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Atomistic models for crystal defects

by

Maciej Buze

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Declarations

I, Maciej Buze, to the best of my knowledge have presented only my original work and the outcomes of my collaboration with Prof. Christoph Ortner, unless specifically referenced or cited in the bibliography. It has not been submitted for another degree or qualification at the University of Warwick or any other higher-education institution.
Abstract

This thesis aims to present the theory behind a class of atomistic models for crystal defects. In particular, we provide a detailed account of the theoretical treatment of a model for the anti-plane screw dislocation and extend it to a similar model for the anti-plane shear mode of crack, which constitutes the novelty of this work. We prove that such a model is well-defined and, using the tools from bifurcation analysis, establish existence of a solution for small enough parameter $\epsilon$, which represents the pull on the crack.
Chapter 1

Introduction

1.1 Motivation

In many solid materials, atoms form a crystalline arrangement, which is prone to a variety of defects: point defects such as vacancies, line defects such as dislocations and other defects such as cracks. In order to get more insight into material behaviour, one would like to model such occurrences mathematically. Since it is argued in physics that any such a defective configuration of atoms corresponds to a local minimum of the energy of the system (cf. [24]), one can formulate a suitable energy minimisation problem as a mathematical model of a defect.

The usual continuum models can prove prohibitively inaccurate in the region very close to the core of a defect, thus, with the rise of high-power computing resources capable of tackling many particle simulations, atomistic and multiscale models have been proposed as an appealing alternative [5].

In particular, in recent years discrete lattice models for defects such as point defects as well as straight line dislocations have been developed (cf. [6],[11]), which serve as a starting point to our analysis.

1.2 Outline

The general aim of this report is to provide a detailed discussion about the aforementioned models and to extend the atomistic modelling for crystal defects to the case of a crack (see Figure 1.2).

The starting point is to look at lattice domains and how they can be used to describe defects in crystalline structures. The next step is to see how the variational approach for PDEs can be translated to a discrete setting, so that we can phrase
the modelling as a minimisation problem for a suitable energy functional.

We then proceed to give a detailed account of the theory of screw dislocations (see Figure 1.1), where we can no longer work with a simple energy functional and instead the crucial concepts of energy difference and decomposition of displacement into a far-field predictor and a core corrector are being introduced. The analysis also includes the decay estimates for the corrector.

![Figure 1.1: A lattice before and after applying a screw-dislocation.](image)

The ultimate aim is to apply the same machinery to the case of a crack, carefully looking at how the differences between these settings affect the results. In particular, since the crucial construction of the predictor takes into account the delicacies of the underlying geometry in a deformed lattice, we make several readjustments to ensure that a crack configuration can be treated with this method. As it will turn out, in the crack case an instance of a bifurcation analysis arises, as we have a non-negative scalar parameter $\epsilon$, which represents the strength of the pull of atomic planes. Thus we also provide a brief introduction to the bifurcation theory.

![Figure 1.2: An example of a crack defect with atomistic modelling (red dots) near the core.](image)
in Banach spaces and then make some initial steps at applying it to the crack model. This part of analysis is far from complete and will remain a focal point of further work in the PhD study of the author.

Another aspect open to further study is the translation of the decay estimates results from the screw dislocation to the case of crack.

1.3 Notation

Throughout the report we use notational conventions:

- by $f \lesssim g$ we mean that there exists a constant $C > 0$ independent of $f$ and $g$, such that $f \leq Cg$;

- by $\nabla_\rho$ we mean $\nabla u \cdot \rho$;

- by $|\nabla^j f(x)|$ we mean
  - $j = 1$: the modulus of the gradient,
  - $j = 2$: a norm of the Hessian matrix,
  - $j = 3$: a norm of the third-order tensor,
  - etc.
Chapter 2

Background

In this chapter we provide a brief description of the mathematical setting of the investigation. We first introduce the concept of the Bravais lattice, which serves the purpose of the domain for the analysis.

In the second part we describe the process of ‘going from continuum to discrete’, which allows to translate the standard variational approach for PDEs to a discrete setting.

In the final section we introduce the theory of bifurcations for Banach spaces, which is applicable to the crack model and will be investigated in Section 4.3.

2.1 Lattices and crystal defects

The basis of the analysis is the domain of an infinite lattice, where each site is identified with an atom. Primarily, we work with a particular instance of the Bravais lattice, which is defined as follows in [3].

**Definition 2.1.1.** A Bravais lattice is a set $\Lambda = AZ^d$, where $d = 1, 2$ or $3$ and $A \in \mathbb{R}^{d \times d}$ is a non-singular matrix.

In this work we solely focus on the case when $d = 2$ and $A = A_{\text{tri}}$, where

$$A_{\text{tri}} := \begin{pmatrix} 1 & \cos(\pi/3) \\ 0 & \sin(\pi/3) \end{pmatrix} = \begin{pmatrix} 1 & 1/2 \\ 0 & \sqrt{3}/2 \end{pmatrix}.$$ 

It results in a homogeneous triangular lattice, which we refer to as $\Lambda_{\text{hom}}$ (see Figure 2.1). In this configuration each site has six nearest-neighbour directions:

$$a_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad a_2 = \begin{pmatrix} 1/2 \\ \sqrt{3}/2 \end{pmatrix}, \quad a_3 = -\begin{pmatrix} 1/2 \\ \sqrt{3}/2 \end{pmatrix}, \quad a_4 = -a_1, \quad a_5 = -a_2, \quad a_6 = -a_3.$$ 

(2.1)
Figure 2.1: A homogeneous triangular lattice $\Lambda^{\text{hom}}$ in two dimensions with a set of bonds $B$.

It is often convenient to work with bonds between lattice sites, thus we use the nearest-neighbour directions from (2.1) to define the set of bonds between sites

$$B := \{(l, l + a_i) \mid l \in \Lambda^{\text{hom}}, i = 1, 2, 3\}. \quad (2.2)$$

Restricting $i$ up to 3 allows us to avoid double-counting. Both $\Lambda^{\text{hom}}$ and $B$ can be modified to account for certain defects, in particular a crack.

The above can be viewed as a two dimensional toy model of real-life crystalline configurations in three dimensions (e.g. face-centered cubic or body-centered cubic, see [3] for more on that), but also as a projection of these arrangements along particular directions. In this way any lattice function $f : \Lambda^{\text{hom}} \to \mathbb{R}$, can be viewed as a displacement in that direction, thus allowing us to recover the 3D configuration via a graph-like representation $(l, f(l)) \in \mathbb{R}^3$. A more rigorous discussion of this concept will be introduced later.

In reality, the abstract perfect crystalline arrangement is broken by a number of possible defects and it is their introduction and how it affects the structure that we would like to model. In this work we focus on two types of defects: screw dislocations and cracks. The analysis of the first has been subject to intense study (cf. [3]), results of which we recall in order to introduce the machinery. We then use it to treat the case of a crack, which constitutes the novelty of this work.

In the following subsections we briefly introduce each defect being considered, with a particular focus on the domain, which we choose to work with in each instance.

### 2.1.1 (Screw) dislocation

We begin with a defect known as a dislocation. Different types of dislocations can prove somewhat hard to visualise and the most intuitive way to understand
them is to construct them following the so-called Volterra construction. We take a homogeneous lattice, make a half-plane cut through and move the resulting two parts of the lattice in opposite directions relative to each other by one atomic spacing. We consider an edge dislocation if the direction of the slip (known as the Burgers vector) is orthogonal to the dislocation line (end line of the half-plane inserted) and a screw dislocation if the Burgers vector is parallel to the dislocation line. See Figure 2.2.

Due to its similarities in structure with the crack defect we focus on the screw dislocation. Its name comes from the fact that if we jump in a loop between atoms around the dislocation line, we go up one atomic plane with each loop - a movement similar to following the threads of a screw. Crucial to the analysis is the fact that a screw dislocation, which is a three dimensional deformation, can be considered using a two dimensional lattice, as described at the beginning of this section (under a reasonable assumption of $e_3$-periodicity). Thus when we work with a screw dislocation, our domain is simply the two dimensional triangular domain $\Lambda^{\text{hom}}$. Furthermore, since after applying the slip the atomic planes on opposite sides of the cut match perfectly, working with the set of bonds $B$ defined in (2.2) also makes sense.

### 2.1.2 Crack defect

In this subsection we briefly discuss the setting for a crack defect. As is known from Fracture Mechanics (see e.g. [8]), there are three main types of cracks: the opening mode, the sliding mode and the one of interest to us, the tearing mode, also-called 'out-of-plane shear' (see Figure 2.3). Being an 'anti-plane' defect in nature, we can immediately resort to the same argument as in Section 2.1.1 to justify the use of a
two dimensional lattice domain. The thing that differs is how lattice sites interact with one another, which results in a change in the set of bonds under consideration. To be precise, we define

$$B^{cr} := B \setminus B^{cr\text{def}}, \text{ where } B^{cr\text{def}} = \bigcup_{i=0}^{\infty} \left\{ (ia_4, ia_4 + a_2) \right\} \cup \left\{ (ia_4, ia_4 + a_3) \right\}. \quad (2.3)$$

To visualise this definition, see Figure 2.4.

Figure 2.4: A reference lattice and bonds for a crack. Note the absence of bonds between atoms on the opposite sides of the crack. We denote such a set of bonds by $B^{cr}$.

### 2.2 Going from continuum to discrete

With the domain under consideration discrete, we need to develop further machinery to accommodate the transition from the continuum setting, where the models for defects can be cast as standard variational problems related to PDEs on infinite domains. Let us thus briefly recall the most basic example and then see how each part can be translated into a discrete setting.
2.2.1 Linear PDE

We consider

$$
\min_{u \in X} \int_{\mathbb{R}^d} \frac{1}{2} |\nabla u|^2 - f u \, dx,
$$

(2.4)

where a suitable function space $X$ is the homogeneous Sobolev space

$$
X = H^1(\mathbb{R}^d) := \{ u \in H^1_{\text{loc}}(\mathbb{R}^d) \mid \nabla u \in L^2(\mathbb{R}^d) \}
$$

and a given function $f$ with properties appropriate to represent a defect in a homogeneous medium, namely $f \in C^\infty(\mathbb{R}^d)$, $\text{supp} f \subset B$ (some finite ball) and $\int f = 0$. This minimisation problem is equivalent to the PDE

$$
-\Delta u = f \quad \text{on } \mathbb{R}^d,
$$

(2.5)

which in turn has the weak formulation of the form

$$
\int_{\mathbb{R}^d} \nabla u \cdot \nabla v = \int_{\mathbb{R}^d} f v \quad \text{for all } v \in C^\infty_c(\mathbb{R}^d)
$$

(2.6)

Without going into too much detail, we also note that a solution to (2.5) can be constructed via the Green’s function approach (see [15] for a broad treatment of this topic), i.e.

$$
u = G * f \quad \text{where } G(x) = \begin{cases} 
C|x|^{2-d}, & d \geq 3, \\
C \log |x|, & d = 2.
\end{cases}
$$

Further analysis reveals that

$$
|\nabla^j u(x)| \lesssim |x|^{1-d-j} \quad \text{for } j \geq 1.
$$

(2.7)

2.2.2 Linear lattice problem

Let us now formulate a similar problem in a discrete setting. For the ease of exposition we let $d = 2$ and replace $\mathbb{R}^d$ with the triangular lattice $\Lambda_{\text{hom}}$ introduced in the previous section. The second step is to replace derivatives with finite differences with nearest neighbours, using the notation $D_{\rho} u(l) = u(l + \rho) - u(l)$.

Recalling (2.1), we can already see that the analogue of the minimisation problem (2.4) is thus to find $u_* \in \mathcal{X}$ (some discrete function space to be specified below) such that

$$
E(u_*) = \min_{u \in \mathcal{X}} E(u)
$$

(2.8)
with
\[
E(u) := \sum_{l \in \Lambda^{\text{hom}}} \sum_{i=1}^{3} \frac{1}{2} |D_{a_i}u(l)|^2 - \langle f, u \rangle_{\Lambda^{\text{hom}}},
\] (2.8)

where summing over three consecutive directions (which we can refer to as forward stencils) allows us to avoid double-counting of bonds.

