GEOMETRY EQUILIBRATION OF CRYSTALLINE DEFECTS IN QUANTUM AND ATOMISTIC DESCRIPTIONS

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Abstract. We develop a rigorous framework for modelling the geometry equilibration of crystalline defects. We formulate the equilibration of crystal defects as a variational problem on a discrete energy space and establish qualitatively sharp far-field decay estimates for the equilibrium configuration. This work extends [13] by admitting infinite-range interaction which in particular includes some quantum chemistry based interatomic interactions.

1. Introduction

The study of crystalline defects is one of the primary tasks in material modelling. Even small defect concentrations can have a major influence on key physical and chemical properties of materials. Two of the most common and important classes are point defects and dislocations.

In computational simulations of defects, a small finite domain is employed, while the far-field behaviour is described via an artificial boundary condition. Different approaches (see, e.g. [35, Ch. 6]) include cluster calculations, where a cluster containing the defect is defined with clamped boundary conditions; supercell methods, where the system is confined to a large box with periodic boundary conditions; and embedded cluster methods, which attempt to remedy some of the deficiencies of the other two methods by embedding the cluster in a simpler representation of the surrounding lattice (for example, if the cluster is described quantum mechanically, the embedding region may use interatomic potentials; if the cluster is simulated by interatomic potentials, the embedding region may use continuum models).

The literature devoted to assessing the accuracy and in particular the cell size effects of such simulations is relatively sparse; see e.g. [1, 2, 19, 25] and references therein for a representative sample. In particular, we refer to [13] for an extensive study of this problem, which develops a rigorous framework within which the accuracy of different boundary conditions can be precisely assessed. A key restriction of [13] is the assumption that each atom only interacts with a finite range neighbourhood. This assumption is in particular not satisfied for electronic structure models. The aim of the present work is to extend the rigorous analysis to such cases where interaction has infinite-range, though we will require some control on the rate of decay of interaction at infinity. Important models satisfying our assumptions include Lennard-Jones, Thomas–Fermi–von Weizsäcker and tight binding.

In the mathematics literature, considerable progress has been made on studying electronic ground states corresponding to local defects in crystals e.g. [3, 4, 5]. Much less is understood about the related geometry optimisation (or, lattice relaxation) problem [21, 13, 29], but in particular the coupling between electronic and geometry relaxation is essentially open. The present work addresses this coupling and establishes some key

2000 Mathematics Subject Classification. 65L20, 65L70, 70C20, 74G40, 74G65.

Key words and phrases. crystal lattices, defects, dislocations, regularity, error estimates, convergence rates.
results: we give general conditions under which the geometry relaxation problem can be formulated as a variational problem on a Hilbert space, and we establish sharp rates of decay of the discrete equilibrium configurations.

The main results of this paper are presented in Sections 3.2 and 3.3, including the formulation of equilibration as a variational problem and the generic decay estimate:

\[ |D\bar{u}(\ell)| \leq C(1 + |\ell|)^{-d} \log^2(2 + |\ell|), \]

(1.1)

where \( \bar{u} \) is the equilibrium corrector displacement, \( Du(\ell) \) is the finite-difference stencil defined in Section 1, \( d \) is the dimension, \( t = 0 \) for point defects and \( t = 1 \) for dislocations.

The results have a range of consequences, for example: (1) present a mathematical model for a defect in an atomistic description of a crystalline solid, which is an ideal benchmark problem for computational multi-scale methods, but can also be used as a building block for the analytical coarse-graining of material models; (2) provide a foundation for the analysis of boundary conditions for defect core simulations; and (3) allow us to perform rigorous error estimates for QM/MM coupling methods [10, 11]. We remark that the QM/MM coupling constructions and analysis described in [10] can be applied verbatim to electronic structure satisfying the locality properties in Section 2.2, such as tight binding and TFW (see Section 4).

1.1. Outline. In Section 2 we formulate lattice relaxation as a variational problem: we specify the reference configuration of a defective system and introduce the displacement and site energy formulations, construct suitable discrete function spaces that will be used in our analysis; and define the energy difference functional on which the variational formulation is based. In Section 3 we state our main results on the decay of discrete equilibrium displacement fields for point defects and dislocations. In Section 4, we show that our relaxation framework can be applied to several practical models, that are not covered by previous works. In Section 5, we make concluding remarks and discuss future perspectives. All proofs and technical details are gathered in the appendixes.

1.2. Notation. We define the following spaces with dimension \( d \) and index \( k \)

\[ \mathcal{L}_{k,d} := \{ w \in L^1([0, \infty)), \|w\|_{\mathcal{L}_{k,d}} := \int_0^\infty x^{k+d-1}w(x)\,dx < \infty, \]

\[ w > 0 \text{ and is a monotonically decreasing function} \} \quad \text{and} \]

\[ \mathcal{L}^{\log}_{k,d} := \{ w \in \mathcal{L}_{k,d}, \|w\|_{\mathcal{L}^{\log}_{k,d}} := \int_0^\infty x^{k+d-1}\log^2(1+x)w(x)\,dx < \infty \}. \]

(1.2)

(1.3)

For example, we have \((1 + x)^{-k-d-x} \in \mathcal{L}_{k,d} \cap \mathcal{L}^{\log}_{k,d}\) for all \( \varepsilon > 0 \); and \( e^{-\alpha x} \in \mathcal{L}_{k,d} \cap \mathcal{L}^{\log}_{k,d}\) for all \( \alpha > 0 \) and index \( k > 0 \). Whenever it is clear, we will omit the dimension \( d \) and write \( \mathcal{L}_k = \mathcal{L}_{k,d}, \mathcal{L}_k^{\log} = \mathcal{L}^{\log}_{k,d} \).

The symbol \( \langle \cdot, \cdot \rangle \) denotes an abstract duality pairing between a Banach space and its dual. The symbol \( \| \cdot \| \) normally denotes the Euclidean or Frobenius norm, while \( \| \cdot \| \) denotes an operator norm.

For a differentiable function \( f \), \( \nabla f \) denotes the Jacobi matrix and \( \nabla_r f = \nabla f \cdot r \) defines the directional derivative. For \( E \in C^2(\mathcal{X}) \), the first and second variations are denoted by \( \langle \delta E(u), v \rangle \) and \( \langle \delta^2 E(u)w, v \rangle \) for \( u, v, w \in \mathcal{X} \). For higher variations of \( E \in C^j(\mathcal{X}) \), we will use the notation \( \langle \delta^j E(u), v \rangle \) with \( v = (v_1, \ldots, v_j) \).

Throughout the article we use the following notation, that for \( b \in A \), we denote \( A \setminus b = A \setminus \{b\} \) and \( A - b = \{a - b | a \in A \setminus b\} \).

The symbol \( C \) denotes a generic positive constant that may change from one line to the next. When estimating rates of decay or convergence, \( C \) will always remain independent.
of the system size, lattice position or the choice of test functions. The dependence of $C$ on model parameters will normally be clear from the context or stated explicitly.

1.3. List of assumptions and symbols. Our analysis requires a number of assumptions on the model or the underlying atomistic geometry. We list these with page references and brief summaries. We also list the symbols that are most frequently used in the paper.

| Symbol | Page | Description |
|--------|------|-------------|
| (RC)   | 3    | assumptions for reference configurations |
| (S)    | 5    | assumptions for site strain potential |
| (H)    | 8    | assumptions for homogeneous lattices |
| (LS)   | 9    | assumptions for lattice stability |
| (P)    | 9    | assumptions for point defects |
| (D)    | 11   | assumptions for dislocations |
| $\mathcal{L}_{k,d}$ | 2 | spaces for weight functions |
| $\mathcal{L}^\log_{k,d}$ | 2 | |
| $\Lambda, \Lambda^h, \Lambda^*_h$ | 3, 4 | reference configuration |
| $D, \bar{D}$ | 3, 44 | finite difference and elastic strain (permuted finite-diff.) |
| $\|D\cdot\|_{\ell_p}^\per$ | 4 | norm over nearest neighbour bonds |
| $\mathcal{W}^{1,2}, \mathcal{W}^c$ | 4 | energy space, compact displacements |
| $\mathcal{A}^p, \mathcal{A}^c$ | 4 | spaces of admissible configurations |
| $\mathcal{V}, \mathcal{V}^\ell, \Phi, \Phi^\ell$ | 5, 11 | site strain potential and site energy |
| $\|D\cdot\|_{\ell_p}^\per$ | 5 | norm with weighted stencils |
| $I^h_1, I^h_2, I^d$ | 7, 8 | energy difference functionals |
| $S, S_0, S^*$ | 44 | slip operators |
| $e$ | 44 | elastic strain, predictor configuration |

2. Preliminaries

2.1. Reference and deformed configuration. We consider a single defect embedded in a homogeneous crystalline bulk. Let $d \in \{2,3\}$ denote the dimension of the reference configuration, $A \in \mathbb{R}^{d \times d}$ be a nonsingular matrix, then we define a homogeneous crystal reference configuration by the Bravais lattice $\Lambda^h := A\mathbb{Z}^d$. It is also convenient to define $\Lambda^h_0 = \Lambda^h \setminus 0 = \Lambda^h - 0$, which satisfies $\Lambda^h_\ell = \Lambda^h - \ell$ for all $\ell \in \Lambda^h$.

