

Finally, we consider a general word made up of only the operators H_i and H_{i+1} . Now consider a word of the form $H_{i+1}H_i^mH_{i+1}$. If m is even, then we can generate a new word corresponding to a shortest path $H_{i+1}^2H_i^m$. If m is odd, then we can write a new shortest path as

$$H_{i+1}H_iH_{i+1}H_i^{m-1}.$$

But then using (3), this must be able to be written either as

$$H_{i+1}^3H_i^{m-1}, \quad \text{or} \quad H_{i+2}H_{i-1}H_{i+2}H_i^{m-1},$$

where the second case results in a contradiction. It is now possible to check that this implies the full conclusion, since by these arguments we can always transform a general word composed of H_i and H_{i+1} into one of the form (A.1). $\square$

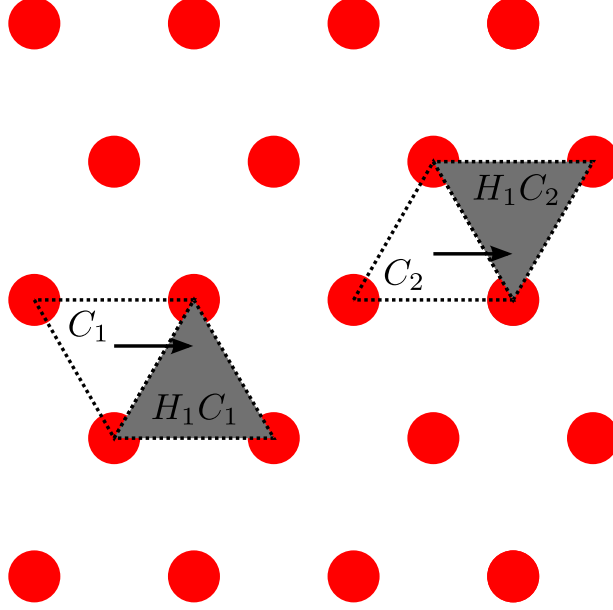


Figure A.1: This illustration shows the action of the operator H_{a_1} on two representative cells, C_1 and C_2 .

A.3 Proof of Lemma 4.3.8

To prove this lemma, we use Lemma 4.3.3 to assert that z should be made up of straight cuts. This will allow us to make estimates for each straight segment which depend upon on the orientation of each segment. We divide the lattice into ‘sextants’ by defining

$$\mathcal{S}^i := \{x \in \mathbb{R}^2 \mid \exists \lambda > 0, \mu \geq 0 \text{ such that } x = \lambda a_i + \mu a_{i+1}\}$$

and rings $\mathcal{R}^i$ by defining $\mathcal{R}^{-1} = \emptyset$, $\mathcal{R}^0 := C_0$, and then

$$\mathcal{R}^i = \text{clos} \bigcup \{C \in \mathcal{C} \setminus (\mathcal{R}^{i-1} \cup \mathcal{R}^{i-2}) \mid \text{clos}(C) \cap \text{clos}(\mathcal{R}^{i-1}) \neq \emptyset\}.$$

We will say a straight cut z is:

1. *tangential* if $\text{supp}\{z\} \subseteq \mathcal{S}^i$ and the cut direction is a_{i+2} , or equivalently $\text{supp}\{z\} \subseteq \mathcal{S}^i \cap \mathcal{R}^r$ for some r , and
2. *radial* if $\text{supp}\{z\} \subseteq \mathcal{S}^i$ and it has direction a_i or a_{i+1} .

It may be checked that for any straight cut, there exist $C^+, C^- \in \mathcal{C}$ such that

$$\int_{\partial C^\pm} z = \pm 1.$$

We separate the full result into 2 further lemmas, which give precise estimates for each of these classes of straight cuts, before combining them to complete the proof for the general case. By Taylor expanding $\psi'(\hat{\alpha}_b)$ around 0 we write

$$\sum_{b \in \mathcal{B}} \psi'(\hat{\alpha}_b) z_b = \sum_{b \in \mathcal{B}} \psi''(0) \hat{\alpha}_b z_b + \frac{1}{6} \psi^{(4)}(s_b) (\hat{\alpha}_b)^3 z_b. \quad (\text{A.4})$$

We proceed to estimate the first terms in the summand, by estimating on the radial and tangential straight segments of z^m separately.