Here \( \langle f, u \rangle_{\Lambda^{\text{hom}}} = \sum_{l \in \Lambda^{\text{hom}}} f(l)u(l) \) and to mimic the continuum setting, we require \( f : \Lambda^{\text{hom}} \to \mathbb{R} \) with \( \text{supp} f \) compact and \( \sum_{l \in \Lambda^{\text{hom}}} f(l) = 0 \). Note that, equivalently, we can cast \( E \) in the form
\[
E(u) = \sum_{b \in B} \frac{1}{2} |Du_b|^2 - \langle f, u \rangle_{\Lambda^{\text{hom}}},
\] (2.9)

where \( B \) as in (2.2) and
\[
Du_b = D_{a_i}u(l) \text{ whenever } b = (l, l + a_i).
\]

This is a convenient formulation, as it is natural to use \( B \) to compute finite differences in the functional and \( Du_b \) represents the strain applied to the bond \( b \). We can thus think of \( Du \) as a function from \( B \) to \( \mathbb{R} \).

The next step is to find an appropriate discrete function space \( X \) so that the problem is well-defined. Using the bond notation, we choose
\[
X = \mathcal{H}^1 := \{ u : \Lambda^{\text{hom}} \to \mathbb{R} \mid Du \in \ell^2(B) \},
\] (2.10)

where \( \Lambda^{\text{hom}} \) denotes the lattice and \( B \) denotes the (potentially defective) set of bonds under consideration. This way we ensure that \( E(u) \) remains finite for all \( u \in X \). It will always be clear from the context which set of bonds is used to define \( \mathcal{H}^1 \). Note that this is an example of a discrete homogeneous Sobolev space.

**Remark 2.2.1.** \( \|D \cdot\|_{\ell^2(B)} \) defines only a semi-norm on \( \mathcal{H}^1 \), as for any constant function \( u_c \) we have \( \|D(u_c)\|_{\ell^2(B)} = 0 \). On the other hand, \( E \) is translation-invariant, since for any constant \( c \), \( E(u+c) = E(u) \) (here in particular due to summation requirement on \( f \)), thus we can simply fix the constant shift in an arbitrary way to regain the Hilbert space structure.

Following the usual variational approach, we see that any solution to (2.8) satisfies the Euler–Lagrange equation
\[
\sum_{b \in B} Du_b Dv_b = \langle f, v \rangle_{\Lambda^{\text{hom}}} \text{ for all } v \in X,
\] (2.11)
where $\langle f, v \rangle_{\Lambda^{\text{hom}}} := \sum_{l \in \Lambda^{\text{hom}}} f(l)v(l)$. This in turn points us to a lattice analogue of (2.5), which is

$$Hu = f \quad \text{where} \quad (Hu)(l) := \sum_{i=1}^{3} D_{-a_i} D_{a_i} u(l). \quad (2.12)$$

To go from (2.12) to (2.11), we begin with $\langle Hu, v \rangle_{\Lambda^{\text{hom}}}$ and ‘sum by parts’, which, since we are on an infinite discrete domain, consists in a relabelling of terms in the sum.

As in the continuous problem, a solution to the lattice problem (2.8) can be constructed via the Green’s function approach. In particular it uses the so-called semi-discrete Fourier transform (see [22] Chapter 2) and we quote a technical result from [3], which ensures the validity of this approach and will prove immensely useful in the treatment of decay estimates in Section 3.3.

**Theorem 2.2.1.** There exists (Green’s function) $G : \Lambda^{\text{hom}} \rightarrow \mathbb{R}$ such that for all $f : \Lambda^{\text{hom}} \rightarrow \mathbb{R}$ with compact support,

$$H(G * f) = f$$

with decay estimates

$$|D_{\rho} G(l)| \lesssim |l|^{-j}, \quad \text{for} \quad \rho \in \{a_1, \ldots, a_6\}^j, \quad j \geq 0,$$

where $D_{\rho} := D_{\rho_1} \ldots D_{\rho_j}$.

The discrete version of the decay estimate (2.7) can be stated as a simple Corollary of the Theorem 2.2.1.

**Corollary 2.2.2.** If $\bar{u} = G * f$, where the right-hand side as in Theorem 2.2.1, then

$$|D_{\rho} \bar{u}(l)| \lesssim |l|^{-1-j}, \quad \text{for} \quad \rho \in \{a_1, \ldots, a_6\}^j, \quad j \geq 1.$$  

This concludes the procedure of obtaining a discrete analogue of a linear PDE problem. While helpful as a toy problem to understand concepts, the linear nature of interaction between lattice sites is not enough to model real-life material behaviour. In fact, the vast majority of work in atomistic modelling employs non-linear interaction laws, which we will now introduce to the analysis, with the first concrete example being the treatment of the screw dislocation in Chapter 3.
2.2.3 Nonlinear interactions

Any realistic lattice model of material behaviour involves a nonlinear interaction law, introduced via a function \( \phi : \mathbb{R} \to \mathbb{R} \) with small variations in its defining properties. The common ground is that we require \( \phi \in C^k(\mathbb{R}) \), where usually \( k = 5 \) and \( \phi(0) = \phi'(0) = 0 \) and \( \phi''(0) = 1 \). Sometimes we may also require \( \phi'''(0) = 0 \). For the ease of presentation we also assume that \( \|\phi^{(j)}\|_{L^\infty(\mathbb{R})} < \infty \) for \( 0 \leq j \leq k \).

Remark 2.2.2. Depending on the exact setting, some of these restrictions may be imposed without loss of generality and/or may be a natural consequence of symmetry involved. We will discuss this issue on a case-by-case basis.

Thus, at least in the simplest cases, using the notation introduced in Section 2.2.2, we work with the energy functional of the form

\[
E(u) = \sum_{b \in \mathcal{B}} \phi(Du_b),
\]

where we can vary the lattice \( \Lambda_{\text{hom}} \) and/or the set of bonds \( \mathcal{B} \).

Interestingly, however, unlike in the simplest case of a linear lattice problem described in Section 2.2.2, it can be shown (see [3]) that for both a screw dislocation and a crack, it is not feasible to consider the energy functional as in (2.13) as then any configuration involving a screw dislocation (and similarly a crack) will have an infinite energy. To accommodate this issue, we thus formulate a minimisation problem for the energy difference functional, which is of the form

\[
E(u) = \sum_{b \in \mathcal{B}} \left( \phi(D\hat{u}_b + Du_b) - \phi(D\hat{u}_b) \right),
\]

where, crucially, the predictor \( \hat{u} \) is a-priori chosen to impose a defective structure (be it a screw dislocation or a crack) in such a way that \( E \) is well-defined for all \( u \in \hat{H}^1 \).

2.2.4 Estimating infinite sums

Central to the analysis is the ability to estimate infinite sums. To do this, we often use arguments that interchange the bond and site formulations and also use integral arguments similar to the integral test for convergence of series. In this section we illustrate how to do it.

For a bond \( b = (l, l + a_i) \) we define

\[
r_b := \min\{|l|, |l + a_i|\}.
\]
Suppose we have a function \( f : \mathcal{B} \rightarrow \mathbb{R} \) (where, say, \( \mathcal{B} \) corresponds to the lattice \( \Lambda_{\text{hom}} \)) such that for \( r_b > r_* \) (where \( r_* > 0 \)) we have

\[
|f_b| \leq C_1 r_b^{-k} \quad \text{for some } k > 1.
\]

Since \( r_b \leq |l| \) and each site \( l \) can be identified with up to three bonds via equality of the form \( r_b = |l| \), we have

\[
\|f\|_{\ell^2(\mathcal{B})}^2 \leq C_2 + 3C_1 \sum_{l \in \Lambda_{\text{hom}} \setminus B_{r_*}(0)} |l|^{-2k},
\]

where \( C_2 \) corresponds to the finite sum over bonds satisfying \( r_b \leq r_* \). This shows how we can go from bond sums to site sums.

Furthermore,

\[
\sum_{l \in \Lambda_{\text{hom}} \setminus B_{r_*}(0)} |l|^{-2k}
\]

can be estimated by an integral with the integrand being a piecewise constant function \( f_C : \mathbb{R}^2 \setminus B_{r_*}(0) \rightarrow \mathbb{R} \), where on each triangle \( T \) uniquely defined by the set of vertices \( \{l, m, n\} \subseteq \Lambda_{\text{hom}} \),

\[
f_C \big|_T = (\max\{|l|, |m|, |n|\})^{-2k}.
\]

Noting that in this way each site will correspond to at most three triangles and that \( |\cdot|^{-2k} \) is a nonnegative monotone decreasing function, we conclude that

\[
\sum_{l \in \Lambda_{\text{hom}} \setminus B_{r_*}(0)} |l|^{-2k} \leq C_3 \int_{r_*}^{\infty} f_C r^2 dr \lesssim \int_{r_*}^{\infty} r^{1-2k} dr,
\]

where we changed to polar coordinates for convenience. As a result, using a standard calculus fact about convergence of improper integrals and also noting that we can reverse the argument to establish divergence for \( k \) not big enough, we have the following lemma.

**Lemma 2.2.3.** A function \( f : \mathcal{B} \rightarrow \mathbb{R} \) belongs to \( \ell^2(\mathcal{B}) \) if and only if there exists \( r_* > 0 \) such that for all \( r_b > r_* \), \( |f_b| \leq C_1 r_b^{-k} \), where \( k > 1 \).

Finally, we also note that we sometimes use notation of the form \( D u(l) := (D_a u(l))_{a=1}^6 \), as then \( |D u(l)|^2 = \sum_{a=1}^6 (D_a u(l))^2 \), which means we double-count the bonds, which is negligible when trying to show finiteness of a given infinite sum. As
a result, we also use
\[ \|Du\|_{\ell_2(\Lambda^{\text{hom}})} := \left( \sum_{l \in \Lambda^{\text{hom}}} |Du(l)|^2 \right)^{1/2} \quad \text{and} \quad \|Du\|_{\ell_{\infty}(\Lambda^{\text{hom}})} := \sup_{l \in \Lambda^{\text{hom}}} |Du(l)|. \]

(2.17)

### 2.3 Bifurcation theory in Banach spaces

This section follows the treatment of bifurcation theory for Banach spaces described in [4].

The analysis starts with a nonlinear problem of the form
\[ F(v, \epsilon) = 0, \]

(2.18)

where \( F: V \times \mathbb{R} \to V \), for some Banach space \( V \) with norm \( \| \cdot \| \). Here \( \epsilon \) represents a scalar parameter and \( F \) is a \( C^p \) mapping for \( p \geq 3 \). For convenience, for \( j = 0, 1, \ldots \), we denote the Fréchet derivative of \( F \) at \((u_j, \epsilon_j) \in V \times \mathbb{R} \) with respect to \( v \) (respectively \( \epsilon \)) by \( F^j_v \) (resp. \( F^j_\epsilon \)). We also write \( F^j \) for \( F(v_j, \epsilon_j) \). Note that for an \( \epsilon_j \) fixed, \( F^j_v \) is a map from \( V \) to \( V \) and for a \( v_j \) fixed, \( F^j_\epsilon \) is map from \( \mathbb{R} \) to \( V \), however it is possible to identify \( F^j_\epsilon \) with an element of \( v^* \in V \) via the fact that due to continuity, \( F^j_\epsilon \lambda = \lambda v^*_s \) for all \( \lambda \in \mathbb{R} \). Thus we refer to \( F^j_\epsilon \) as an element of \( V \).

Of central interest in this analysis is to describe the following set
\[ S := \{(v, \epsilon) \in V \times \mathbb{R} \mid F(v, \epsilon) = 0\}. \]

(2.19)

It is often possible to identify a trivial member of \( S \), say \((v_0, \epsilon_0)\) and the following theorem, known as the Implicit Function theorem, proves useful (taken from [16]).