The reference configuration for the defect is a set $\Lambda \subset \mathbb{R}^d$ satisfying

$$(RC) \quad \exists R_{\text{def}} > 0, \text{ such that } \Lambda \setminus B_{R_{\text{def}}} = \Lambda^h \setminus B_{R_{\text{def}}} \text{ and } \Lambda \cap B_{R_{\text{def}}} \text{ is finite.}$$

Clearly, choosing $\Lambda = \Lambda^h$ satisfies (RC).

For any $\ell \in \Lambda$, we define the set of its nearest neighbours:

$$\mathcal{N}(\ell) := \left\{ m \in \Lambda \setminus \ell \ \big| \ \exists x \in \mathbb{R}^d \text{ s.t. } |x - \ell| = |x - m| \leq |x - k| \ \forall k \in \Lambda \right\}. \quad (2.1)$$

We remark that for $\Lambda = \Lambda^h = A\mathbb{Z}^d$ and $\ell \in \Lambda$,

$$\mathcal{N}(\ell) \supseteq \{ \ell \pm Ae_i \} \quad \text{with} \quad 1 \leq i \leq d \quad (2.2)$$

When the matrix $A$ is well chosen (there are infinitely many matrices $A$ such that $\Lambda = A\mathbb{Z}^d$). Throughout this paper, we will assume that the matrix $A$ is chosen such that (2.2) is satisfied.

Let $d_s \in \{2,3\}$ denote the physical dimension of the system, then for $u : \Lambda \to \mathbb{R}^{d_s}$ and $\ell \in \Lambda$, $\rho \in \Lambda - \ell$, we define the finite-difference

$$D_\rho u(\ell) := u(\ell + \rho) - u(\ell) \quad (2.3)$$
and $Du(\ell) := \{D_\rho u(\ell)\}_{\rho \in \Lambda - \ell}$. We consider $Du(\ell) \in (\mathbb{R}^d)^{\Lambda - \ell}$ to be a finite-difference stencil with infinite range. For a stencil $Du(\ell)$, we define the norms

$$
|Du(\ell)|_N := \left( \sum_{\rho \in N(\ell) - \ell} |D_\rho u(\ell)|^2 \right)^{1/2}, 
\|Du\|_{\ell^2(\Lambda)} := \left( \sum_{\ell \in \Lambda} |Du(\ell)|_{\ell^2(\Lambda)}^2 \right)^{1/2},
$$

and the corresponding functional space of finite-energy displacements

$$
\mathcal{W}^{1,2}(\Lambda; \mathbb{R}^d) := \{ u : \Lambda \rightarrow \mathbb{R}^d \mid \|Du\|_{\ell^2(\Lambda)} < \infty \}.
$$

We also require the following subspace of compact displacements

$$
\mathcal{W}^c(\Lambda; \mathbb{R}^d) := \{ u : \Lambda \rightarrow \mathbb{R}^d \mid \exists R > 0 \text{ s.t. } u = \text{const in } \Lambda \setminus B_R(0) \}.
$$

As we consider $d_s \in \{2, 3\}$ to be fixed, we simply denote $\mathcal{W}^{1,2}(\Lambda; \mathbb{R}^{d_s})$ and $\mathcal{W}^c(\Lambda; \mathbb{R}^{d_s})$ by $\mathcal{W}^{1,2}(\Lambda)$ and $\mathcal{W}^c(\Lambda)$, respectively, from this point onwards. The next lemma follows directly from [30, Proposition 9].

**Lemma 2.1.** If (RC) is satisfied, then $\mathcal{W}^{1,2}(\Lambda)$ is the closure of $\mathcal{W}^c(\Lambda)$ with respect to the norm $\|D \cdot \|_{\ell^2(\Lambda)}$.

Now let $\Lambda_0 \subset \mathbb{R}^{d_s}$ satisfy (RC) with respect to a Bravais lattice $\Lambda_0^b$ (for dislocations we consider $d_0 \neq d_s$, i.e. $\Lambda \neq \Lambda_0$), then define $x : \Lambda_0 \rightarrow \mathbb{R}^{d_s}$ by $x(\ell) = \ell$ and $u_0 : \Lambda_0 \rightarrow \mathbb{R}^{d_s}$ to be a fixed predictor prescribing the far-field boundary conditions and let $y_0 := x + u_0$ denote the corresponding deformation predictor of the atomic or nuclear configuration. In general, we decompose a deformation $y$ into the predictor $y_0$ and a displacement corrector $u$ satisfying $y = y_0 + u$. For systems with point defects or straight line dislocations, the appropriate predictors $u_0$ will be, respectively, specified in Sections 3.2 and 3.3.

### 2.2. Site strain potential

In order to state our assumptions on the the model, we require the following spaces of admissible atomic or nuclear arrangements. For $m, \lambda > 0$, we first define

$$
\mathcal{A}_{m,\lambda}^0(\Lambda_0) := \left\{ y : \Lambda_0 \rightarrow \mathbb{R}^{d_s} \mid B_\lambda(x) \cap y(\Lambda_0) \neq \emptyset \quad \forall x \in \mathbb{R}^{d_s}, \right. \\
\left. \quad |y(\ell) - y(m)| \geq m|\ell - m| \quad \forall \ell, m \in \Lambda_0 \right\},
$$

and

$$
\mathcal{A}^0(\Lambda_0) := \bigcup_{m > 0} \bigcup_{\lambda > 0} \mathcal{A}_{m,\lambda}^0(\Lambda_0).
$$

Analysis requires that the predictor $y_0 \in \mathcal{A}^0(\Lambda_0)$, and we ensure this for the predictors constructed in Sections 3.1–3.3; see in particular Lemma F.1.

The parameter $\lambda > 0$ ensures that there are no large regions that are devoid of nuclei. We require the constraint $\lambda < \infty$ for the definition of the TFW site energy, see Section 4.4. The condition $m > 0$ prevents the accumulation of atoms which is necessary for many interatomic interactions, including Lennard–Jones, TFW and tight binding, to define the site energies; see Sections 4.1, 4.3 and 4.4.

Using $\mathcal{A}^0(\Lambda_0)$, we define the space of admissible configurations $\mathcal{A}(\Lambda)$ for point defects and dislocations.

For point defects, we consider $\Lambda = \Lambda_0$, $\Lambda^b = \Lambda_0^b$, $d = d_s \in \{2, 3\}$ and define the admissible space of arrangements to be $\mathcal{A}(\Lambda) = \mathcal{A}^0(\Lambda)$.

To model dislocations, we consider $d = 2$, $d_s = 3$ and let $\Lambda_0 \subset \mathbb{R}^3$ be a Bravais lattice. We consider configurations $y \in \mathcal{A}^0(\Lambda_0)$ that are periodic in the $e_3$-direction. As a result,
we can project \( \Lambda_0 \) onto the plane \( \{ x_3 = 0 \} \) to obtain a Bravais lattice \( \Lambda = \Lambda^h \subset \mathbb{R}^2 \) and also define the projected configuration \( \tilde{y} : \Lambda \rightarrow \mathbb{R}^3 \) via the relation: for all \( \ell = (\ell_1, \ell_2, \ell_3) \in \Lambda_0, \)
\[
y(\ell) = \tilde{y}(\ell_1, \ell_2) + (0, 0, \ell_3). \tag{2.8}
\]

It is convenient to identify \( y \in A^0(\Lambda_0) \) with \( \tilde{y} \), hence we define the admissible space
\[
A(\Lambda) := \left\{ \tilde{y} : \Lambda \rightarrow \mathbb{R}^3 \mid y \text{ given by (2.8) satisfies } y \in A^0(\Lambda_0) \right\}. \tag{2.9}
\]

Let \( \tilde{y}_0 \in A(\Lambda) \) correspond to \( y_0 \in A^0(\Lambda_0) \) and define \( \tilde{u}_0 : \Lambda \rightarrow \mathbb{R}^3 \) by \( \tilde{u}_0(\ell) = \tilde{y}_0(\ell) - \ell \).

We commit a minor abuse of notation by subsequently denoting \( \tilde{y}_0 \) and \( \tilde{u}_0 \) by \( y_0 \) and \( u_0 \), unless specified otherwise. The modelling of dislocations is discussed further in Section 3.3.

It is also convenient to introduce the following spaces, which represent displacements corresponding to a subset of \( A(\Lambda) \):
\[
\mathcal{H}(\Lambda) := \left\{ u \in \mathcal{W}^{1,2}(\Lambda) \mid y_0 + u \in A(\Lambda) \right\}, \quad \text{and}
\]
\[
\mathcal{C}(\Lambda) := \left\{ u \in \mathcal{W}^{c}(\Lambda) \mid y_0 + u \in A(\Lambda) \right\}. \tag{2.10}
\]

We also define \( \mathcal{H}_{m,\lambda}(\Lambda) \) analogously using \( A_{m,\lambda}(\Lambda) \). We also note that as \( y_0 \in A(\Lambda) \), it follows that
\[
\mathcal{H}(\Lambda) = \left\{ u \in \mathcal{W}^{1,2}(\Lambda) \mid |(y_0 + u)(\ell) - (y_0 + u)(m)| \neq 0 \quad \forall \ell, m \in \Lambda \right\},
\]

hence it is a suitably rich space to pose our variational problem.