Lemma A.3.1. *For a tangential cut z^{tan} with $\|z^{\text{tan}}\|_1 = \text{hop}_2(C^+, C^-) = l$ on ring $\mathcal{R}^r$, we have the following estimate:*

$$\sum_{b \in \mathcal{B}} z_b^{\text{tan}} \hat{\alpha}_b \geq -\frac{1}{2\pi} \arctan \left(\frac{2 \lfloor \min(l, 2r-l)/2 \rfloor + 1}{(r-2/3)\sqrt{3}} \right) - O(r^{-1}).$$

Proof. First, we appeal to symmetry. If $b = (\xi, \xi + a_j) \in \mathcal{S}_i$, then applying the reflection

$$R = \frac{1}{3} (a_i + a_{i+1}) \otimes (a_i + a_{i+1}) - a_{i+2} \otimes a_{i+2},$$

it is straightforward to check that if $b' = (R\xi, R\zeta)$, then

$$\hat{\alpha}_b = -\hat{\alpha}_{b'}.$$

This means that if a tangential cut crosses the line of symmetry $\{t(a_i + a_{i+1}) \mid t \in \mathbb{R}\}$, then some of the bond contributions cancel. It follows that we need only consider the case where all bonds in the support on z^{tan} lie on one side of this line of symmetry, since this is the worst case. For such cuts, it may be checked that $l \leq r$.

Identifying z^{tan} with a dual lattice path, we may enumerate $b_k \in \text{supp}\{z^{\text{tan}}\}$ ‘along the path’, and elementary geometry now shows that $\hat{\alpha}_{b_k}$ has alternating sign as k increases. Letting $\xi^r := \frac{1}{2}(r - \frac{2}{3})(a_i + a_{i+1})$ if i is odd, $\xi^r := \frac{1}{2}(r - \frac{1}{3})(a_i + a_{i+1})$ if i is even, it is straightforward to show that each bond b_k can be represented as one of

$$(\xi^r + sa_{i+2}, \xi^r + sa_{i+2} + a_i) \quad \text{or} \quad (\xi^r + sa_{i+2}, \xi^r + sa_{i+2} + a_{i+1})$$

where $s \in \{0, \frac{1}{2}, \dots, \frac{r-1}{2}\}$. Elementary trigonometry now allows us to calculate that

$$\begin{aligned} 2\pi \hat{\alpha}_b z_b^{\text{tan}} &= \pm \left[\arctan \left(\frac{s + 1/2}{|\xi^{r+1}|} \right) - \arctan \left(\frac{s}{|\xi^r|} \right) \right] \\ &\text{or } \pm \left[\arctan \left(\frac{s - 1/2}{|\xi^{r+1}|} \right) - \arctan \left(\frac{s}{|\xi^r|} \right) \right] \end{aligned}$$

respectively for the cases above. We therefore have that

$$2\pi \sum_b z_b^{\tan} \hat{\alpha}_b = \sum_{t=1}^{\lfloor l/2 \rfloor} \arctan\left(\frac{t+s_0+1/2}{|\xi^{r+1}|}\right) - 2 \arctan\left(\frac{t+s_0}{|\xi^r|}\right) + \arctan\left(\frac{t+s_0-1/2}{|\xi^{r+1}|}\right) + O(r^{-1}),$$

$$\text{or} = \sum_{t=1}^{\lfloor l/2 \rfloor} \arctan\left(\frac{t+s_0+1/2}{|\xi^r|}\right) - 2 \arctan\left(\frac{t+s_0}{|\xi^{r+1}|}\right) + \arctan\left(\frac{t+s_0-1/2}{|\xi^r|}\right) + O(r^{-1}),$$

where $s_0 \in \{0, \frac{1}{2}, \dots, \frac{r-1}{2}\}$, and the $O(r^{-1})$ term arises from the contribution of at most 2 bonds we have neglected, whose contribution we estimate using (4.5). In the second case, the fact that $-\arctan$ is convex for positive arguments implies that the sum is bounded below by 0. In the first case, for all t in the range of summation,

$$\frac{t+s_0+1/2}{|\xi^{r+1}|} \geq \frac{t+s_0}{|\xi^r|} \quad \text{and trivially} \quad \frac{t+s_0}{|\xi^{r+1}|} \leq \frac{t+s_0}{|\xi^r|}.$$