**Theorem 2.3.1 (Implicit Function Theorem).** Let \( X, Y, Z \) be Banach spaces. Let the mapping \( F: X \times Y \to Z \) be continuously Fréchet differentiable with respect to both \( x \) and \( y \). If \((x_0, y_0) \in X \times Y, f(x_0, y_0) = 0 \) and the mapping \( y \mapsto Df(x_0, y_0)(0, y) \) is a Banach space isomorphism from \( Y \) onto \( Z \), then there exist neighbourhoods \( U \) of \( x_0 \) and \( V \) of \( y_0 \) and a Fréchet differentiable function \( g: U \to V \) such that \( f(x, g(x)) = 0 \) and \( f(x, y) = 0 \) if and only if \( y = g(x) \), for all \((x, y) \in U \times V \).

Thus, if we can show that \( F^j_v \) is an isomorphism on \( V \) then Theorem 2.3.1 ensures that there exists a unique smooth path of solutions \( v(\epsilon) \in C^p \) satisfying \( F(v(\epsilon), \epsilon) = 0 \) for \( \epsilon \in [\epsilon_0 - \xi, \epsilon_0 + \xi] \) for some \( \xi > 0 \). We let \( \epsilon_1 = \epsilon_0 + \xi \) with corresponding unique \( v_1 \in V \) and consider what happens at \((v_1, \epsilon_1)\), which is known
as the bifurcation point. There $F^1_v$ ceases to be an isomorphism and several things could happen. In this work we solely focus on the simplest possible case that the bifurcation point is a simple fold (or turning) point. It can be described as follows.

A simple fold point occurs if at $(v_1, \epsilon_1)$, we have $F(v_1, \epsilon_1) = 0$ and $F^1_v$, a bounded linear operator from $V$ to $V$, is singular with algebraically simple zero eigenvalue, which means that there is a single corresponding eigenfunction $\gamma_0 \in V$ ($\gamma_0 \neq 0$) such that $F^1_v \gamma_0 = 0$. We define

$$\text{Ker}(F^1_v) = \text{span}\{\gamma_0\}$$

and let us denote by $\psi_0$ the corresponding basis element of $V^*$, which means that

$$\langle \psi_0, \gamma_0 \rangle = 1 \text{ and } \langle \psi_0, v \rangle = 0$$

for all $v \in V$ orthogonal to $\gamma_0$. Crucially, a simple fold also requires that

$$\langle \psi_0, F^1_\epsilon \rangle \neq 0, \quad (2.21)$$

which means that $F^1_\epsilon$ has a non-zero $\gamma_0$ component.

If all the above holds, we consider the system $H : (V \times \mathbb{R}) \times \mathbb{R} \to V \times \mathbb{R}$ introduced in [14]

$$H(y, t) := \begin{pmatrix} F(v, \epsilon) \\ \langle \psi_0, v - v_1 \rangle + d(\epsilon - \epsilon_1) - t \end{pmatrix},$$

where $d \in \mathbb{R}$ and $y = (v, \epsilon)$. We can apply the so-called 'ABCD' Lemma from [14] to this system to conclude that for $y_1 = (v_1, \epsilon_1)$

$$H_y(y_1, 0) = \begin{pmatrix} F^0_v \\ \langle \psi_0, \cdot \rangle \\ d \end{pmatrix}$$

is an isomorphism on $V \times \mathbb{R}$. As a result, it can be shown that near $\epsilon_1$ there exists smooth functions $v(t), \epsilon(t)$ such that $(v(t), \epsilon(t)) \in V \times \mathbb{R}$ is the unique path of solutions of $F(v(t), \epsilon(t)) = 0$ with $(x(0), \epsilon(0)) = (v_1, \epsilon_1)$. What it informally means is that even though at $(v_1, \epsilon_1)$ we can no longer represent the solution path as $(v(\epsilon), \epsilon)$, parametrising it via parameter $t \in \mathbb{R}$ still works. Please refer to Figure 2.5 for a schematic visualisation.

This concludes the abstract treatment of bifurcation theory. We will apply it to a specific example in Section 4.3, where appearance of a scalar parameter $\epsilon$
prompts a bifurcation analysis.

Figure 2.5: A schematic example of a fold point bifurcation. The missing vertical axis abstractly corresponds to \( v(\epsilon) \). Existence of the path represented by the solid red line is ensured by the Implicit Function Theorem and of the dashed extension by the ABCD Lemma.
Chapter 3

Model for a screw dislocation

3.1 Basics

As described in Section 2.1.1, we begin with a reference configuration $\Lambda^{\text{hom}}$ and work with a setting of a scalar anti-plane displacement field $u : \Lambda^{\text{hom}} \to \mathbb{R}$. Employing the machinery introduced in Section 2.2.3, we thus consider the energy difference functional

$$E(u) = \sum_{b \in \mathcal{B}} \left( \phi (e_b + D u_b) - \phi (e_b) \right),$$

(3.1)

where (recalling that $b = (l, l + a_i)$)

$$e_b = \int_b \nabla a_i \hat{u} \, dx,$$

(3.2)

where $\hat{u}$ is the far-field predictor, which will be constructed in such way that $E$ is well-defined for $u \in \mathcal{H}^1$. Defining $e_b$ in this way is convenient, as away from the half-plane cut $e_b = D \hat{u}_b$ (so that (3.1) agrees with (2.14)) and for bonds crossing the cut, as described in Section 2.1.1, the integral encodes the presence of the jump. See also Figure 3.1.

We assume that $\phi \in C^4(\mathbb{R})$, $\phi(0) = \phi'(0) = 0$ and $\phi''(0) = 1$. In addition, since the corresponding three dimensional structure is assumed to be $e_3$-periodic (cf. Section 3.1), it is natural to require $\phi$ to be 1-periodic. This follows from the fact that thanks to $e_3$-periodicity, for any site $l$, both (a) $u(l) = r$ and (b) $u(l) = r + z$, where $z \in \mathbb{Z}$, result in the same 3D configuration. Finally, for the ease of presentation, we also assume that $\|\phi'\|_{L^\infty} < \infty$, for $j \leq 4$.

In the subsequent sections we will first analyse the energy difference functional $E$ and its properties, with a particular focus on the construction of the predictor and how it affects the structure of $E$. We will then proceed to discuss the
decay estimates of solutions - a task significantly harder than in the toy problem described in Section 2.2.2.

3.2 Analysis of the energy difference functional

In this section we would like to describe the properties of $E$. A preliminary observation is that we can rewrite $E$ by adding and subtracting same quantity

$$E(u) = \sum_{b \in B} \left( \phi(e_b + Du_b) - \phi(e_b) - \phi'(e_b)Du_b \right) + \sum_{b \in B} \phi'(e_b)Du_b$$

$$=: \hat{E}(u) + \langle \delta E(0), u \rangle .$$

Remark 3.2.1. We can assume $\phi'(0) = 0$ without loss of generality, as for $\phi'(0) \neq 0$ we can safely subtract from (3.3) a term of the form

$$\sum_{b \in B} \phi'(0)Du_b ,$$

which informally means that in $\langle \delta E(0), u \rangle$ we replace $\phi'(r)$ by $\phi'(r) - \phi'(0)$. This yields a cancellation after we Taylor expand $\phi'(e_b)$ around 0 (see Section 3.2.2).

We can use Taylor expansion to show growth restrictions on infinite sums involved in $\hat{E}$, which ensure their finiteness for any $u \in \dot{H}^1$. Using the defining properties of $\phi$, we can immediately conclude that

$$|\phi(e_b + Du_b) - \phi(e_b) - \phi'(e_b)Du_b| \leq \frac{\|\phi''\|_{L^\infty}}{2}|Du_b|^2 ,$$

which implies $\hat{E}$ is well-defined on $\dot{H}^1$. Thus we focus $\langle \delta E(0), u \rangle$.

In the subsequent sections we will first describe the construction of the predictor and then show how it allows us to conclude that $\delta E(0)$ is a bounded linear functional defined on $\dot{H}^1$.

3.2.1 Construction of the predictor

The linear lattice problem and the linear PDE mentioned in Section 2.2 can be seen as approximations of one another, thus it is an intuitive approach to obtain the predictor $\hat{u}$ by solving a standard continuum linear elasticity equation for a screw dislocation (cf. [10]). We define a branch-cut

$$\Gamma := \left\{ \left( x_1, \frac{\sqrt{3}}{4} \right) \mid x_1 \leq \frac{1}{2} \right\} ,$$
where \( \hat{x} := \left( \frac{1}{2}, \frac{\sqrt{3}}{2} \right) \) is the dislocation core, chosen to correspond to the mid-point between two atomic plates and also so that it lies in the middle of a triangular cell of three lattice sites with one being at the origin. Thus, as is known from [10], the far-field predictor \( \hat{u} \) satisfies a system of equations

\[-\Delta \hat{u} = 0 \text{ in } \mathbb{R}^2 \setminus \Gamma, \tag{3.5}\]
\[\hat{u}(x^+) - \hat{u}(x^-) = 1 \text{ on } \Gamma \setminus \hat{x}, \tag{3.6}\]
\[\partial_{x^2} \hat{u}(x^+) - \partial_{x^2} \hat{u}(x^-) = 0 \text{ on } \Gamma \setminus \hat{x}, \tag{3.7}\]

where \( f(x^\pm) \) is to be understood as \( \lim_{t \to 0} f(x_1, x_2 \pm t) \). The jump conditions encode both the slip and the fact that atomic planes match perfectly on the opposite sites of the cut.

It is straightforward to see that this system has a solution

\[\hat{u}(x) = \frac{1}{2\pi} \arg((x_1 - \hat{x}_1) + i(x_2 - \hat{x}_2)) \tag{3.8}\]

and we choose the branch-cut \( \mathbb{R}^- \) for the arg. See Figure 3.1 for a plot. One can also quite easily establish that \( \nabla \hat{u} \in C^\infty(\mathbb{R}^2 \setminus \{0\}) \) and

\[|\nabla^j \hat{u}(x)| \lesssim |x|^{-j}. \tag{3.9}\]

Figure 3.1: Linear elasticity predictor \( \hat{u} \) for a screw dislocation. The presence of the jump motivates why \( e_b \) is defined via integration.

Using this result, we can now proceed to show several properties of the energy difference functional \( E \).
3.2.2 Well-definedness and differentiability

The contribution of this section can be summarised in the following theorem, which we will subsequently prove.

**Theorem 3.2.1.** Assuming that \( e_b \) is given by (3.2), where \( \hat{u} \) is given by (3.8), the energy difference functional \( E \) given by (3.3) is well-defined for all \( u \in \dot{H}^1 \) and in fact \( E \in C^3(\dot{H}^1) \) with a formula for subsequent Fréchet derivatives given by

\[
\delta^j E(u)[v^1, \ldots, v^j] = \sum_{b \in B} \phi^{(j)}(e_b + Du_b)Dv^1_b \ldots Dv^j_b,
\]

where \( j = 1, \ldots, 3 \) and \( v^i \in \dot{H}^1 \) for each \( i \).

**Proof.** Well-definedness: Recalling the preliminary observation from the preface of Section 3.2, in order to establish well-definedness we have to ensure that \( \delta E(0) \) is a bounded linear functional on \( \dot{H}^1 \). Exploiting the \( \phi'(0) = 0 \) and \( \phi''(0) = 1 \), we use a Taylor expansion around zero to get

\[
\langle \delta E(0), u \rangle = \sum_{b \in B} \phi'(e_b)Du_b = \sum_{b \in B} (e_b + g^{(1)}_b)Du_b = (e, Du)_B + (g^{(1)}, Du)_B, \quad (3.10)
\]

where \( (\cdot, \cdot)_B \) denotes the inner product corresponding to the Hilbert space \( \ell^2(B) \). Here \( g^{(1)}_b \) denotes the Lagrange form of the quadratic remainder. Using \( r_b \) as in (2.15) we conclude that

\[
|g^{(1)}_b| \lesssim |e_b|^2 \approx |\nabla \hat{u}(l)|^2 \lesssim r_b^{-2},
\]

which by Lemma 2.2.3 implies that \( g^{(1)} \in \ell^2(B) \) and thus by Cauchy-Schwarz we have

\[
(g^{(1)}, Du)_B \lesssim \|g^{(1)}\|_{\ell^2(B)} \|Du\|_{\ell^2(B)}.
\]

Hence it only remains to show a similar estimate for the term \( (e, Du)_B \) in (3.10).