The following result is a consequence of Lemma 2.1, whose proof is given in Appendix C.1.

**Lemma 2.2.** If (RC) is satisfied, then \( \mathcal{H}(\Lambda) \) is dense in \( \mathcal{H}(\Lambda) \) with respect to the norm \( \| D \cdot \|_{L^2(\Lambda)} \).

Given \( \ell, m \in \Lambda \), we denote \( r_{\ell m}(y) = |y(\ell) - y(m)| \). When it is clear from the context, we simply denote \( r_{\ell m} \) by \( r_{\ell m}(y) \). Let \( \ell \in \Lambda \) with \( \Lambda \) satisfying (RC), then for a collection of mappings \( V_\ell : \text{Dom}(V_\ell) \rightarrow \mathbb{R} \) with
\[
\text{Dom}(V_\ell) := \left\{ D(u_0 + u)(\ell) \mid x + u_0 + u \in A(\Lambda) \right\}, \tag{2.11}
\]
we call them **site strain potentials** if the following assumptions (S) are satisfied. In the following, we consider \( u \) such that \( y_0 + u \in \mathcal{A}_{m,\lambda}(\Lambda) \) with \( m, \lambda > 0 \).

**(S.R) Regularity:** For all \( \ell \in \Lambda \), \( V_\ell(Du(\ell)) \) possess partial derivatives up to \( n \)-th order, where \( n \geq 3 \) for point defects and \( n \geq 4 \) for dislocations. We denote the partial derivatives by \( V_{\ell,\rho}(Du(\ell)) \) with \( \rho = (\rho_1, \cdots, \rho_j) \in (\Lambda - \ell)^j \), \( j = 1, \cdots, n \) and
\[
V_{\rho}(g) := \frac{\partial^j V(g)}{\partial g_{\rho_1} \cdots \partial g_{\rho_j}} \quad \text{for} \quad g \in (\mathbb{R})^{\Lambda - \ell}. \tag{2.12}
\]

**(S.L) Locality:** For \( j = 1, \cdots, n \), there exist constants \( C_j = C_j(m, \lambda) > 0 \) and \( w_j : \mathbb{R}_{\geq 0} \rightarrow \mathbb{R}_{\geq 0} \) independent of \( y, m, \lambda \), such that
\[
|V_{\ell,\rho}(Du(\ell))| \leq C_j \sum_{\{A_1, \cdots, A_k\} \in \mathcal{P}(j)} \left( \prod_{1 \leq i \leq k} w_{|A_i|}(|\rho_{\ell_i}|) \prod_{m \in A_i} \delta_{\rho_{\ell_i}, \rho_m} \right) \tag{2.13}
\]
\[
\forall \ell \in \Lambda, \quad \rho = (\rho_1, \cdots, \rho_j) \in (\Lambda - \ell)^j,
\]
where \( \mathbf{w}_j \in \mathcal{L}_j \) for the homogeneous lattice and point defects, \( \mathbf{w}_j \in \mathcal{L}^{\log}_{j+2} \) for dislocations, and
\[
P(j) := \{ \mathcal{A} = \{ A_1, \ldots, A_k \} : \mathcal{A} \text{ is a partition of } \{ n_1, \ldots, n_j \} \},
\]
(2.14)
\(|A_i|\) denotes the cardinality of the subset \( A_i \), \( i' \) is the smallest element in \( A_i \).

**(S.H)** Homogeneity: There exist \( V^h_i \) on the host homogeneous lattice \( \Lambda^h = AZ^d \), satisfying the assumptions (S.L) and (S.R) with \( \Lambda^h \) replacing \( \Lambda \). Moreover, there exists \( s > d/2 \) and \( \mathbf{w}_1 \in \mathcal{L}_1 \) such that if \( y_1 \in \mathcal{A}_{m,\lambda}(\Lambda) \), \( y_2 \in \mathcal{A}_{m,\lambda}(\Lambda^h) \) and for any \( \ell_1 \in \Lambda \), \( \ell_2 \in \Lambda^h \) and \( r > 0 \) satisfying
\[
\{ y_1(n_1) - y_1(\ell_1) \mid n_1 \in \Lambda, \ r_{\ell_1 n_1}(y_1) \leq r \} = \{ y_2(n_2) - y_2(\ell_2) \mid n_2 \in \Lambda^h, \ r_{\ell_2 n_2}(y_2) \leq r \}
\]
(2.15)
(see Figure 1), there exist \( C_h = C_h(m, \lambda) \) such that for \( u_i = y_i - x \ (i = 1, 2) \) and any \( n_1 \in \Lambda \setminus \ell_1 \) satisfying \( r_{\ell_1 n_1}(y_1) \leq r \), we have
\[
|V_{\ell_1 n_1 \ell_1}(Du_1(\ell_1)) - V^h_{\ell_2 n_2 \ell_2}(Du_2(\ell_2))| \leq C_h(1 + r)^{-s}\mathbf{w}_1(|\ell_1 - n_1|),
\]
(2.16)
where \( n_2 \) is the unique element of \( \Lambda^h \setminus \ell' \) satisfying \( y_1(n_1) - y_1(\ell_1) = y_2(n_2) - y_2(\ell_2) \).

**(S.PS)** Point symmetry: The homogeneous site strain potential \( V^h_i \) given in (S.H) satisfies
\[
V^h_i((-g_{-p})_{p \in \Lambda^h}) = V^h_i(g) \quad \forall g \in (\mathbb{R}^d)^{\Lambda^h}.
\]
(2.17)

**Figure 1.** A diagram representing the assumption (2.15) appearing in (S.H).

**Remark 2.3.** We require stronger locality estimates are for the analysis of dislocations, hence in (S.L) we assume \( \mathbf{w}_i \in \mathcal{L}^{\log}_{i+2} \) as opposed to \( \mathbf{w}_i \in \mathcal{L}_i \) for point defects. The reason for this additional requirement is shown in detail in Sections 3.1–3.3.

We now give examples of (2.13) when \( j \in \{1, 2\} \):
\[
|V_{\ell, p}(Du(\ell))| \leq C_1\mathbf{w}_1(|\rho|),
\]
\[
|V_{\ell, p, \rho}(Du(\ell))| \leq C_2\mathbf{w}_1(|\rho|)\mathbf{w}_1(|\varsigma|) \quad \text{with } \rho \neq \varsigma, \quad \text{and}
\]
\[
|V_{\ell, p, \rho}(Du(\ell))| \leq C_2(\mathbf{w}_1(|\rho|)^2 + \mathbf{w}_2(|\rho|)),
\]
where \( \mathbf{w}_i \in \mathcal{L}_i \) for point defects and \( \mathbf{w}_i \in \mathcal{L}^{\log}_{i+2} \) for dislocations, for \( i \in \{1, 2, 3\} \).
Remark 2.4. The homogeneity assumption (S.H) will only be necessary in the analysis of point defects, since $\Lambda \neq \Lambda^h$ in this case. In the dislocation case, we have $\Lambda = \Lambda^h$, hence (S.H) is automatically satisfied.

In addition to showing (2.16) for the interaction models discussed in Section 4, it is also possible to derive an additional homogeneity estimate: suppose that $y_1, y_2 \in \mathcal{A}(\Lambda)$ satisfy $y_1(\ell) = y_2(\ell)$ for all $\ell \in \Lambda \setminus B_{R_{\text{def}}}$, then for $u_i = y_i - x$ ($i = 1, 2$), we have

$$|V(\ell)(Du_1(\ell)) - V(\ell)(Du_2(\ell))| \leq C \tilde{w}_h(\gamma r), \quad \text{for all } \Lambda \setminus B_{R_{\text{def}}} \text{ and } 0 < r < |\ell| - R_{\text{def}}, \quad (2.18)$$

where $\tilde{w}_h : \mathbb{R}_{>0} \to \mathbb{R}_{>0}$ decays at infinity. This estimate is not required to study the relaxation problem, however, it allows us to interpret $V^h_\ell$ as the far-field limit of $V_\ell$, in the following sense: as (RC) ensures that $\Lambda \setminus B_{R_{\text{def}}} = \Lambda^h \setminus B_{R_{\text{def}}}$, from (2.18) we deduce that

$$V(\ell)(Du_1(\ell)) - V(\ell)(Du_2(\ell)) \to 0 \quad \text{as } |\ell| \to \infty.$$

Due to the periodicity of the lattice, the space $\text{Dom}(V^h_\ell)$ is independent of $\ell \in \Lambda^h$. Moreover, using $\Lambda^h - \ell = \Lambda^h$ for all $\ell \in \Lambda^h$, we have that the homogeneous site strain potential $V^h_\ell$ is independent of the site $\ell \in \Lambda^h$, hence $V^h_\ell(Du(\ell)) \equiv V(Du(\ell))$ for all $\ell \in \Lambda^h$ and $u \in \mathcal{H}(\Lambda^h)$. For convenience, we will use $V$ instead of $V^h_\ell$ to denote the homogeneous site strain potential hereafter. Then the point symmetry assumption (2.17) becomes

$$V((-g - \rho)_{\rho \in \Lambda^h}) = V(g) \quad \forall \ g \in (\mathbb{R}^d)^{\Lambda^h}. \quad \Box$$

Remark 2.5. By writing the site strain potential as a function of $Du(\ell)$, we have already assumed that the model is invariant under translations. The assumption (S.PS) can also be derived from the isometric and permutational symmetries of the model (see (S.I) and (S.P) in Section 4). These assumptions are satisfied when all atoms in the system are of the same species. We can extend the assumptions to admit multiple species of atoms, e.g. [29]. However, the generalisation will introduce notation that is significantly more complex, so we will not pursue this here. \square

We conclude by noting that (S.R) implies the following result.