Since $\arctan$ is increasing, we obtain the lower bound

$$2\pi \sum_b z_b^{\tan} \hat{\alpha}_b \geq \sum_{t=1}^{\lfloor l/2 \rfloor} \left\{ \arctan\left(\frac{t+s_0-1/2}{|\xi^r|}\right) - \arctan\left(\frac{t+s_0}{|\xi^r|}\right) \right\} + O(r^{-1})$$

$$\geq -\arctan\left(\frac{\lfloor l/2 \rfloor + 1/2}{|\xi^r|}\right) + O(r^{-1}),$$

using the fact that $\arctan$ is positive and increasing for positive arguments. Finally, note that in the case where $l > r$, i.e. the tangential cut crosses the line of symmetry, and we obtain the same estimate but with $2r-l$ in place of l in the formula above, so using the definition of ξ^r gives the result. $\square$

Lemma A.3.2. *For a radial cut z^{rad} such that $\|z^{\text{rad}}\|_1 = \text{hop}_2(C^+, C^-) = l$, either $|x^{C^+}| < |x^{C^-}|$ and*

$$\sum_{b \in \mathcal{B}} z_b^{\text{rad}} \hat{\alpha}_b \geq 0,$$

or else $|x^{C^+}| > |x^{C^-}|$, and if $C^- \in \mathcal{R}^r$, then

$$\sum_{b \in \mathcal{B}} z_b^{\text{rad}} \hat{\alpha}_b \geq -\frac{1}{\pi} \text{arcsinh}\left(\frac{2\lfloor l/2 \rfloor}{\sqrt{3}(r-2/3)}\right) - O(r^{-1}).$$

Proof. First, we enumerate the bonds in $b_k \in \{b \in \mathcal{B} \mid z_b^{\text{rad}} > 0\}$, beginning with the bond for which d_b is smallest, and proceeding outwards along the cut. Elementary geometry shows that the terms $z_{b_k}^{\text{rad}} \hat{\alpha}_{b_k}$ are all positive in the case where b_1 is in one of the directions a_{i+1} , a_{i+2} or a_{i+3} , which corresponds to having $|x^{C^+}| < |x^{C^-}|$; this immediately provides the first bound.

In the second case (4.5) implies

$$\hat{\alpha}_{b_k} \geq -\frac{1}{2\pi d_{b_k}}.$$

Without loss of generality, we assume the cut direction is a_i , the case with direction a_{i+1} being similar. There are now two cases: b_1 is either in the direction a_{i-1} , or a_{i-2} . Further elementary geometry allows us to conclude that in the first case, $d_{b_1} = |x|$ for some $x \in \mathcal{S}^i$, and in the second, $d_{b_1} > |x|$ with $x = x^{C^-} \in \text{clos}(\mathcal{S}^i)$. In either case, d_{b_2} satisfies the same lower bound as d_{b_1} , and further, we have that

$$d_{b_{2n-1}}, d_{b_{2n}} \geq |x + na_i|.$$

Noting that as $x \in \text{clos}(\mathcal{S}^i)$, it follows that $a_i \cdot x \geq 0$ and

$$\frac{1}{|x + ta_i|} = \frac{1}{\sqrt{|x|^2 + 2t a_i \cdot x + t^2}} \leq \frac{1}{\sqrt{|x|^2 + t^2}},$$

which is a decreasing function of t , so we estimate

$$\sum_{k=1}^l \hat{\alpha}_{b_k} \geq -\frac{1}{\pi} \sum_{i=0}^{\lfloor l/2 \rfloor} \frac{1}{|x + na_i|} \geq -\frac{1}{\pi} \left(\frac{1}{|x|} + \int_0^{\lfloor l/2 \rfloor} \frac{1}{\sqrt{|x|^2 + s^2}} ds \right).$$

Evaluating the integral, and noting further that $|x| \geq \frac{\sqrt{3}}{2}(r - 2/3)$, we obtain the conclusion. $\square$

We now combine the estimates of Lemma A.3.1 and Lemma A.3.2 to obtain an estimate for a general cut z^m made up of two straight segments. As we showed in Lemma 4.3.3, each z^m is made up of at most 2 straight segments. It may be checked that each of these segments is either purely radial, purely tangential, or changes from tangential to radial part way along its length, with one bond which crosses $\partial\mathcal{S}^i$. All possible cuts satisfying the **DMCP** and made up of 2 straight segments can therefore be decomposed as either