To this end we use the properties of \( \hat{u} \) and identify \( u \in \dot{H}^1 \) with its piecewise linear interpolant defined on a triangulation \( \mathcal{T} \) induced by the lattice sites (cf. [2]). First, by turning the set of equations (3.5)–(3.7) into the weak form by multiplying by \( u \), integrating over \( \mathbb{R}^2 \setminus B_\epsilon(\hat{x}) \) for sufficiently small positive \( \epsilon \) and integrating by parts, we see that

\[
\int_{\mathbb{R}^2 \setminus B_\epsilon(\hat{x})} \nabla \hat{u} \cdot \nabla u dx = \int_{\partial B_\epsilon(\hat{x})} \nabla \hat{u} \cdot \nu u ds = 0,
\]

where the last equality follows from the fact that \( \nabla \hat{u} \) is orthogonal to the unit outer
normal of a ball. Since it works for any \( \epsilon > 0 \) small enough, then we can define the integral over the whole \( \mathbb{R}^2 \) as a limit \( \epsilon \to 0 \) and thus conclude that

\[
\int_{\mathbb{R}^2} \nabla \hat{u} \cdot \nabla u = 0. \tag{3.11}
\]

In order to work with derivatives in the \( a_i \)-directions, we note the simple calculation that \( \nabla \hat{u} \cdot \nabla u = \frac{2}{3} \sum_{i=1}^{3} \nabla_{a_i} \hat{u} \nabla_{a_i} u \), which in turn, using the tessellation of \( \mathbb{R}^2 \), allows us to conclude

\[
0 = \int_{\mathbb{R}^2} \nabla \hat{u} \cdot \nabla u = \frac{2}{3} \sum_{C \in T} \sum_{i=1}^{3} \int_{C} \nabla_{a_i} \hat{u} \, dx \, D_{a_i} u(l^C_i), \tag{3.12}
\]

where we have used the fact that on each triangle \( C \), \( \nabla_{a_i} u = D_{a_i} u(l^C_i) \) is constant. Here \( l^C_i \) is a lattice site that is a vertex of a triangle \( C \).

Noting that each bond \( b \) appears twice in the double-sum in the RHS of (3.12), we define \( \omega_b \) to be the union of two triangles sharing bond \( b \) and thus we can rephrase (3.12) in terms of bonds to get

\[
0 = \int_{\mathbb{R}^2} \nabla \hat{u} \cdot \nabla u = \sum_{b \in B} \frac{1}{\sqrt{3} |\omega_b|} \int_{\omega_b} \nabla_{a_i} \hat{u} \, dx \, D_{a_i} u_b. \tag{3.13}
\]

This superconvergence result (cf. [18]) proves useful to treat \( (e, Du)_B \). Adding zero in the form of (3.13) we have the identity

\[
(e, Du)_B = \sum_{b \in B} g_b^{(2)} D_{a_i} u_b,
\]

where

\[
g_b^{(2)} = e_b - \frac{1}{|\omega_b|} \int_{\omega_b} \nabla_{a_i} \hat{u} \, dx
\]

provided that \( b \) does not belong to the triangle with the dislocation core.

Furthermore, for \( b = (l, l + a_i) \) a standard vector calculus result is that

\[
e_b = \int_{0}^{1} \nabla_{a_i} \hat{u}(l + ta_i) \, dt. \tag{3.14}
\]

Since both \( b \) and \( \omega_b \) have the same mid-point, we can proceed as follows. Suppose for simplicity that we try to estimate

\[
I_f = \int_{b} f \, dx - \frac{1}{|\omega_b|} \int_{\omega_b} f \, dx,
\]
where \( f \) is function of one variable and both \( b \) and \( \omega_b \) are intervals sharing the same mid-point denoted by \( m_b \) (in particular note that \(|b| = 1\)). Then Taylor expansion around \( m_b \) of both integrands yields

\[
I_f = \left( f(m_b) \int_b dx + f'(m_b) \int_b (x - m_b) \, dx + f''(\xi_1) \int_b (x - m_b)^2 \, dx \right) - \left( f(m_b) \int_{\omega_b} dx + f'(m_b) \int_{\omega_b} (x - m_b) \, dx + \frac{f''(\xi_2)}{|\omega_b|} \int_{\omega_b} (x - m_b)^2 \, dx \right).
\]

Using the fact that mid-point approximation is exact for linear functions, we can conclude that terms involving constant and linear integrands cancel each other. Thus we can conclude that

\[
I_f \lesssim \| f'' \|_{L^\infty(\omega_b)}.
\]

A two-dimensional analogue of this argument applied to \( f = \nabla_a \hat{u} \) allows us to conclude that

\[
|g^{(2)}_b| \lesssim \| \nabla^3 \hat{u} \|_{L^\infty(\omega_b)} \lesssim r_b^{-3},
\]

which, applying Lemma 2.2.3, implies that

\[
\langle \delta E(0), u \rangle \lesssim \| Du \|_{\ell^2},
\]

hence ensuring \( E \) is well-defined.

**Remark 3.2.2.** Note that using a simpler argument allows to obtain \(|e_b| \lesssim r_b^{-2}\), which is already a sufficiently strong result to conclude (3.16). Obtaining the rate \( r_b^{-3} \) will, however, prove useful in the sections to come.

**Differentiability:** To show differentiability in the sense of Fréchet, we have to show that

\[
|E(u + v) - E(u) - \langle \delta E(0), u \rangle| = o(v),
\]

which follows via Taylor expansion around \( e_b + Du_b \):

\[
\phi(e_b + Du_b + Dv_b) = \phi(e_b + Du_b) + \phi'(e_b + Du_b)Dv_b + \frac{\phi''(\xi_b)}{2}Dv_b^2.
\]

Together with the uniform boundedness of \( \phi \) and its derivatives, this implies

\[
|E(u + v) - E(u) - \langle \delta E(u), v \rangle| \lesssim \sum_{b \in B} |Dv_b|^2 = \| Dv \|_{\ell^2(B)}^2,
\]

where the RHS clearly is of order \( o(v) \). Showing that \( E \in C^3(\mathcal{H}^1) \) requires the same argument.
3.3 Decay estimates

Assuming that a minimiser $\bar{u} \in \hat{H}^1$ of (3.1) exists, it is of considerable importance to be able to prove its decay rate, i.e. to find a result similar to Corollary 2.2.2 for the linear lattice problem. It is particularly important in simulations, as it allows to deem the influence of $\bar{u}$ negligible outside a small region near the core. Note that it is extremely difficult to prove existence and it has only been done under additional assumptions (see [11]). Numerical tests, however, clearly show that there is a solution, thus we choose to ignore this issue.

The decay result can be stated as the following theorem.

**Theorem 3.3.1.** Suppose that $\phi'''(0) = 0$. Let $\bar{u}$ be a minimiser of (3.1) over the space $\hat{H}^1$. Then, for $\rho \in \{a_1, \ldots, a_6\}^j$ ($j = 0, \ldots, 3$), we have

$$|D_{\rho} \bar{u}(l)| \lesssim |l|^{-1-j},$$

(3.17)

where $D_{\rho}$ as in Theorem 2.2.1.

In order to prove it, we proceed through a number of lemmas.

**Lemma 3.3.2.** Under the assumptions of Theorem 3.3.1, $\bar{u}$ satisfies

$$(H\bar{u}, v)_{\Lambda^{\text{hom}}} = (g + h, Dv)_B$$

for all $v \in \hat{H}^1$, (3.18)

where $H$ is the linear operator defined in (2.12) and

$$g_b = \phi'(e_b) + \phi''(0)D\bar{u}_b - \phi'(e_b + D\bar{u}_b) \quad \text{and} \quad h_b = -\phi'(e_b).$$

Furthermore, for $r_b$ (defined in (2.15)) large enough,

$$|g_b| \lesssim r_b^{-4} + |D\bar{u}_b|^2$$

(3.19)

and

$$|h_b| \lesssim r_b^{-3}.$$  

(3.20)

**Proof.** We begin by noting that if $\bar{u}$ is a minimiser, then it is a critical point of $E$, i.e. it satisfies

$$\langle \delta E(\bar{u}), v \rangle = 0$$

for all $v \in \hat{H}^1$, which, using Theorem 3.2.1, means

$$\sum_{b \in \mathcal{B}} \phi'(e_b + D\bar{u}_b)Dv_b = 0$$

for all $v \in \hat{H}^1$. 

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Furthermore, we recall how $H$ is used in Theorem 2.2.1 (for convenience converting from lattice sites to bonds)
\[(H \bar{u}, v)_{\Lambda_{\text{hom}}} = (D \bar{u}, Dv)_B = \sum_{b \in B} D \bar{u}_b Dv_b.\]

Finally, we note that $\phi'(0) = 0$, $\phi''(0) = 1$, $\phi'''(0) = 0$. Putting all the above together immediately implies (3.18).

For the second part, we use Taylor expansion around 0 to get
\[\phi'(e_b) = \phi'(0) + \phi''(0)e_b + \frac{\phi'''(0)}{2}(e_b + D\bar{u}_b)^2 + \frac{\phi^{(iv)}(\xi)}{6}(e_b + D\bar{u}_b)^3,\]

where $\xi$ lies between 0 and $e_b$ (Lagrange form of the remainder of the Taylor expansion). Furthermore:
\[\phi'(e_b + D\bar{u}_b) = \phi'(0) + \phi''(0)(e_b + D\bar{u}_b) + \frac{\phi'''(0)}{2}(e_b + D\bar{u}_b)^2 + \frac{\phi^{(iv)}(\xi_2)}{6}(e_b + D\bar{u}_b)^3.\]

Thus, using the fact that $\phi'''(0) = 0$, we get
\[|g_b| = |\phi'(e_b) + \phi''(0)D\bar{u}_b - \phi'(e_b + D\bar{u}_b)| = \left|\frac{\phi^{(iv)}(\xi_1) - \phi^{(iv)}(\xi_2)}{6} e_b^3 - (e_b + D\bar{u}_b)^3\right|.
\]

Now, for $a, b \in \mathbb{R}_+ \cup \{0\}$ we have $|a^3 - (a + b)^3| = |3a^2b + 3ab^2 + b^3| = |b(3a^2 + b^2) + 3b(ab)|$ and $ab^2 = b(ab) \lesssim b(a^2 + b^2)$, so we get an estimate
\[|g_b| \lesssim \left(|e_b|^2|D\bar{u}_b| + |D\bar{u}_b|^3\right).
\]

Next we apply Cauchy-Schwarz to the first term and note that $\bar{u} \in \mathcal{H}^1$, thus in particular $D\bar{u} \in \ell^2(B) \subset \ell^\infty(B)$ and so
\[|D\bar{u}_b|^3 \leq ||Du||_{\ell^\infty} |Du_b|^2.
\]

With these two results in hand and noting the property of the predictor that $|e_b| \lesssim r_b^{-1}$, we obtain (3.19).

Now we turn to $h_b$. We know that $h_b = -\phi'(e_b)$, thus $(h, Dv)_B = -(\delta E(0), v)$, which, by (3.10) implies that $(-h, Dv)_B = (g^{(1)}, Dv)_B + (g^{(2)}, Dv)_B$. Thanks to the additional assumption that $\phi'''(0) = 0$, the quadratic term in the Taylor expansion disappears and so $g_b^{(1)}$ now corresponds to the Lagrange form of the cubic remainder of Taylor expansion. Thus $g_b^{(1)} \lesssim e_b^3$ and hence both $g^{(1)}$ and $g^{(2)}$ decay with the rate of $r_b^{-5}$, which implies that so does $h_b$, i.e. we get (3.20). \[\square\]
Lemma 3.3.3. Let a function $v_1 : \Lambda^{\text{hom}} \to \mathbb{R}$ be defined by $v(m) = D_\rho \mathcal{G}(l - m)$, where $\mathcal{G}$ is the Green’s function introduced in Theorem 2.2.1. Then $v_1 \in \dot{H}^1$ and

$$(H \bar{u}, v_1)_{\Lambda^{\text{hom}}} = D_\rho \bar{u}(l),$$  

(3.21)

where the notation as in Theorem 3.3.1.