Proposition 2.6. For all $\ell \in \Lambda$ and $u \in \mathcal{H}(\Lambda)$, $V_\ell(Du(\ell))$ is $(n - 1)$-times continuously differentiable with respect to $\|D \cdot \|_{L^2}$.\!

The justification of this result requires the construction of alternate norms for lattice displacements, which we introduce in Appendix A. As we show a more general result while proving Theorem 2.7 (iii) in Appendix C.2, we omit the proof of Proposition 2.6 for the sake of brevity.

2.3. The energy difference functional. Let $\Lambda$ satisfy (RC). With a given predictor $y_0 = x + u_0$, we first formally define the energy-difference functional for a displacement $u \in \mathcal{H}(\Lambda)$:

$$\mathcal{E}(u) = \sum_{\ell \in \Lambda} \left( V_\ell(Du_0(\ell) + Du(\ell)) - V_\ell(Du_0(\ell)) \right).$$

The following lemma states that the energy difference functional is defined on $\mathcal{H}(\Lambda)$, which we prove in Appendix C.2.

Theorem 2.7. Suppose that (S.R) and (S.L) hold, $y_0 \in \mathcal{A}(\Lambda)$ and also that $F : \mathcal{H}(\Lambda) \to \mathbb{R}$, given by

$$\langle F, u \rangle := \sum_{\ell \in \Lambda} \langle \delta V_\ell(Du_0(\ell)), Du(\ell) \rangle = \sum_{\ell \in \Lambda} \sum_{\rho \in \Lambda - \ell} V_{\ell, \rho}(Du_0(\ell))^T D_{\rho} u(\ell), \quad (2.19)$$

is a well-defined bounded linear functional on $(\mathcal{H}(\Lambda), \|D \cdot \|_{L^2})$. Then

(i) $\mathcal{E} : \mathcal{H}(\Lambda) \to \mathbb{R}$ is well-defined and $\delta \mathcal{E}(0) = F$. \!\!


Remark 2.8. For where \( h \) is the defect-free homogeneous system \( \Lambda \) in Section 3.3.

Remark 2.9. The condition that \( F \) is a bounded linear functional is justified for the defect-free homogeneous system \( \Lambda^h \) in Section 3.1, for point defects in Section 3.2 and for dislocations in Section 3.3.\[\square\]

Under the conditions of Theorem 2.7 we can formulate the variational problem

Find \( \bar{u} \in \arg \min \{ \mathcal{E}(u) \mid u \in \mathcal{H}(\Lambda) \} \),

where \( \mathcal{E} \) is understood in the sense of local minimality with respect to the \( \| D \cdot \|_{\mathcal{H}(\Lambda)} \) norm. If \( \bar{u} \) is a minimiser, then \( \bar{u} \) is a first-order critical point satisfying

\[
\langle \delta \mathcal{E}(\bar{u}), v \rangle = 0 \quad \forall \ v \in \mathcal{H}^c(\Lambda).
\]

We shall only be concerned with the structure of solutions to (2.20) or (2.21) in our analysis, assuming their existence.

3. Main Results

We will first discuss the homogeneous lattice as a preparation for defective systems, and then present our results on point defects and dislocations respectively.

3.1. Preliminary results on the homogeneous lattice. For homogeneous systems the setting is as follows:

\( \text{(H)} \quad \Lambda = \Lambda^h = AZ^d, \ d = d_s \in \{2, 3\}, \ x(\ell) = \ell \) and \( u_0(\ell) = 0 \) for all \( \ell \in \Lambda^h \).

In this setting, let \( \mathcal{E}^h(u) := \mathcal{E}(u) \) be the energy difference functional defined by (2.19), which has the form

\[
\mathcal{E}^h(u) = \sum_{\ell \in \Lambda^h} \left( V(Du(\ell)) - V(0) \right),
\]

where \( V \) is the homogeneous site strain potential introduced in Section 2.2.

Once we establish the following result, it will immediately follow from Theorem 2.7 that \( \mathcal{E}^h \) is defined. We will readily make use of this fact in the analysis of the relaxation problem for point defects. The proof of the following result is given in Appendix E.1.

Lemma 3.1. If the assumptions (S.R), (S.L), (S.PS) and (H) are satisfied, then for all \( u \in \mathcal{H}^c(\Lambda^h) \), \( \ell, \rho \mapsto V^h(0) \cdot D_\rho u(\ell) \in \mathcal{L}^1(\Lambda^h \times \Lambda^h) \). Moreover,

\[
\sum_{\ell \in \Lambda^h} \langle \delta V^h(0), Du(\ell) \rangle = \sum_{\ell \in \Lambda^h} \sum_{\rho \in \Lambda^h} V^h(0)^T D_\rho u(\ell) = 0 \quad \forall \ u \in \mathcal{H}^c(\Lambda^h).
\]
For a defective system with Λ satisfying (RC) with site strain potentials \( \{ V_\ell \}_{\ell \in \Lambda} \), we denote by \( V \) the far-field limit site strain potential on the host homogeneous lattice \( \Lambda^h = AZ^d \) and define the homogeneous difference operator \( H : \mathcal{W}^{1,2}(\Lambda^h) \rightarrow \mathcal{W}^{-1,2}(\Lambda^h) \) by
\[
\langle Hu, v \rangle := \sum_{\ell \in \Lambda^h} \langle \delta^2 V(0) Du(\ell), Dv(\ell) \rangle
= \sum_{\ell \in \Lambda^h} \sum_{\rho, \zeta \in \Lambda^h} D\zeta v(\ell)^T \cdot V_{\rho,\zeta}(0) \cdot D_{\rho} u(\ell) \quad \forall \ v \in \mathcal{W}^{1,2}(\Lambda^h). \tag{3.3}
\]

In our analysis of defect systems, we will require the following strong stability of the host homogeneous lattice.

**Lattice stability:** There exists a constant \( c_L > 0 \) depending only on \( \Lambda^h \), such that
\[
\langle Hu, v \rangle \geq c_L \| Dv \|^2_{\mathcal{L}_\Lambda^c} \quad \forall \ v \in \mathcal{W}^c(\Lambda^h).
\]

The analysis of the homogeneous difference operator will be presented in Appendix D, which will be heavily used in our decay estimate proofs.

### 3.2. Point defects

For systems with point defects, we consider the following setting:

1. **(P)** \( \Lambda \) satisfying (RC) with respect to \( \Lambda^h = AZ^d \), \( d = d_s \in \{2, 3\} \), \( x(\ell) = \ell \) and \( u_0(\ell) = 0 \) for any \( \ell \in \Lambda^h \).

With this setting, let \( \mathcal{E}(u) \) be the energy difference functional defined by (2.19). The following result together with Theorem 2.7 implies that \( \mathcal{E} \) is defined on \( \mathcal{H}(\Lambda) \) and \( \mathcal{E} \in C^{n-1}(\mathcal{H}(\Lambda), \| D \cdot | D_{\mathcal{L}_\Lambda^c}(\Lambda) \|) \).

**Theorem 3.2.** Suppose that the assumptions \( (S) \) and \( (P) \) are satisfied with \( s > d/2 \) in \( (S.H) \). Then \( F : \mathcal{W}^c(\Lambda) \rightarrow \mathbb{R} \), given by
\[
\langle F, u \rangle := \sum_{\ell \in \Lambda} \langle \delta V_\ell(0), Du(\ell) \rangle = \sum_{\ell \in \Lambda} \sum_{\rho \in \Lambda - \ell} V_{\ell,\rho}(0)^T D_{\rho} u(\ell). \tag{3.4}
\]
defines a bounded linear functional on \( \mathcal{W}^c(\Lambda), \| D \cdot | D_{\mathcal{L}_\Lambda^c}(\Lambda) \| \). That is, there exists \( C > 0 \) such that \( \|\langle F, u \rangle\| \leq C \| Du \|^2_{\mathcal{L}_\Lambda^c} \) for all \( u \in \mathcal{W}^c(\Lambda) \).