1. a tangential cut and 2 radial cuts or
2. a tangential cut, a radial cut and tangential cut,

where any of these segments could possibly have length 0, and neglecting the extra bonds mentioned above for now. Recall the result of Corollary 4.3.2 which states that

$$\text{hop}_2(C_0, C_m^-) \geq \text{hop}_2(C_0, C_m^+).$$

Consider the first case, letting the two radial segments be of length l_1 and l_2 respectively, and the tangential segment of length $l - l_1 - l_2$. If $|x^{C_m^+}| < |x^{C_m^-}|$ and the radial cuts are of non-zero length, then the radial segments have the trivial lower bound, by Lemma A.3.2. In the worst case, where $l - l_1 - l_2 = r$, we have the bound

$$\sum_{b \in \mathcal{B}} z_b^m \hat{\alpha}_b \geq -\frac{1}{2\pi} \arctan\left(\frac{r+1}{(r-2/3)\sqrt{3}}\right) - O(r^{-1}) = -\frac{1}{12} - O(r^{-1}).$$

Otherwise, $|x^{C_m^+}| > |x^{C_m^-}|$, so applying Corollary 4.3.2, we have that for $C' \in \mathcal{R}^r$,

$$2r \geq \text{hop}_2(C_0, C') \geq \text{hop}_2(C_m^+, C') = l_1 + l_2. \quad (\text{A.5})$$

Therefore, applying Lemma A.3.1 and Lemma A.3.2,

$$\begin{aligned} \sum_{b \in \mathcal{B}} z_b \hat{\alpha}_b \geq & -\frac{1}{2\pi} \left(\arctan\left(\frac{2\lfloor(l-l_1-l_2)/2\rfloor+1}{(r-2/3)\sqrt{3}}\right) + 2 \operatorname{arcsinh}\left(\frac{2\lceil l_1/2 \rceil}{\sqrt{3}(r-2/3)}\right) \right. \\ & \left. + 2 \operatorname{arcsinh}\left(\frac{2\lceil l_2/2 \rceil}{\sqrt{3}(r+\lfloor l_1/2 \rfloor-2/3)}\right) + O(r^{-1}) \right). \end{aligned}$$

By ignoring the floor functions, it is possible to check that under the bound (A.5), the function in parentheses is increasing in both l_1 and l_2 if r is suitably large; we therefore have that the maximum must occur when $l = l_1 + l_2$. Hence putting $l_2 = l - l_1$, we have

$$\sum_{b \in \mathcal{B}} z_b \hat{\alpha}_b \geq -\frac{1}{\pi} \left(\operatorname{arcsinh}\left(\frac{2\lceil l_1/2 \rceil}{\sqrt{3}(r-2/3)}\right) + \operatorname{arcsinh}\left(\frac{2\lceil(l-l_1)/2\rceil}{\sqrt{3}(r+\lfloor l_1/2 \rfloor-2/3)}\right) + O(r^{-1}) \right).$$

Dropping the floor and ceiling functions, this estimate is convex in l_1 . The worst cases are therefore $l_1 = 0$ or $l_1 = l$ and $2\lceil l/2 \rceil = 2r + 1$, giving the value

$$\sum_{b \in \mathcal{B}} z_b \hat{\alpha}_b \geq -\frac{1}{\pi} \operatorname{arcsinh}\left(\frac{2r+1}{\sqrt{3}(r-2/3)}\right) + O(r^{-1}) = -\frac{\operatorname{arcsinh}(2/\sqrt{3})}{\pi} + O(r^{-1}).$$

In the case where we have tangential, radial and tangential segments, similar arguments show that, once more, the worst possible bound arises in the case where the cut is purely radial, giving the same lower bound.

We now return to the lower order terms in (A.4). Then by crudely estimating

$$\left| \sum_{b \in \mathcal{B}} \frac{1}{6} \psi^{(4)}(s_b) (\hat{\alpha}_b)^3 z_b^m \right| \lesssim \sum_{d_b \geq r} d_b^{-3} \lesssim \frac{1}{r}$$

and noting that the worst bounds occur when $\text{hop}_2(C_0, C_m^-) \simeq r$, we have

$$\sum_{b \in \mathcal{B}} z_b^m \psi'(\hat{\alpha}_b) \geq -\psi''(0) \frac{\operatorname{arcsinh}(2/\sqrt{3})}{\pi} - c_0 \text{hop}_2(C_0, C_m^-)^{-1}.$$

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