Proof. For any suitable $\rho$ (notation introduced in Theorem 2.2.1) the fact that $v_1 \in \dot{H}^1$ follows from Lemma 2.2.3, which can be applied due to the decay estimate for $\mathcal{G}$ mentioned in Section 2.2.2. For simplicity we show the basic case $\rho = a_i$ as for any higher-order $\rho$ the argument can be reduced to the basic case due to the following observation. Since $D_{a_i} \bar{u}(l) = \bar{u}(l + a_i) - \bar{u}(l)$, then

$$(H \bar{u}, \mathcal{G}(l - \cdot + a_i) - \mathcal{G}(l - \cdot)) = (H \bar{u}, \mathcal{G}(l - \cdot + a_i)) - (H \bar{u}, \mathcal{G}(l - \cdot)).$$

Hence (3.21) for $\rho = a_i$ will follow if we can show that

$$(H \bar{u}, v_2)(l) = \bar{u}(l), \text{ where } v_2(m) = \mathcal{G}(l - m).$$  

(3.22)

Similarly, for any higher-order $\rho$ we can always reduce the argument to considering $v_2$. And (3.22) follows by Theorem 2.2.1, which we apply to a sequence of compactly supported functions $(u_n)_{n=1}^\infty \subset \dot{H}^1$ with the property that $u_n \to \bar{u}$. For each $n$ we have

$$H(\mathcal{G} \ast u_n)(l) = u_n(l).$$

Furthermore, we show that for any $u \in \dot{H}^1$ (so in particular for $u_n$ and $\bar{u}$)

$$(Hu, v_2)(l) = H(\mathcal{G} \ast u)(l),$$  

(3.23)

where $v_2$ as in (3.22). It can be established by writing both sides in full

$$H(\mathcal{G} \ast u)(l) = \sum_{i=1}^3 D_{-a_i}D_{a_i}(\mathcal{G} \ast u)(l) = \sum_{i=1}^3 D_{-a_i}D_{a_i} \left( \sum_{m \in \Lambda^{\text{hom}}} \mathcal{G}(l - m)u(m) \right)$$  

(3.24)

and

$$(Hu, v_2)(l) = \sum_{m \in \Lambda^{\text{hom}}} \left( \sum_{i=1}^3 D_{-a_i}D_{a_i}u(m) \right) \mathcal{G}(l - m).$$  

(3.25)

By noting that in (3.24), the difference operator $D_{a_i}$ is applied with respect to $l$, it is a simple matter of relabelling to obtain (3.23).

Since $u \mapsto (Hu, v_2)$ is a bounded mapping, then we can pass to the limit and
thus obtain
\[ \tilde{u} = \lim_{n \to \infty} u_n = \lim_{n \to \infty} H(G \ast u_n) = \lim_{n \to \infty} (Hu_n, v_2) = (H\tilde{u}, v_2), \]
which establishes (3.22) and thus proves the lemma.

\[ \text{Lemma 3.3.4. Let } g \text{ and } h \text{ be as in Lemma 3.3.2 and } v_1 \text{ as in Lemma 3.3.3 with } \rho = a_i. \text{ Then} \]
\[ |(h, Dv_1)_B(l)| \lesssim |l|^{-2} \]
and
\[ |(g, Dv_1)_B| \lesssim |l|^{-2} + \|D\tilde{u}\|_{\ell^2(\Lambda^{\text{hom}} \setminus B_{|l|/2}(0))} \|D\tilde{u}\|_{\ell^\infty(\Lambda^{\text{hom}} \setminus B_{|l|/2}(0))}, \]
where the norms defined on a lattice as in (2.17).

\[ \text{Proof.} \text{ We consider each term separately. Note that in this proof we will extensively use ideas developed in Section 2.2.4.} \]
\[ \text{PART 1: } (h, Dv_1)_B. \]
Thanks to the decay estimates of the Green’s function we know that for \( b = (m, m + a_i) \), \(|Dv_1_b| \lesssim |m|^{-2}\) and we also recall (3.20) (as well as how we define \( r_b \) in (2.15)).

We can hence estimate
\[ |(h, Dv_1)_B| \lesssim \sum_{m \in \Lambda^{\text{hom}}} (1 + |m|)^{-3}(1 + |m - l|)^{-2}, \]
where +1 in the second term comes from the fact that we can choose the constant big enough to have \(|m - l|^{-2} \leq C(1 + |m - l|)^{-2}\) as long as \( m \neq l \), which is acceptable, as we are interested in the far-field. Similarly, +1 in the first term together with the constant in front reflects the fact that (3.20) holds for large enough \( b \). Next we split the domain by defining
\[ \Omega := \Lambda^{\text{hom}} \cap B_{|l|/2}(l). \]
Basic algebra tells us that \( m \in \Omega \implies |m| \geq \frac{|l|}{2}. \) Thus \((1 + |m|)^{-3} \lesssim |l|^{-3}\). Hence
\[ |(h, Dv_1)_B| \lesssim |l|^{-3} \sum_{m \in \Omega} (1 + |m - l|)^{-2} + \sum_{m \in \Lambda^{\text{hom}} \setminus \Omega} (1 + |m|)^{-3}(1 + |m - l|)^{-2}. \]
As \(|l| \to \infty\), the first sum tends to a convergent infinite sum, thus the first term can be bounded by \( C|l|^{-4}\). The second sum can be controlled by noting that \( m \in \Lambda^{\text{hom}} \setminus \Omega \implies |m - l| \geq \frac{|l|}{2} \implies (1 + |m - l|)^{-2} \leq \frac{4}{(2 + |l|)^2} \leq 4|l|^{-2}. \) Thus we can...
conclude that

\[ \sum_{m \in \Lambda_{\text{hom}} \setminus \Omega} (1 + |m|)^{-3}(1 + |m - l|)^{-2} \leq 4|l|^{-2} \sum_{m \in \Lambda_{\text{hom}} \setminus \Omega} (1 + |m|)^{-4} \lesssim 4|l|^{-2}. \]

Looking at the both terms together, we hence obtain (3.26).

\[ \text{PART 2: } |(g, Dv_1)|_B. \]

Starting again with \( |Dv_1| \lesssim |m - l|^{-2} \) and (3.19), we estimate

\[ |(g, Dv)|_B \lesssim \sum_{m \in \Lambda_{\text{hom}}} (1 + |m|)^{-4}(1 + |m - l|)^{-2} + \sum_{m \in \Lambda_{\text{hom}}} |D\tilde{u}(m)|^2(1 + |m - l|)^{-2}. \]

We immediately recognise that thanks to the argument in Part 1, the first term decays with the rate \(|l|^{-2}\).

For the second term we use a technique originating from the regularity theory for systems of elliptic PDEs ([9]). Using \( \Omega \) defined in (3.28), we proceed as follows

\[ \sum_{m \in \Lambda_{\text{hom}} \setminus \Omega} |D\tilde{u}(m)|^2(1 + |m - l|)^{-2} = \]

\[ \sum_{m \in \Lambda_{\text{hom}} \setminus \Omega} |D\tilde{u}(m)|^2(1 + |m - l|)^{-2} + \sum_{m \in \Omega} |D\tilde{u}(m)|^2(1 + |m - l|)^{-2}. \]

We will treat both sums separately. The first one can be estimated as in Part 1, namely

\[ \sum_{m \in \Lambda_{\text{hom}} \setminus \Omega} |D\tilde{u}(m)|^2(1 + |m - l|)^{-2} \leq 4|l|^{-2} \sum_{m \in \Lambda_{\text{hom}} \setminus \Omega} |D\tilde{u}(m)|^2 \leq 4\|Du\|^2_2 |l|^{-2}. \]

For the second sum we note that for \( l \) fixed this is a finite sum and so we can easily replace one power of \( |D\tilde{u}(m)| \) by the supremum over all \( m \in \Omega \) and apply Cauchy-Schwarz inequality to the rest:

\[ \sum_{m \in \Omega} |D\tilde{u}(m)|^2(1 + |m - l|)^{-2} \lesssim \|Du\|_{\ell^\infty(\Omega)} \|Du\|_{\ell^2(\Omega)} \left( \sum_{m \in \Omega} (1 + |m - l|)^{-4} \right)^{1/2} \]

\[ \lesssim \|Du\|_{\ell^\infty(\Omega)} \|Du\|_{\ell^2(\Omega)} \|1 + |\cdot - l|^{-2}\|_{\ell^2(\Lambda_{\text{hom}})} \]

\[ \lesssim \|D\tilde{u}\|_{\ell^2(\Lambda_{\text{hom}} \setminus B_{|l|/2}(0))} \|D\tilde{u}\|_{\ell^\infty(\Lambda_{\text{hom}} \setminus B_{|l|/2}(0))}, \]

where the last equality follows from the fact that \( \Omega \subset \Lambda_{\text{hom}} \setminus B_{|l|/2}(0) \). Note that the last term in the second line gets incorporated into the constant, as it does not depend on \( l \).

Putting everything together, we obtain (3.27). \( \square \)
We can now proceed to prove Theorem 3.3.1, starting with the case when \( \rho = a_i \).

**Proof of Theorem 3.3.1.** Let \( \rho = a_i \). Thanks to Lemma 3.3.2 \( \bar{u} \) satisfies (3.18) and we test it with \( v_1 \) from Lemma 3.3.3. Thanks to (3.21) and Lemma 3.3.4, we have that there exists \( R_1 > 0 \) such that for all \( |l| \geq R_1 \)

\[
|D_{\rho \gamma} \bar{u}(l)| \leq C \left(|l|^{-2} + \|D\bar{u}\|_{L^2(\Lambda^{\text{hom}} \setminus B_{|l|/2}(0))}\|D\bar{u}\|_{L^\infty(\Lambda^{\text{hom}} \setminus B_{|l|/2}(0))}\right).
\]

We define \( \omega(r) := \|D\bar{u}\|_{L^\infty(\Lambda^{\text{hom}} \setminus B_r(0))} \) and note that there exists \( R_2 > 0 \) such that \( \|D\bar{u}\|_{L^\infty(\Lambda^{\text{hom}} \setminus B_r(0))} \leq \frac{1}{C} 2^{-3} \) for \( r \geq R_2 \) (a consequence of the fact that this term goes to 0 as \( r \to \infty \)). Thus for \( r \geq R_3 = \max\{R_1, R_2\} \), we have for all \( |l| \geq R_3 \)

\[
|D_{\rho \gamma} \bar{u}(l)| \leq C |l|^{-2} + 2^{-3} \|D\bar{u}\|_{L^\infty(\Lambda^{\text{hom}} \setminus B_{|l|/2}(0))}.
\]  

(3.29)

Taking the supremum over all \( |l| \geq R_3 \) of (3.29), we deduce

\[
\omega(r) \leq Cr^{-2} + 2^{-3} \omega(r/2) \quad \text{for} \quad r \geq R_3.
\]  

(3.30)

Thus

\[
r^2 \omega(r) \leq C + \frac{1}{2} \left(\frac{r}{2}\right)^2 \omega\left(\frac{r}{2}\right) \quad \text{for} \quad r \geq R_3.
\]

But if \( r/2 \geq R_3 \), then we apply (3.30) to \( \omega(r/2) \) and we continue to iterate this argument, that is: if \( \frac{r}{2^n} \geq R_3 \) then

\[
r^2 \omega(r) \leq C \left(1 + \frac{1}{2} + \cdots + \frac{1}{2^{n-1}}\right) + \frac{1}{2^{n+1}} \left(\frac{r}{2^{n+1}}\right)^2 \omega\left(\frac{r}{2^{n+1}}\right)
\]

and we impose \( \frac{r}{2^n} < 2 R_3 \) \( \iff \) \( \frac{r}{2^{n+1}} < R_3 \) so that we cannot go any step further. Noting that the sum in the bracket can be bounded by 2 and that \( \omega(\cdot) \) is monotonically decreasing, which implies that \( \omega(\frac{r}{2^{n+1}}) \leq \omega(R_3) \), we obtain

\[
r^2 \omega(r) \leq 2C + (2R_3)^2 \omega(R_3) \iff \omega(r) \lesssim r^{-2},
\]

which proves (3.17) for \( \rho = a_i \).