The proof of Theorem 3.2 is given in Appendix E.2.

Next, we consider the variational problem (2.20). We establish the rate of decay for a minimising displacement \( \bar{u} \) in the following result, whose proof is given in Appendix E.3.

**Theorem 3.3.** Suppose that the conditions in Theorem 3.2 and (LS) hold, then for any \( \bar{u} \) solving (2.21), there exists \( C > 0 \) depending on \( \bar{u} \) and \( s \), such that
\[
| D_{\rho} \bar{u}(\ell) | \leq C|\rho| \begin{cases} (1 + |\ell|)^{-d} & \text{if } s > d, \\ (1 + |\ell|)^{-s} \log(2 + |\ell|) & \text{if } \frac{d}{2} < s \leq d, \end{cases} \tag{3.5}
\]
for all \( \ell \in \Lambda \) and \( \rho \in \Lambda - \ell \), where \( s \) is the parameter in \( (S.H) \).

In the case \( s > d \), an immediately conclusion of this theorem is
\[
| D\bar{u}(\ell) | \leq C(1 + |\ell|)^{-d},
\]
for either \( |D\bar{u}(\ell)| := |D\bar{u}(\ell)|_{W_{E,k}} \) or \( |D\bar{u}(\ell)| := |D\bar{u}(\ell)|_{L^2} \), as shown in (1.1). Similar to [13, Theorem 2.3], we also have decay estimates for higher order derivatives: for \( j \leq n - 1 \), there exist constants \( C_j > 0 \) such that
\[
| D_{\rho}^j \bar{u}(\ell) | \leq C_j \left( \prod_{i=1}^{j} |\rho_i| \right) (1 + |\ell|)^{1-d-j} \tag{3.6}
\]
for $\rho = (\rho_1, \ldots, \rho_j) \in (\Lambda^h \cap B_{R_c}(0))^j$ with some cutoff $R_c > 0$ and $\ell \in \Lambda \setminus B_{R_{def}}$ with $|\ell|$ sufficiently large. The proof is a straightforward combination of the arguments used in [13] and the techniques developed in the present paper, hence we omit it. It is not clear whether the higher-order decay generalises to arbitrarily large $\rho_i$.

3.3. Dislocations. The following setting for dislocations can be found in [13]. We consider a model for straight line dislocations obtained by projecting a 3D crystal. Given a Bravais lattice $\Lambda_0 = BZ^3$ with dislocation direction parallel to $e_3$ and Burgers vector $b = (b_1, 0, b_3)$, we consider displacements from $BZ^3$ to $\mathbb{R}^3$ (hence $d_s = 3$) that are periodic in the direction of the dislocation direction $e_3 \in BZ^3$. Thus, we choose a projected reference lattice $\Lambda := AZ^2 = \Lambda^h = \{(\ell_1, \ell_2) \mid \ell = (\ell_1, \ell_2, \ell_3) \in BZ^3\}$ (hence $d = 2$), which is again a Bravais lattice as $A$ is non-singular. It is convenient to identify $\ell = (\ell_1, \ell_2) \in AZ^2$ with corresponding $(\ell_1, \ell_2, \ell_3) \in BZ^3$. This projection gives rise to a projected 2D site strain potential, for $y \in \mathcal{A}(\Lambda)$, with the additional invariance

$$V_\ell(Du(\ell)) = V_\ell(D(u + ze_3)(\ell)) \quad \forall z : \Lambda \to b_3\mathbb{Z} \quad (3.7)$$

Let $\hat{x} \in \mathbb{R}^2$ be the position of the dislocation core and

$$\Gamma := \{x \in \mathbb{R}^2 \mid x_2 = \hat{x}_2, x_1 \geq \hat{x}_1\}$$

be the “branch cut”, with $\hat{x}$ chosen such that $\Gamma \cap \Lambda = \emptyset$. Following [13], we define the far-field predictor $u_0$ by

$$u_0(\ell) := u_0^\text{lin}(\xi^{-1}(\ell)) + u^c(\ell), \quad \text{for all } \ell \in \Lambda, \quad (3.8)$$

where $u_0^\text{lin} \in C^\infty(\mathbb{R}^2 \setminus \Gamma; \mathbb{R}^3)$ and $u^c \in C_c^\infty(\mathbb{R}^2; \mathbb{R}^3)$. We introduce the function $u^c$ to ensure that $y_0 \in \mathcal{A}(\Lambda)$, see Lemma F.1 for more details. The displacement $u_0^\text{lin}$ is the continuum linear elasticity solution solving $\sum_{\rho_i \in \Lambda^h} V_{\rho_i}(0) \nabla_x \nabla_{\varepsilon_i} u_0^\text{lin}(x) = 0$ (see [13, Appendix A] for more details). In particular, under the lattice stability assumption (LS) there exists a solution of the form

$$u_i^\text{lin}(\hat{x} + x) = \text{Re} \left( \sum_{n=1}^3 B_{i,n} \log(x_1 + p_n x_2) \right) \quad \text{with } B_{i,n}, p_n \in \mathbb{C}, i,n = 1,2,3 \quad (3.9)$$

and

$$\xi(x) = x - b_{12} \frac{1}{2\pi} \eta \left( \frac{|x - \hat{x}|}{\tilde{r}} \right) \arg(x - \hat{x}), \quad (3.10)$$

where $\arg(x)$ denotes the angle in $(0, 2\pi)$ between $x$ and $b_{12} = (b_1, b_2) = (b_1, 0)$, $\eta \in C(\mathbb{R})$ with $\eta = 0$ in $(-\infty, 0]$, $\eta = 1$ in $[1, \infty)$ and $\tilde{r} > 0$ is sufficiently large to ensure that $\xi : \mathbb{R}^2 \setminus \Gamma \to \mathbb{R}^2 \setminus \Gamma$ is a bijection. Then we have [13, Lemma 3.1]

$$|\nabla^nu_0(x)| \leq C|x|^{-n} \quad \forall x \in \mathbb{R}^2 \setminus (\Gamma \cup B_{\ell}), \quad \text{for all } n \in \mathbb{N}. \quad (3.11)$$

Remark 3.4. It is necessary that $y_0 \in \mathcal{A}(\Lambda)$ and while it is straightforward to observe that $y_0$ satisfies the required properties in the far-field, some care is needed to ensure no collisions occur around the defect core. 

The predictor $y_0 = x + u_0$ is constructed in such a way that $y_0$ jumps across $\Gamma$, which encodes the presence of the dislocation. Alternatively, constructing the jump over the left-hand plane $\{x_1 \leq \hat{x}_1\}$ also achieves this. The role of $\xi$ in the definition of $u_0$ allows us to map $y_0$ to an equivalent far-field predictor that characterises the dislocation with a left-hand plane branch-cut. This is shown in detail in Appendix F.2.

Remark 3.5. One can treat anti-plane models of pure screw dislocations by admitting displacements of the form $u_0 = (0, 0, u_{0,3})$ and $u = (0, 0, u_3)$. Similarly, one can treat
the in-plane models of pure edge dislocations by admitting displacements of the form $u_0 = (u_{0,1}, u_{0,2}, 0)$ and $u = (u_1, u_2, 0)$ (see [13]).

In summary, we treat dislocations in the following setting (D):

(D) $\Lambda = \Lambda^h = \mathbb{Z}^2$, $d = 2$, $d_s = 3$, $x(\ell) = \ell$ and $u_0$ is given by (3.8).

With this setting, let $\mathcal{E}(u)$ be the energy difference functional defined by (2.19). The following lemma together with Theorem 2.7 implies that $\mathcal{E}$ is well-defined and that $\mathcal{E} \in C^{n-1}(\mathcal{H}, \|D \cdot \|_{\Lambda^h(\Lambda^c)})$. The proof is given in Appendix F.2.

Theorem 3.6. Suppose the assumptions (S.R), (S.L), (S.PS) and (D) are satisfied, then $F: \mathcal{W}^c(\Lambda) \to \mathbb{R}$, given by

$$\langle F, u \rangle := \sum_{\ell \in \Lambda^h} \langle \delta V_\ell(Du_0(\ell)), Du(\ell) \rangle = \sum_{\ell \in \Lambda^h} \sum_{\rho \in \Lambda^h} V_{\ell,\rho}(Du_0(\ell))^T D_\rho u(\ell),$$

defines a bounded linear functional on $(\mathcal{W}^c(\Lambda), \|D \cdot \|_{\Lambda^h(\Lambda^c)})$. That is, there exists $C > 0$ such that $|\langle F, u \rangle| \leq C\|Du\|_{\Lambda^h(\Lambda^c)} < \infty$, for all $u \in \mathcal{W}^c(\Lambda)$.

We now consider the variational problem (2.20). We establish the rate of decay for a minimising displacement $\bar{u}$ in the following result, whose proof is given in Appendix E.3.