For the higher order \( \rho \), we note that thanks to the result for the basic case, from (3.19) we obtain that \( g \) introduced in Lemma 3.3.2 decays with the rate

\[
|g_b| \lesssim r_b^{-4}.
\]  

(3.31)

Using decay estimates of the Green’s function for higher-order \( \rho \) (cf. Corollary 2.2.2)
and repeating the argument in Part 1 of the proof of Lemma 3.3.4 we immediately obtain

\[ |(h, Dv_1)_B(l)| + |(g, Dv_1)_B(l)| \lesssim |l|^{-1-j}, \tag{3.32} \]

which thanks to Lemma 3.3.3 concludes the proof.

This proof serves as an indicator of techniques to be used to derive corresponding estimates for the model of a crack defect, on which we will next focus.


Chapter 4

Model for a crack defect

4.1 Basics

Having considered a model for screw dislocation, we now proceed to treat a crack defect in anti-plane shear mode. Both models share many features.

As before, we start with a reference configuration $\Lambda^\text{hom}$ and have a scalar anti-plane displacement field $u : \Lambda^\text{hom} \to \mathbb{R}$. Furthermore, since as in a screw dislocation case, we pull both sides of the cut in opposite directions, we again resort to considering the energy difference functional, which differs slightly due to the fact now we sum over a defective set of bonds $B^\text{cr}$ (recall Figure 2.4) and use a different far-field predictor $\bar{u}$, which introduces the the crack structure. Thus, in a sense the far-field predictor can be though as an a-priori imposed boundary condition. We again consider

$$E(u) = \sum_{b \in B^\text{cr}} \left( \phi(e_b + D\hat{u}_b) - \phi(e_b) \right), \quad (4.1)$$

with the difference being the absence of bounds crossing the half-plane cut. As a result we can safely let $e_b = D\bar{u}_b$, where the construction of the predictor will ensure that $E$ is well-defined for $u \in \mathcal{H}^1$ (note that in the definition of $\mathcal{H}^1$ we now use $\Lambda^\text{hom}$ and $B^\text{cr}$, see the discussion in Section 2.1.2). The potential $\phi$ retains the same properties as in Chapter 3 with the additional one being that $\phi'''(0) = 0$. Since we think of $u$ as an anti-plane displacement, this is a natural assumption, as then $\phi(-r) = \phi(r)$.

In the next section we discuss how we construct the predictor and show its decay properties. Subsequently we use it to present the argument for well-definedness of $E$ - a task which highlights how the crack model technically differs from the screw dislocation, due to the absence of bonds on the opposite sites of the
crack.

We then proceed to translate the bifurcation theory introduced in Section 2.3 to this particular instance. In the conclusions we will also briefly mention the decay estimates for the crack. The work on them is far from complete and will be subject to further study in the coming months of the PhD project.

Note that in the section to follow, we will extensively refer to results obtained in Chapter 3.

4.2 Analysis of the energy difference functional

In the preface to this section we verbatim repeat the preliminary observation of Section 3.2, which states that we can rewrite $E$ as

$$E(u) = \sum_{b \in B^{cr}} \left( \phi(e_b + Dv_b) - \phi(e_b) - \phi'(e_b)Dv_b \right) + \sum_{b \in B^{cr}} \phi'(e_b)Dv_b$$

$$=: \hat{E}(u) + \langle \delta E(0), u \rangle$$

and that $\hat{E}$ is well-defined for $u \in \mathcal{H}^1$ thanks to a Taylor expansion argument as in (3.4). Thus we again focus on $\langle \delta E(0), u \rangle$, where the construction of the predictor is crucial. To proceed with the derivation of the equation, we note that

$$\langle \delta E(0), v \rangle = (e,Dv)_{B^{cr}} + (g,Dv)_{B^{cr}}$$

where $(\cdot,\cdot)_{B^{cr}}$ is the inner product of the space $\ell^2(B^{cr})$. Here $g$ comes from the fact that as in the screw dislocation case, we can expand:

$$\phi'(e_b) = \phi'(0) + \phi''(0)e_b + \frac{\phi'''(0)}{2}e_b^2 + \frac{\phi''''(0)(\xi)}{6}e_b^3,$$

and since we assume $\phi'(0) = \phi''(0) = 0$ and $\phi'''(0) = 1$ we can define $g_b$ to be the remainder, i.e. $g_b = \frac{\phi'''(0)(\xi)}{6}e_b^3$ and thus $|g_b| \lesssim |e_b|^3$.

4.2.1 Construction of the predictor

As in the case of a screw dislocation, we would like to solve a fitting continuum equation to obtain the predictor. We derive it from looking at $(e,Dv)_{B^{cr}}$. Similarly to the screw dislocation, we identify $v \in \mathcal{H}^1$ with its piecewise linear interpolant on the triangulation $\mathcal{T}^{cr}$, which is obtained from $\mathcal{T}$ (triangulation induced by lattice sites $\Lambda^{hom}$) by excluding the set of triangles $\mathcal{T}(B^{crdef})$ (recall (2.3)), for which a
bond \( b \in B^{\text{crdef}} \) is an edge. Thus

\[
T^{\text{cr}} := T - T(B^{\text{crdef}})
\]

For the continuum domain, we hence define

\[
\Omega = \bigcup_{T \in T^{\text{cr}}} T \text{ and } \Gamma = \partial \Omega.
\]

(4.3)

See Figure 4.1.

![Figure 4.1: Identification of different regions in the domain. Neglecting the erraticism of the core of the crack (represented as a triangle inside the yellow circle), \( \Gamma \) outside the crack core corresponds to green lines. \( \Gamma_0 \) is the red line.](image)

We can then show that in fact

\[
(e, v)_{B^{\text{cr}}} = \int_{\Omega} \mu \nabla I \hat{u} \cdot \nabla v + \int_{\Gamma} \mu' \nabla_t I \hat{u} \cdot \nabla_t v,
\]

(4.4)

where \( \mu = \frac{1}{\sqrt{3}} \), \( \mu' = \frac{1}{2} \) and \( I \hat{u} \) is the piecewise linear interpolant, same which is used for the identification of \( v \) at the beginning of this section. To show this we employ an argument similar to (3.12). First we note that

\[
(e, Dv)_{B^{\text{cr}}} = \sum_{b \in B^{\text{cr}}} D \hat{u}_b Dv_b = \sum_{T \in T^{\text{cr}}} \sum_{b \in B^{\text{cr}} \subset T} \frac{1}{2} D \hat{u}_b Dv_b + \sum_{b \subset \Gamma} \frac{1}{2} D \hat{u}_b Dv_b.
\]

This follows from the fact that we split the strain of each bond into two halves, assigning one to each triangle. The last term accounts for the bonds at the boundary of \( T^{\text{cr}} \), which have only one neighbouring triangle. On the other hand

\[
\int_{\Omega} \nabla I \hat{u} \cdot \nabla v \, dx = \sum_{T \in T^{\text{cr}}} \int_T \sum_{i=1}^3 \frac{2}{3} \nabla a_i I \hat{u} \nabla a_i v \, dx = \sum_{T \in T^{\text{cr}}} \frac{4|T|}{3} \sum_{b \in B^{\text{cr}} \subset T} \frac{1}{2} D \hat{u}_b Dv_b
\]
and
\[ \int_{\Gamma} \nabla_t I \hat{u} \nabla_t v \, dx = \sum_{b \subset \Gamma} \int_b D \hat{u}_b D v_b. \]
Since \(|T| = \frac{\sqrt{3}}{4}\), then indeed \(\mu = \frac{1}{\sqrt{3}}\), \(\mu' = \frac{1}{2}\).

To obtain the corresponding continuum equation, we introduce \(u_\epsilon(x) = \epsilon u(x/\epsilon)\) and let \(\epsilon \to 0\). As a result, \(\Gamma\) collapses to a single line \(\Gamma_0\), where we place the end point at \(\hat{x} = \left(\frac{1}{2}, \frac{\sqrt{3}}{4}\right)\) (see Figure 4.1) and we also replace \(\Omega\) by \(\Omega_0 := \mathbb{R}^2 \setminus \Gamma_0\).

Thus, formally, we obtain the following equation for \(\hat{u}\) to satisfy:
\begin{align*}
0 &= \int_{\Omega_0} \mu \nabla \hat{u} \cdot \nabla v \, dx + \int_{\Gamma_0} \mu' \nabla_t \hat{u} \nabla_t v \, dx \\
&= \int_{\Omega_0} (-\nu \Delta \hat{u}) v \, dx - \int_{\Gamma_0} (-\mu' \nabla_t^2 \hat{u} + \mu \nabla_n \hat{u}) v \, dx,
\end{align*}
where the second line follows by applying integration by parts. Instead of specifying set of admissible \(v\)'s and keeping the weak version, we refer to the strong formulation and state that \(\hat{u}\) satisfies
\[ -\Delta \hat{u} = 0 \quad \text{and} \quad \mu \nabla_n \hat{u} - \mu' \nabla_t^2 \hat{u} = 0. \quad (4.5) \]
It can be readily checked that \(\hat{u}\) of the following form satisfies (4.5)
\[ \hat{u}(r, \theta) = \epsilon \left\{ r^{1/2} \sin \left(\frac{\theta}{2}\right) + \frac{\mu'}{2\mu} r^{-1/2} \cos \left(\frac{\theta}{2}\right) \right\}, \quad (4.6) \]
where \(r\) and \(\theta\) are the usual polar coordinates defined via \(x_1 = r \cos \theta, x_2 = r \sin \theta\). Note the introduction of nonnegative scalar parameter \(\epsilon\), which represents the strength of the pull on the crack. With the appearance of powers of \(r = |x|\), it is easy to see that
\[ |\nabla^j \hat{u}(x)| \approx |x|^{1/2-j}, \quad (4.7) \]
which is significantly worse rate than of the predictor for the screw dislocation. This is exactly why we require \(\phi'''(0) = 0\) as otherwise our proof that \(E\) is well-defined fails.

With a formula for \(\hat{u}\) in hand, we can now proceed to prove \(E\) is well-defined.

### 4.2.2 Well-definedness and differentiability

In this section we prove the following theorem.

**Theorem 4.2.1.** Assuming that \(e_b = D \hat{u}_b\), where \(\hat{u}\) is given by (4.6), the energy difference functional \(E\) given by (4.2) is well-defined for all \(u \in \dot{H}^1\) and in fact
$E \in C^3(\mathcal{H}^1)$ with a formula for subsequent Fréchet derivatives given by

$$
\delta^j E(u)[v^1, \ldots, v^j] = \sum_{b \in \mathcal{B}} \phi^{(j)}(e_b + Du_b)Dv^1_b \ldots Dv^j_b,
$$

where $j = 1, \ldots, 3$ and $v^i \in \mathcal{H}^1$ for each $i$.

**Proof.** Recalling the preliminary observation from the preface to Section 4.2, we have to show that $\delta E(0)$ is a bounder linear functional on $\mathcal{H}^1$. First of all, we see that

$$
\langle \delta E(0), v \rangle = (e, Dv)_{\mathcal{B}^\sigma} + (g, Dv)_{\mathcal{B}^\sigma},
$$

where, thanks to $\phi'''(0) = 0$, $|g| \lesssim |e|^3$, thus, using (4.7), we have

$$
|g| \lesssim |r|^{-3/2},
$$

which due to Lemma 2.2.3 is enough to conclude that $g \in \ell^2(\mathcal{B}^\sigma)$, thus $(g, Dv)_{\mathcal{B}^\sigma} \lesssim ||g||_{\ell^2(\mathcal{B}^\sigma)} ||Dv||_{\ell^2(\mathcal{B}^\sigma)}$. Hence we focus on $(e, Dv)_{\mathcal{B}^\sigma}$.

For $(e, Dv)_{\mathcal{B}^\sigma}$ we use the fact that $\hat{u}$ satisfies the Laplace equation on $\Omega_0$, so we multiply both side sof this equation by $v$, which is the piecewise linear interpolant identification of $v \in \mathcal{H}^1$, as described at the beginning of Section 4.2.1. We then integrate over $\Omega \subset \Omega_0$ and apply integration by parts to obtain

$$
0 = \int_{\Omega} (-\Delta \hat{u}) v = \int_{\Omega} \nabla \hat{u} \cdot \nabla v - \int_{\Gamma} (\nabla \hat{u} \cdot \nu) v. \tag{4.8}
$$

Recalling (4.4), we add and subtract same two terms corresponding to $\hat{u}$:

$$
(e, v)_{\mathcal{B}^\sigma} = \int_{\Omega} \mu \left( \nabla I \hat{u} - \nabla \hat{u} \right) \cdot \nabla v + \int_{\Omega} \mu' \left( \nabla_t \hat{u} - \nabla_t \hat{u} \right) \nabla_t v + \int_{\Omega} \mu \nabla \hat{u} \cdot \nabla v + \int_{\Gamma} \mu' \nabla_t \hat{u} \cdot \nabla_t v \tag{4.9}
$$

The standard FEM interpolation estimates [2] tell us that

$$
||\nabla I \hat{u} - \nabla \hat{u}||_{L^\infty(T)} \lesssim ||\nabla^2 \hat{u}||_{L^\infty(T)}, \quad \text{and} \quad ||\nabla_t \hat{u} - \nabla_t \hat{u}||_{L^\infty(T)} \lesssim ||\nabla^2 \hat{u}||_{L^\infty(T)}
$$

and (4.7) implies $|\nabla^2 \hat{u}| \lesssim r^{-3/2}$, which due to Lemma 2.2.3 is enough to conclude that the first two terms of (4.9) decay fast enough. For the third term we use (4.8), so that after applying integration by parts to the last term, we conclude that in the end we work with

$$
\int_{\Gamma} \left( \mu \nabla \hat{u} \cdot \nu - \mu' \nabla_t^2 \hat{u} \right) v.
$$

33
Since $E$ is translation invariant, we can subtract a term $v(0)$ and thus consider
\[ \int_\Gamma \left( \mu \nabla \hat{u} \cdot \nu - \mu' \nabla^2 \hat{u} \right) \left( v(x) - v(0) \right). \]

Noting the notational change $\nabla \hat{u} \cdot \nu \equiv \nabla_n \hat{u}$, we define
\[ s := \mu \nabla_n \hat{u} - \mu' \nabla^2 \hat{u}, \]
and observe that thanks to (4.5) $s = 0$ on $\Gamma_0$. So if $x_0 \in \Gamma_0$, we can Taylor-expand
\[ s(x) = s(x_0) + \nabla s(\xi) \cdot (x - x_0), \]
where clearly $s(x_0) = 0$. For any $x \in \Gamma$ we choose $x_0 \in \Gamma_0$ such that they both have the same $e_1$-coordinate, so that $x - x_0 = (0, \pm \sqrt{3} 4)$. See Figure 4.2 for visualisation.

![Figure 4.2: Points in black represent choosing $x_0 \in \Gamma_0$ corresponding to an arbitrary $x \in \Gamma$ away from the defect core.](image)

As a result, we can conclude that $s$ is of order $O(|\nabla s|)$ and $|\nabla s| \approx |\nabla^2 \hat{u}| \lesssim r^{-3/2}$, which implies that we can estimate
\[ s(x) \lesssim |x|^{-3/2}. \]

**Remark 4.2.1.** This can be shown differently. Observing what tangential and normal derivatives on $\Gamma$ away from the core are and letting all constants equal to 1 for convenience, as it does not alter the analysis, allows us to directly calculate $s$. We obtain
\[ s(r, \theta) = \frac{2r^2 \cos \left( \frac{\theta}{2} \right) - 3 \left( r \sin \left( \frac{3\theta}{2} \right) + \cos \left( \frac{5\theta}{2} \right) \right)}{4r^{5/2}} = O(r^{-1/2}) = O(|x|^{-1/2}) \quad (4.10) \]
As $r = |x|$ (for $x \in \Gamma$) increases, we get arbitrarily close to $\theta = \pi$, which means the term of order $O(r^{-1/2})$ in (4.10) goes away. Thus we can directly state that for $r$ large enough, we can estimate $s(x) \leq C|x|^{-3/2}$.
As a result,

\[ \int_{\Gamma} s(x)(v(x) - v(0)) \lesssim \int_{\Gamma} |x|^{-3/2}(v(x) - v(0)). \tag{4.11} \]

In order to proceed, we need to generalise the result from [20] (Proposition 12) to the case of a defective set of bonds, which we state as a proposition and prove in Appendix A.

**Proposition 4.2.2.** If \( v \in \dot{H}^1 \) (where, crucially, the set of bonds \( B^{cr} \) is used to define this space), then for any \( l \in \Gamma \)

\[ |v(l) - v(0)| \lesssim ||Dv||_{L^2(B^{cr})}(1 + \log |l|). \tag{4.12} \]

Applying this result to (4.11) we conclude that

\[ \int_{\Gamma} |x|^{-3/2}(v(x) - v(0)) \lesssim ||Dv||_{L^2} \left[ \int_{\Gamma} |x|^{-3/2} + |x|^{-3/2} \log |x| \right] \]

and the integral term is finite, as \( \Gamma \) is one-dimensional. Hence we conclude that \( \langle \delta E(0), v \rangle \lesssim ||Dv||_{L^2} \), i.e. that \( \delta E(0) \) is a bounded linear functional on \( \dot{H}^1 \). Therefore \( E \) is well-defined for all \( v \in \dot{H}^1 \).

For the differentiability, since \( E \) is of the same form as in the screw dislocation, Theorem 3.2.1 applies.

\[ \square \]

### 4.3 Bifurcation analysis

Starting with the energy difference functional

\[ E(u) = \sum_{b \in B^{cr}} \left[ \phi(D\hat{u}_b + Du_b) - \phi(D\hat{u}_b) \right], \]

we recall (4.5) and rephrase the predictor as \( \hat{u}(x) = \epsilon u^\text{CP}(x) \), where

\[ u^\text{CP}(r, \theta) = r^{1/2} \sin \left( \frac{\theta}{2} \right) + \frac{\mu'}{2\mu} r^{-1/2} \cos \left( \frac{\theta}{2} \right) \]

and hence we work with

\[ E(u, \epsilon) = \sum_{b \in B^{cr}} \left[ \phi(\epsilon e_b + Du_b) - \phi(ee_b) \right], \]
where $e_b = Du^0_{b}^{\text{CP}}$. In particular $E : V \times \mathbb{R} \to \mathbb{R}$, where we define

$$V := \{ v \in \mathcal{H}^1 | v(0) = 0 \},$$

as the constant shift has to be specified in order to have a Hilbert space structure, which is particularly important here. The inner product of this space is defined as

$$(v, w)_V := (Dv, Dw)^{B_{cr}} = \sum_{b \in B_{cr}} Dv_b Dw_b.$$

Furthermore, Theorem 4.2.1 ensures $E$ has a Fréchet derivative with respect to $v$ at $(u_0, \epsilon_0)$ given by

$$\delta u E(u_0, \epsilon_0) \in V^* \text{ with } \langle \delta u E(u_0; \epsilon_0), v \rangle = \sum_{b \in B^{cr}} \phi'(\epsilon e_b + Du_b) Dv_b \text{ for all } v \in V.$$

Furthermore, since $V$ is a Hilbert space, by the Riesz Representation theorem there exists unique $k^0 (= k(u_0, \epsilon_0)) \in V$ such that

$$\langle \delta u E(u_0, \epsilon_0), v \rangle = (k^0, v)_V = \sum_{b \in B^{cr}} Dk^0_b Dv_b \text{ for all } v \in V. \quad (4.13)$$

If for a fixed $\epsilon_0$, $u_0$ solves the minimisation problem, then it necessarily is a critical point satisfying

$$\langle \delta u E(u_0; \epsilon_0), v \rangle = 0 \text{ for all } v \in V. \quad (4.14)$$

In order to apply Bifurcation theory for Banach spaces from Section 2.3 we need a map $F : V \times \mathbb{R} \to V$ and some $(u_0, \epsilon_0)$ such that $F(u_0, \epsilon_0) = 0$. We thus recast (4.14) in this way using the Riesz map $R : V^* \to V$ as described in (4.13). That is, we define

$$F := R \circ \delta u E \quad (4.15)$$

in particular since $\delta u E : V \times \mathbb{R} \to V^*$. We now proceed with the following proposition.

**Proposition 4.3.1.** At $(u_0, \epsilon_0) \in V \times \mathbb{R}$, the map $F$ defined in (4.15) has Fréchet derivatives $F^0_v = F_v(u_0, \epsilon_0)$ and $F^0_{\epsilon} = F_{\epsilon}(u_0, \epsilon_0)$ given by

$$F^0_v = R \circ \delta u^2 E(u_0, \epsilon_0) \quad (4.16)$$

and

$$F^0_{\epsilon} = R \circ G, \quad (4.17)$$
where $G : \mathbb{R} \to V^*$ is defined as

$$\langle G\lambda, v \rangle = \sum_{b \in B^*} \phi''(\epsilon_0 e_b + Du_{0_b})\lambda e_b Dv_b = \lambda \sum_{b \in B^*} \phi''(\epsilon_0 e_b + Du_{0_b})e_b Dv_b.$$  

Proof. We proceed in two steps.

**PART 1:** $F^0_v$.

Starting with $E(u_0; \epsilon_0)$ (fixed $\epsilon_0$), we know from Theorem 4.2.1 that

$$d^2 u E(u_0, \epsilon_0)[v, w] = \sum_{b \in B} \phi''(\epsilon_0 e_b Du_{0_b}) Dv_b Dw_b$$

and that $d^2 u E(u_0; \epsilon_0) : V \to V^*$, so

$$[R \circ \delta^2 u E(u_0, \epsilon_0)](v) \in V.$$  

The claim in (4.16) can be shown by considering

$$F(v + h) - F(v) - F^0_v h = R \circ \delta u E(v + h) - R \circ \delta u E(v) - [R \circ \delta^2 u E(u_0, \epsilon_0)] h.$$  

The Riesz mapping is an isometric isomorphism, so in particular it is additive, so the result is by true by Theorem 3.2.1.

**PART 2:** $F^0_\epsilon$.

For a fixed $u_0 \in V$, this is in principle a map $F^0_\epsilon : \mathbb{R} \to V$ and it satisfies

$$F(u_0, \epsilon + \lambda) - F(u_0, \epsilon) - F^0_\epsilon \lambda = o(\lambda). \quad (4.18)$$  

Mimicking the argument in Part 1, we again neglect $R$ and to confirm the claim just work with

$$\sum_{b \in B^*} \phi'(\epsilon_0 + \lambda) e_b Du_{0_b} Dv_b - \sum_{b \in B^*} \phi'(\epsilon_0 e_b + Du_{0_b}) Dv_b - \sum_{b \in B^*} \phi''(\epsilon_0 e_b + Du_{0_b})\lambda e_b Dv_b$$

Using Taylor expansion we can readily conclude that this can be bounded by a term of the form $C\lambda^2$, which is enough to say that it is of order $o(\lambda)$, hence proving (4.17).

**Remark 4.3.1.** As mentioned in Section 2.3 we can identify $F^0_\epsilon$ with an element of $v_s \in V$ via the fact that $F^0_\epsilon \lambda = \lambda v_s$ for all $\lambda \in \mathbb{R}$. Due to Riesz Representation Theorem we identify $F^0_\epsilon$ with $v_s \in V$ such that

$$\sum_{b \in B^*} \phi''(\epsilon_0 e_b + Du_{0_b}) e_b Dv_b = (v_s, v)_V \quad \text{for all } v \in V.$$  

So whenever we write $F^0_\epsilon$ we mean $v_s$. 

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With $F$ and its derivatives explicitly stated, we proceed with a proposition.

**Proposition 4.3.2.** For $\epsilon$ sufficiently small, there exists a unique corrector $u(\epsilon) \in V$, which minimises the energy difference functional $E$ given by (4.1).