Theorem 3.7. Suppose that the conditions in Theorem 3.6 and (LS) hold, then for any $\bar{u}$ solving (2.21), there exists $C > 0$ depending on $\bar{u}$, such that

$$|D_\rho \bar{u}(\ell)| \leq C|\rho|(1 + |\ell|)^{-2}\log(2 + |\ell|)$$

for all $\ell \in \Lambda$ and $\rho \in \Lambda - \ell$.

An immediately conclusion of this theorem is

$$|D\bar{u}(\ell)| \leq C(1 + |\ell|)^{-2}\log(2 + |\ell|)$$

for either $|D\bar{u}(\ell)| := |D\bar{u}(\ell)|_{\mathfrak{m}_\ell}$ or $|D\bar{u}(\ell)| := |D\bar{u}(\ell)|_N$, as shown in (1.1).

Similar to [13, Theorem 3.5], we also have a decay estimate for higher order derivatives: For $j \leq n - 2$ there exist constants $C_j > 0$ such that

$$|\tilde{D}_\rho \bar{u}(\ell)| \leq C_j \left(\prod_{i=1}^{j} |\rho_i|\right)(1 + |\ell|)^{-1-j}\log(2 + |\ell|)$$

for $\rho = (\rho_1, \ldots, \rho_j) \in (\Lambda^h \cap B_{R_c}(0))^j$ with some cutoff $R_c > 0$ and $\ell \in \Lambda^h$ with $|\ell|$ sufficiently large. The finite-difference operator $\tilde{D}$ appearing in (3.14) is a permutation of $D$, accounting for plastic slip, and is described in more detail in Appendix F.1. Similarly as for (3.6), the proof of (3.14) follows from a straightforward combination of the arguments used in [13] and the techniques developed in the present paper, hence we omit it.

4. Discussions of practical models

In the previous sections, we developed an abstract formulation for the relaxation of crystalline defects. We now demonstrate that this framework applies to several physical models from molecular mechanics to quantum mechanics, that were previously untreated.

Instead of the site strain potential $V_\ell(Du(\ell))$, we discuss the physical models through the site energy $\Phi_\ell: \mathcal{S}(\Lambda) \to \mathbb{R}$ in this section. For $y = y_0 + u$, the site energy $\Phi_\ell(y)$ can be viewed as a replacement of site strain potential $V_\ell(Du_0(\ell) + Du(\ell))$:

$$\Phi_\ell(y) = \Phi_\ell(y_0 + u) = V_\ell(Du_0(\ell) + Du(\ell)).$$

(4.1)
Note that $\Phi_\ell$ is a function of atomic configuration $y$ and is more convenient to describe practical models. We will discuss them in detail in the following subsections for different models.

In the following, we consider models for three-dimensional systems, hence $d \in \{2, 3\}$, $d_\delta = 3$ and we suppose $\Lambda \subset \mathbb{R}^d$, $\Lambda_0 \subset \mathbb{R}^3$ satisfy (RC) with respect to Bravais lattices $\Lambda^h \subset \mathbb{R}^d$, $\Lambda^h_0 \subset \mathbb{R}^3$, respectively. In the following subsections, for each model, we define $\Phi_\ell(y)$, for each $\ell \in \Lambda_0$ and $y \in \mathcal{A}(\Lambda_0)$.

In the case of point defects, we have $d = d_\delta = 3$, $\Lambda = \Lambda_0$ and $\mathcal{A}(\Lambda)$ is the projection of $\Lambda_0$ onto the plane $\{x_3 = 0\}$ as $\Lambda \neq \Lambda_0$, we use (2.8) to identify $y \in \mathcal{A}(\Lambda)$ with $\tilde{y} \in \mathcal{A}(\Lambda_0)$. Then for $\ell = (\ell_1, \ell_2, \ell_3) \in \Lambda_0$, we define $\Phi_{\ell_1}(y) := \Phi_\ell(\tilde{y})$ to be the corresponding site energy for $y \in \mathcal{A}(\Lambda)$ and $\ell_1 \in \Lambda$ and remark that this is well-defined.

Using (4.1), we can easily rewrite the assumptions (S.R), (S.L) and (S.H) in terms of the site energy $\Phi_\ell$ (we skip the details for simplicity of presentations). In addition, we require that the site energy is invariant under permutations and isometries as in the following assumptions (S.P) and (S.I), from which (S.PS) can be derived.

(S.P) **Symmetry under permutations:** If $y \circ \pi \in \mathcal{A}(\Lambda)$ and $\Phi_{\pi(y)}(y) = \Phi_{\ell}(y)$.

(S.L) **Symmetry under isometries:** If $\phi : \mathbb{R} \rightarrow \mathbb{R}$ is an isometry, then $\phi \circ y \in \mathcal{A}(\Lambda)$ and $\Phi_{\phi(y)}(\phi(y)) = \Phi_{\ell}(y)$.

4.1. Lennard-Jones. The Lennard-Jones potential [22] is a simple model that approximates the interaction between a pair of neutral atoms or molecules, in three dimensions. The most common expression for the Lennard-Jones potential is

$$\phi_{\text{LJ}}(r) := 4\varepsilon \left( \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right),$$  \hspace{1cm} (4.2)

where $\varepsilon$ is the depth of the potential well, $\sigma$ is the finite distance at which the inter-particle potential is zero. We consider the more general model

$$\phi_{\text{LJ}}^{(p,q)}(r) := C_1 r^{-p} - C_2 r^{-q},$$  \hspace{1cm} (4.3)

with $p > q > 0$ and $C_1, C_2 > 0$. Then the Lennard-Jones site energy is given by

$$\Phi_{\ell}(y) := \frac{1}{2} \sum_{k \in \Lambda_0, k \neq \ell} \phi_{\text{LJ}}^{(p,q)}(r_{\ell k}),$$  \hspace{1cm} (4.4)

where $r_{\ell k} = |y(\ell) - y(k)|$. Note that by fixing the parameters $C_1, C_2$ in the potential, we have assumed that all atoms of the system belong to the same species.

We obtain from a simple calculation that if $q > 3$, then the assumptions (S) are satisfied by the Lennard-Jones site energy (4.4) for point defects, and if $q > 5$, (S) are satisfied for dislocations as well.

We briefly justify that (S.H) holds with arbitrary $s > 0$. Let $\Phi^h_\ell$ be the site energy on $\Lambda^h$ satisfying (S), $y \in \mathcal{A}(\Lambda_0)$ and $y' \in \mathcal{A}(\Lambda^h)$. Then for $\ell \in \Lambda_0$ and $\ell' \in \Lambda^h_0$ satisfying

$$\{y(n) - y(\ell) \mid n \in \Lambda_0, r_{\ell n}(y) \leq r\} = \{y'(n') - y'(\ell') \mid n' \in \Lambda^h_0, r_{\ell' n'}(y') \leq r\},$$  \hspace{1cm} (4.5)

with $r > 0$, we have that there exists $n \in \Lambda_0$ and $n' \in \Lambda^h_0$ such that $y(\ell) - y(n) = y(\ell') - y(n')$ and

$$\Phi_{\ell, n}(y) = \phi_{\text{LJ}}(r_{\ell n}(y)) \frac{y(n) - y(\ell)}{r_{\ell n}(y)} = \phi_{\text{LJ}}(r_{\ell' n'}(y')) \frac{y'(n') - y'(\ell')}{r_{\ell' n'}(y')} = \Phi^h_{\ell, n'}(y'),$$

hence as $|\Phi_{\ell, n}(y) - \Phi^h_{\ell, n'}(y')| = 0$, (S.H) is satisfied with arbitrary $s > 0$. 

Similarly, we can construct the site energy for general pair potential models $\Phi_\ell(y) = \frac{1}{2} \sum_{k \neq \ell} \phi(r_{\ell k})$ and show that the assumptions (S) are satisfied for most of the practical models, such as Morse potential [26], as long as $|\phi^{(j)}(r)| \lesssim r^{-q-j}$ with $q > 3$ for point defects and $q > 5$ for dislocations.

4.2. Embedded atom model. The site energy of the embedded atom model (EAM) [12] can be written as (a pair potential contribution is omitted from the standard EAM formula since we have discussed them in the previous subsection)

$$\Phi_\ell(y) := F_\alpha \left( \sum_{k \in \Lambda_0, k \neq \ell} \rho_\beta(r_{\ell k}) \right),$$

(4.6)

where $r_{\ell k} = |y(\ell) - y(k)|$, $\rho_\beta$ is the contribution to the electron charge density from atom $k$ of type $\beta$ at the location of atom $\ell$, and $F_\alpha$ is an embedding function that represents the energy required to place atom $\ell$ of type $\alpha$ into the electron cloud.

In most of the practical EAM models, there is a cutoff $R_c$ established and interactions between atoms separated by more than $R_c$ are ignored, i.e. the sum in (4.6) is taken over $k \in \Lambda_0$ satisfying $r_{\ell k} \leq R_c$. We consider here a more general model with infinite range of interaction. This serves as a simple study of the kind of decay required for many-body interaction.

Let $y \in \mathcal{A}_{m,\lambda}^0(\Lambda_0)$. We assume a smooth and positive density contribution: $\rho_\beta \in C^\infty((0, \infty))$ and $\rho_\beta(r) > 0, \forall r > 0$. We also require a decay property of $\rho_\beta$ that

$$\rho_\beta^{(j)}(r) \leq C(1 + r)^{-q-j} \quad \forall r > 0, \ 0 \leq j \leq n \quad \text{with some} \ q > 0.$$  

(4.7)

Since $y \in \mathcal{A}_{m,\lambda}^0(\Lambda_0)$ and $\rho_\beta$ is bounded, we have that the range of electron density $\sum_{k \in \Lambda_0, k \neq \ell} \rho_\beta(r_{\ell k})$ lies in a bounded interval $[\underline{\sigma}_{m,\lambda}, \overline{\sigma}_{m,\lambda}]$, with $0 < \underline{\sigma}_{m,\lambda} < \overline{\sigma}_{m,\lambda} < \infty$ depending on $m$ and $\lambda$.

Further, we assume that the embedding function $F_\alpha$ is smooth and bounded for admissible electron densities: $F_\alpha \in C^\infty((0, \infty))$ and

$$|F_\alpha^{(j)}(x)| \leq C_{m,\lambda} \quad \forall x \in [\underline{\sigma}_{m,\lambda}, \overline{\sigma}_{m,\lambda}], \ 1 \leq j \leq n$$

(4.8)

where $C_{m,\lambda} > 0$ depends on $m$ and $\lambda$. This assumption is satisfied for most practical models as $F_\alpha(\cdot)$ is usually a polynomial or $\sqrt{\cdot}$ (Gupta and Finnis–Sinclair models).

Assume that all atoms of the system belong to the same species (i.e. $F_\alpha \equiv F$ and $\rho_\beta \equiv \rho$). We have from a direct calculation that if $q > 3$, then the assumptions (S.L) are satisfied by the EAM site energy (4.6) for point defects; and if $q > 5$, than (S.L) are satisfied for dislocations.

To see the conditions for (S.H), we compare two configurations $y$ and $y'$ satisfying (4.5), for some $r > 0$. Define

$$\rho_1(y) = \sum_{k \neq \ell, r_{\ell k}(y) \leq r} \rho(r_{\ell k}(y)), \quad \rho_1(y') = \sum_{k' \neq \ell', r_{\ell' k'}(y') \leq r} \rho(r_{\ell' k'}(y')),$$

$$\rho_2(y) = \sum_{k \neq \ell, r_{\ell k}(y) > r} \rho(r_{\ell k}(y)), \quad \rho_2(y') = \sum_{k' \neq \ell', r_{\ell' k'}(y') > r} \rho(r_{\ell' k'}(y')).$$
The condition (4.5) ensures that \( \rho_1(y) = \rho_1(y') \). With the site energy (4.6), we have for some \( \theta \in (0, 1) \)

\[
\left| \Phi_{\ell,n}(y) - \Phi_{\ell,n}(y') \right| = \left| F'(\rho_1(y) + \rho_2(y)) - F'(\rho_1(y') + \rho_2(y')) \right| \left| \rho'(r_{\ell n}(y)) \right|
\leq \left| F'(\rho(y) + \theta(\rho_2(y) - \rho_2(y'))) \right| \left| \rho_2(y) - \rho_2(y') \right| \left| \rho'(r_{\ell n}(y)) \right|
\leq C (|\rho_2(y)| + |\rho_2(y')|) \left| \rho'(r_{\ell n}(y)) \right|
\]

where we have used the assumption that \( F' \) is bounded is used in the last estimate. Now a necessary condition for \((S, H)\) is \( |\rho_2(y)| + |\rho_2(y')| \leq C(1 + r)^{-s} \) with \( s > 3/2 \). Using the form of \( \rho \) in (4.7), we therefore require \( q > 9/2 \).

In summary, if \( q > 9/2 \), then the assumptions \((S)\) are satisfied by the EAM site energy (4.6) for point defects; and if \( q > 5 \), than \((S)\) are satisfied for dislocations.

In particular, for all interatomic potentials with similar form as (4.6), such as second moment tight binding model [16], Gupta potential [18], Finnis-Sinclair potential [15, 33], the assumptions \((S)\) are satisfied.

### 4.3. Tight binding

Whereas the Lennard-Jones and EAM model are classical interatomic potentials, we now give examples of three quantum mechanical (QM) models that can be treated within the assumptions of our work. The first QM model that we consider is the tight binding model. For simplicity of presentation, we consider an orthogonal two-centre tight binding model [17] with a single orbital per atom. All results can be extended directly to general non-self-consistent non-orthogonal tight binding models with multiple orbitals, as described in [9].

For a finite system with reference configuration \( \Omega \subset \Lambda_{0} \) and \#\( \Omega = N \), the two-centre tight binding model is formulated in terms of a discrete Hamiltonian, with matrix elements

\[
(H^\Omega(y))_{\ell k} = \begin{cases} 
  h_{\text{ons}} \left( \sum_{j \in \Omega, \ell} \varrho \left( |y(\ell) - y(j)| \right) \right) & \text{if } \ell = k \\
  h_{\text{hop}} \left( |y(\ell) - y(k)| \right) & \text{if } \ell \in \Omega \setminus k,
\end{cases}
\]

where \( R_{c} \) is a cut-off radius, \( h_{\text{ons}} \in C^{n}([0, \infty)) \) is the on-site term, with \( \varrho \in C^{n}([0, \infty)) \), \( \varrho = 0 \) in \([R_{c}, \infty)\), and \( h_{\text{hop}} \in C^{n}([0, \infty)) \) is the hopping term with \( h_{\text{hop}}(r) = 0 \) for all \( r \in [R_{c}, \infty) \).

Note that \( h_{\text{ons}} \) and \( h_{\text{hop}} \) are independent of \( \ell \) and \( k \), which indicates that all atoms of the system belong to the same species. We observe that the formulation (4.9) satisfies all the assumptions on Hamiltonian matrix elements in [9, Assumptions H.tb, H.loc, H.sym, H.emb].

With the above tight binding Hamiltonian \( H^\Omega \), we can obtain the band energy of the system

\[
E^\Omega(y) = \sum_{s=1}^{N} f(\varepsilon_{s}), \quad \text{where} \quad H^\Omega(y)\varepsilon_{s} = \varepsilon_{s}\varepsilon_{s} \quad s = 1, 2, \cdots, N.
\]

A canonical choice of for modelling solids is the grand-canonical potential,

\[
f(\varepsilon) = 2k_{B}T \ln(1 - f(\varepsilon)) \quad \text{where} \quad f(\varepsilon) = \left( 1 + e^{(\varepsilon - \mu)/(k_{B}T)} \right)^{-1},
\]

\( f \) is the Fermi-Dirac distribution function and \( \mu \) the chemical potential of the crystal (see [7] for more details of its derivation), \( k_{B} \) Boltmann’s constant, and \( T > 0 \) the temperature of the system. Other choices of \( f \) are also possible [9].

Tight binding models typically also include a pairwise repulsive potential, which can be treated purely classically [9], hence we do not consider this.

A crucial assumption justified in [7] is that the chemical potential \( \mu \) is independent of the configuration \( y \). Under this assumption, following [9, 16], we can distribute the energy
to each atomic site
\[ E^\Omega(y) = \sum_{\ell \in \Omega} \Phi^\Omega_\ell(y) \quad \text{with} \quad \Phi^\Omega_\ell(y) := \sum_s f(\varepsilon_s) |\psi_s(\ell)|^2. \tag{4.11} \]

It is then shown in [9, Theorem 3.1] that the site energy on an infinite lattice can be defined via the thermodynamic limit:
\[ \Phi_\ell(y) := \lim_{R \to \infty} \Phi^{B_R(\ell)}_\ell(y), \tag{4.12} \]
and that the resulting site energy is local: if \( y \in \mathcal{A}_{m,\lambda}(\Lambda_0) \) then
\[ |\partial_{y(n_1)} \cdots \partial_{y(n_j)} \Phi_\ell(y)| \leq C \exp \left( -\gamma \sum_{i=1}^j |y_{n_i} - y_{\ell}| \right), \tag{4.13} \]
where \( C, \gamma \) depends only on \( m, \lambda \) but is independent of \( y \). This already justifies (S.L) with weight functions \( w_j(r) = e^{-\gamma/2r} \) (the factor 1/2 is due to a subtle technicality).

Along similar lines, under assumptions of (S.H), [10, Lemma B.1] establishes
\[ |\Phi_{\ell_1,n_1}(Dy_1(\ell_1)) - \Phi_{\ell_2,n_2}(Dy_2(\ell_2))| \leq C \exp \left( -\gamma (r + |\ell_1 - n_1|) \right), \tag{4.14} \]
where \( C, \gamma \) may be chosen the same as in (4.13) without loss of generality. This establishes (S.H) with arbitrary \( s > 0 \).

Thus, the tight binding model (4.11) fulfills all assumptions (S) on the site energy.

### 4.4. The Thomas–Fermi–von Weizsäcker (TFW) Model

The second QM model for which we verify that it fits within our general framework is the orbital-free TFW model.