**Proof.** It is trivial to see that $(u_0, \epsilon_0) = (0, 0) \in V \times \mathbb{R}$ is one possible choice to kick-start bifurcation analysis, as $F(0, 0) = 0$, which in particular due to the definition of $F$ ensures that $u_0$ is a minimiser of $E$. Thanks to $\phi''(0) \neq 0$, $F^0_v : V \to V$ is an isomorphism: for $v$ fixed, we can identify it with $k_v$ via

$$\langle d^2_{\epsilon}E(u_0, \epsilon_0)v, w \rangle = (Dk_v, Dw)_{B^c_r} \text{ for all } w \in V,$$

which at $(0, 0)$ means

$$\sum_{b \in B^{c_r}} \phi''(0) Dw_b Dw_b = \sum_{b \in B^{c_r}} Dk_v Dw_b$$

Thus we have $Dk_v = \frac{1}{\phi'(0)} Dw_b$ for all $b \in B^{c_r}$, thus establishing $F^0_v$ as an isomorphism. Hence Implicit Function Theorem (Theorem 2.3.1) implies that there exists $\epsilon_1 > 0$ such that for any $\epsilon \leq \epsilon_1$, we have unique $u(\epsilon)$ such that $F(u(\epsilon), \epsilon) = 0$.  

**Remark 4.3.2.** It is interesting to note that while in the screw dislocation case the existence of a minimiser is very difficult to establish and has only been proven under restrictive assumptions, in the crack case it arises naturally from the bifurcation analysis.

The central aim of the analysis is to describe what happens at $\epsilon_1$ and the corresponding $u_1$. Here many things can potentially happen and it largely remains a problem to be solved.

As a gentle step towards describing the bifurcation point, let us briefly discuss the possibility that at $\epsilon_1$ we have a simple fold point.

Recalling discussion in Section 2.3, we assume that $(u_1, \epsilon_1)$ is a simple fold point and translate the machinery to the current setting. Since $(u_1, \epsilon_1) \in S$ (as defined in (2.19)), $F(u_1, \epsilon_1) = 0$, which means

$$\sum_{b \in B^{c_r}} \phi'(\epsilon_1 e_b + Du_{1_b}) Dw_b = 0 \text{ for all } w \in V. \quad (4.19)$$

Furthermore, since at $(u_1, \epsilon_1)$ the mapping $F^1_v : V \to V$ ceases to be an isomorphism, we have $F^1_v \gamma_0 = 0$ (where $\gamma_0$ as in (2.20)), which means

$$\sum_{b \in B^{c_r}} \phi''(\epsilon_1 e_b + Du_{1_b}) D\gamma_0 Dw_b = 0 \text{ for all } w \in V.$$
A defining property for the occurrence of a fold point is the fact that $F_1^1$ is not orthogonal to $\gamma_0$. For now let us assume for simplicity that in fact it is a multiple of it, i.e. that $F_1^1 = C \gamma_0$. Thus we have

$$\sum_{b \in B^r} \phi''(\epsilon_1 e_b + Du_{1_b})Dv_{s_b}Dw_b = 0 \quad \text{for all } w \in V, \quad (4.20)$$

where $v_s$ is such that

$$(v_s, w)_V = \sum_{b \in B^r} Dv_{s_b}Dw_b = \sum_{b \in B^r} \phi''(\epsilon_1 e_b + Du_{1_b})e_bDw_b.$$

Hence the general aim is to establish conditions which allow (4.19) and (4.20) to hold at the same time.

This, as well a similar treatment of other possible bifurcation points will be subject to further study.
Chapter 5

Conclusions

The purpose of this work was to present the mathematical theory behind a class of atomistic models for defects in crystals, with a particular focus on theoretical treatment of the anti-plane screw dislocation model and the anti-plane shear mode of crack model.

The essence of this approach was introduced in Chapter 2, where we first described how lattice domains can be used in atomistic modelling and how we can obtain discrete analogues of minimisation problems known from PDE theory. In Chapter 3 a detailed account of the theory for an anti-plane screw dislocation was given and the crucial results concerning well-definedness and decay estimates were proven. In the final chapter, which constitutes the novelty of this work, we extended this theory to the case of a crack, primarily focusing on proving that the model is well-defined and on the treatment of the arising bifurcation problem.

5.1 Further work

As mentioned in the Introduction, this MSc thesis leads on to a PhD research project, which will be centred around the ideas introduced in this report. In particular, we plan to investigate the following.

**Decay estimates for the crack model.** The aim is to translate the decay estimate result for a screw dislocation (cf. Section 3.3). A variant of the argument from [6] used for edge dislocation can be applied in the part of the domain away from the crack. Near the crack, in a cone with apex at the origin, this approach fails and we have to consider a discrete analogue of the so-called surface Green’s function (cf. [13]). To the best of our knowledge, there are no rigorous results on decay estimates for surface Green’s function.
**Full bifurcation analysis for the crack model.** The bifurcation analysis in Section 4.3 provides background information, which we aim to apply to fully describe the bifurcation phenomena in the crack model. In particular, we hope to find conditions on $\phi$, for which a given instance of a bifurcation point can/cannot occur. In a broader sense, this analysis should result in a full understanding of the crack model for any $\epsilon \in \mathbb{R}$ in the definition of the far-field predictor $\hat{u}$ in (4.6).

**Removing assumptions of symmetry from the analysis.** For both the decay estimates for a screw dislocation (Theorem 3.3.1) and the well-definedness proof for a crack model (Theorem 4.2.1), we assume that $\phi'''(0) = 0$, which is reasonable as long as we consider an anti-plane displacement, which is a highly symmetric setting. Breaking this symmetry, for example by applying a macroscopic shear, yields a tilted potential, where $\phi'''(0) \neq 0$, which means the arguments used in these theorems are no longer valid. The broad aim is thus to try to increase the generality of the analysis by removing symmetry. In particular, we also lose the symmetry when we consider in-plane modes of crack.

**Computational aspects of molecular modelling.** A broad aim is to also include simulations in the analysis, with the particular focus on the numerical treatment of bifurcations in the crack model. This will require the extension of a implementation of code accommodating the case of a crack, building from pre-existing code in the programming language Julia [1] in the Lujia-Light library [19].

**Further extensions.** In the crack model we implicitly make a very limiting assumption, namely that all bonds on the opposite sides of the cut disappear. In reality, however, bonds close to the tip do not immediately snap, but rather remain in place with an increased strain applied to them. Introducing this idea to the model drastically alters the analysis but has the benefit that it would allows us to consider our model in the context of Transition State Theory (see [7] and [23] for a classical introduction).

Furthermore, a direct calculation in Remark 4.2.1 seems to imply that an alternative, simpler construction of the far-field predictor $\hat{u}$ for the crack model is also a feasible option. Such a predictor, considered classical (cf [17]), does not introduce the $r^{-1/2}$ term. It is of interest to describe this case in detail.
Bibliography


Appendix A

Proof of Proposition 4.2.2

The argument in [20, Proposition 12(ii)] proves the result for the case of a homogeneous set of bonds $\mathcal{B}$. In that setting, the proof follows directly from [21, Theorem 2.2]. For $\mathcal{B}^\tau$, we modify the argument. We distinguish two cases, depending on where $l$ is located on $\Gamma$.

Case 1: Let $l \in \Gamma$ be of the form $l = (\xi_1, 0)$, where $\xi_1 \neq 0$. We consider a sequence of squares $(Q_i)_{i=0}^N \subset \Omega$ (recall the definition of $\Omega$ in (3.28)) aligned in the direction $0-l$ (which is possible due to the assumption on $l$) and defined as follows. $Q_0$ and $Q_N$ are unit squares corresponding to sites 0 and $l$, defined in such a way that 0 (respectively $l$) is the midpoint of the side of $Q_0$ (resp. $Q_N$) which belongs to $\Gamma = \partial \Omega$. The squares $Q_1, \ldots, Q_{N-1}$ are defined to fill the space between 0 and $l$ in such a way that they have disjoint interiors and are such that their side-lengths differ by at most a factor of 2, with one side of the smaller square contained in one side of the larger square. It is easy to see that there is at most $N \leq C_1(2 + \log |l|)$ squares in the sequence. See Figure A.1. For any two neighbouring squares $Q_j, Q_{j+1}$

![Figure A.1](image_url)

Figure A.1: An example of construction of squares. The red dot represents the origin, the green dot a site in Case 1, the brown dot a site in Case 2, the yellow dot is $k$ and the white dot is $m$. 44
it follows from a special case of \[12, \text{Lemma 2}\] that
\[
|Q_{j+1} - Q_j| \leq C_2 \|\nabla v\|_{L^2(\Omega)} = C_2 \|Dv\|_{C(\mathcal{B}^*)}, \tag{A.1}
\]
where
\[
(v)_{Q_j} := \frac{1}{|Q_j|} \int_{Q_j} v(x) \, dx.
\]

The equality on the right-hand side comes from the fact that \(v \in \dot{H}^1\) is identified with its piecewise linear interpolant (cf. discussion preceding (4.8)). As a result
\[
|\left(\frac{u}{Q_N} \right) - (u)_{Q_0}| \leq \sum_{j=1}^N \left| (u)_{Q_j} - (u)_{Q_{j-1}} \right| \tag{A.2}
\]
\[
\leq \sum_{j=1}^N C_2 \|\nabla v\|_{L^2(\Omega)} = N C_2 \|\nabla v\|_{L^2(\Omega)} \leq C_3 (2 + \log |l|) \|\nabla v\|_{L^2(\Omega)},
\]
where \(C_3 = C_1 C_2\).

Furthermore, it is a basic calculus fact that
\[
|\left(\frac{v}{Q_0} \right) - v(0)| \leq \|\nabla v\|_{L^\infty(Q_0)} \quad \text{and} \quad |v(l) - \left(\frac{v}{Q_N} \right)| \leq \|\nabla v\|_{L^\infty(Q_N)} \tag{A.3}
\]
and since on each \(Q_i\), the piecewise linear interpolant \(v\) belongs to a finite-dimensional space, we obtain
\[
\|\nabla v\|_{L^\infty(Q_i)} \leq C_4 \|\nabla v\|_{L^2(Q_i)} \leq C_4 \|\nabla v\|_{L^2(\Omega)} = C_4 \|Dv\|_{C(\mathcal{B}^*)}, \tag{A.4}
\]
where the first inequality follows from the equivalence of norms for finite-dimensional spaces and the second from extending the domain from \(Q_i\) to the whole of \(\Omega\).

With (A.2) and (A.3)-(A.4) in hand, we obtain
\[
|v(l) - v(0)| \leq |v(l) - (v)_{Q_N}| + |(v)_{Q_N} - (v)_{Q_0}| + |(v)_{Q_0} - v(0)| \tag{A.5}
\]
\[
\leq C(1 + \log |l|) \|Dv\|_{C(\mathcal{B}^*)},
\]
which concludes the proof for \(l \in \Gamma\) of the form \((\xi, 0)\).

\textbf{Case 2:} Let \(l \in \Gamma\) be of the form \(l = (\xi_1, \xi_2)\) where \(\xi_1 \neq 0\) and \(\xi_2 \neq 0\), which informally means that \(l\) is on the other side of the crack from the origin and it deems the previous argument invalid, as we can no longer define the sequence of squares aligned with 0-\(l\) which will be a subset of \(\Omega\). Thus we proceed in two 'jumps'. By
defining \( k = a_1 \) and \( m = a_2 \) (recall (2.1)) conclude that

\[
|v(l) - v(0)| \leq |v(l) - v(m)| + |v(m) - v(k)| + |v(k) - v(0)| \\
\leq C \|Dv\|_{\ell^2(B^{cr})}((1 + \log |l - m|) + 1 + \log |m - k| + 1 + \log |k|) \\
\lesssim \|Dv\|_{\ell^2(B^{cr})}(1 + \log |l|),
\]

where the second inequality follows from applying (A.5) three times, in particular because the alignment of \( l - m, m - k \) and \( k - 0 \) allows us to define sequences of squares needed to establish (A.5). The last inequality follows from the fact that both \( k \) and \( m \) are fixed.