Let \( \nu \in C_c^\infty(\mathbb{R}^3) \) satisfying \( \nu \geq 0 \) and \( \int_{\mathbb{R}^3} \nu = 1 \) describe the smeared distribution of a single nucleus with unit charge and let \( Z(\ell) \in \mathbb{N} \) denote the charge of the nucleus at \( \ell \in \Lambda \). We assume that \( Z(\ell) \) is constant for all \( \ell \in \Lambda_0 \setminus B_{R_{\text{def}}} \), where \( \Lambda_0 \setminus B_{R_{\text{def}}} = \Lambda_0^b \setminus B_{R_{\text{def}}} \). For \( y \in \mathcal{A}(\Lambda_0) \), we define the total nuclear distribution corresponding to \( y \) as
\[ g^{\text{nuc}}(y; x) = \sum_{\ell \in \Lambda_0} Z(\ell) \nu(x - y(\ell)). \]

As \( y \in \mathcal{A}(\Lambda) \), it follows immediately that \( g^{\text{nuc}} = g^{\text{nuc}}(y; \cdot) \) satisfies
\[ \sup_{x \in \mathbb{R}^3} \int_{B_1(x)} g^{\text{nuc}}(z) \, dz < \infty \quad \text{and} \quad \lim_{R \to \infty} \inf_{x \in \mathbb{R}^3} \int_{B_R(x)} g^{\text{nuc}}(z) \, dz = +\infty, \]
hence [5, Theorem 6.10] guarantees the existence and uniqueness of the corresponding TFW ground state \( (\varrho, \phi) \in (C^\infty(\mathbb{R}^3))^2 \), \( \varrho \geq 0 \), solving the following coupled elliptic system pointwise
\[ \left( -\Delta + \frac{5}{3} \varrho^{2/3} - \phi \right) \sqrt{\varrho} = 0, \tag{4.15a} \]
\[ -\Delta \phi = 4\pi (\varrho^{\text{nuc}} - \varrho). \tag{4.15b} \]

Here \( \varrho \) represents the ground state electron density and \( \phi \) the electrostatic potential. Using \( (\varrho, \phi) \), we define the ground state energy density corresponding to \( y \),
\[ E_{\text{TFW}}(y; \cdot) = |\nabla \sqrt{\varrho}|^2 + \varrho^{5/3} + \frac{1}{2} \phi (\varrho^{\text{nuc}} - \varrho). \]

One can view (4.15) as the Euler–Lagrange equations corresponding to the formal energy given by \( \int_{\mathbb{R}^3} E_{\text{TFW}}(y; x) \, dx \). We then introduce a family of partition functions
\{\chi_\ell(y; \cdot)\}_{\ell \in \Lambda_0} \text{ satisfying } \chi_\ell(y; \cdot) \in C^\infty(\mathbb{R}^3), \chi_\ell(y; \cdot) \geq 0 \text{ and }
\sum_{\ell \in \Lambda_0} \chi_\ell(y; x) = 1, \quad \text{and (4.16a)}

\left| \frac{\partial^k \chi_\ell(y; x)}{\partial y(j_1) \cdots \partial y(j_k)} \right| \leq Ce^{-\gamma|x-y(\ell)|} \prod_{1 \leq i \leq k} e^{-\gamma|y(j_i)|}, \quad (4.16b)

\text{for some } C, \gamma > 0 \text{ and for all } k \in \mathbb{N}, \ell, i_1, \ldots, i_k \in \Lambda_0 \text{ and } x \in \mathbb{R}^3. \text{ The construction of such partition functions is given in [27, Remark 12, Theorem 5.11] and [28, Remark 9].}

One such example is the following: for } \alpha > 0, \text{ let } \tilde{\chi}(x) = e^{-\alpha|x|^2}, \text{ then for } \ell \in \Lambda_0, \text{ define }
\chi_\ell(y; x) = \frac{\tilde{\chi}(x - y(\ell))}{\sum_{\ell' \in \Lambda_0} \tilde{\chi}(x - y(\ell'))}.

This construction satisfies all of the required conditions.

We then define the TFW site energy as
\Phi_\ell(y) := \int_{\mathbb{R}^3} E_{\text{TFW}}(y; x) \chi_\ell(y; x) \, dx. \quad (4.17)

It is shown in [28] and [27, Proposition 6.3, Theorem 5.11] that this site energy is well-defined and that it satisfies the same locality and homogeneity estimates (4.13) and (4.14) as the tight binding model. Thus, all assumptions (S) are again satisfied (with (S.H) holding for arbitrary } s > 0) by the TFW site energy (4.17).

4.5. Reduced Hartree–Fock with Yukawa potential. The third QM model we consider is the reduced Hartree–Fock model [34], also called the Hartree model in the physics literature. Instead of the long-range Coulomb interaction, we assume that all the particles interact through a short-range Yukawa potential [36]. Similar to the TFW model in Section 4.4, we can define the ground state energy density, and then construct the site energy from a family of partition functions. Assuming that all atoms of the system belong to the same species, we have from [6] that the assumptions (S) are satisfied (with (S.H) holding for arbitrary } s > 0) by the rHF site energy.

5. Conclusions

We have developed a general framework to study the geometry relaxation of crystalline defects embedded in a homogeneous host crystal. Specifically, we formulated energy difference functionals for solid systems with point defects and dislocations, and justified the far-field decay of equilibrium states under a mild far-field stability assumption. The novel aspect of our work is that we can incorporate an infinite interaction neighbourhood in our framework, in particular we showed that we include a wide range of (simplified) quantum chemistry models for interatomic interaction.

Our results are interesting in their own right in classifying properties of crystalline defects, but in addition they provide a foundation for the analysis of different boundary conditions and atomistic multiscale simulation methods, see e.g. [10, 13, 23, 24, 32].

The main restriction of present work is that the locality assumptions in (S.L) are not satisfied for some long-range potentials. Note that for (S.L) in the dislocations case, our assumption requires that the interaction between two particles should decay faster than } r^{-2-d} \text{ with respect to their distance } r. \text{ This is in particular not satisfied by Coulomb or even di-pole interactions. One would therefore need to justify (or assume) that such long-range interactions are screened when we apply the framework and results in this paper. Even in this setting, however, our results help in that we only require mild algebraic decay.
of the screened interaction, which may be easier to justify than the more common and much more stringent assumption of exponential decay.

APPENDIX A. EQUIVALENT NORMS

In addition to the norm $\|D \cdot \|_{\bar{c}_N^i}$ introduced in (2.4), we construct a family of norms that use weighted finite-difference stencils with infinite interaction range. For $k \in \mathbb{N}$, $w \in \mathcal{L}_k$, $\Lambda$ satisfying (RC), $\ell \in \Lambda$ and $u \in \dot{W}^{1,2}(\Lambda)$, define

$$|D u(\ell)|_{w,k} := \left( \sum_{\rho \in \Lambda - \ell} w(|\rho|) |D_{\rho} u(\ell)|^k \right)^{1/k}, \quad (A.1)$$

and the norms

$$\|D u\|_{c_{N,k}} := \left( \sum_{\ell \in \Lambda} |D u(\ell)|_{w,k}^2 \right)^{1/2} \quad \text{for } k = 1, \quad (A.2)$$

$$\|D u\|_{c_{N,k}} := \left( \sum_{\ell \in \Lambda} |D u(\ell)|_{w,k}^k \right)^{1/k} \quad \text{for } k \geq 2. \quad (A.3)$$

To the best of our knowledge, the norms given by (A.2)–(A.3) are new constructions, and are vital for our analysis. The following lemma states the relationships between the norms $\|D \cdot \|_{c_{N,k}}$, $\|D \cdot \|_{\bar{c}_N^i,k}$ and $\|D \cdot \|_{\bar{c}_N^i}$.

**Lemma A.1.** Let $k \in \mathbb{N}$, $w \in \mathcal{L}_k$ and $\Lambda$ satisfy (RC).

1. Suppose $k = 1, 2$ and $\inf_{\ell \in \Lambda} \inf_{\rho \in N(\ell) - \ell} w(|\rho|) = c_0 > 0$, then there exist constants $c_k, C_k > 0$ such that

$$c_k \|D u\|_{\bar{c}_N^i} \leq \|D u\|_{c_{N,k}} \leq C_k \|D u\|_{\bar{c}_N^i} \quad \forall u \in \dot{W}^{1,2}(\Lambda). \quad (A.4)$$

2. Suppose $k > 2$, then there exists $C_k > 0$ such that

$$\|D u\|_{c_{N,k}} \leq C_k \|D u\|_{\bar{c}_N^i} \quad \forall u \in \dot{W}^{1,2}(\Lambda). \quad (A.5)$$

To prove this lemma, we require the following results.

**Lemma A.2.** Let $\Lambda$ satisfy (RC), then for all $\ell \in \Lambda$ and $\rho \in \Lambda - \ell$, there exists a finite path of lattice points $\mathcal{P}(\ell, \ell + \rho) := \{\ell_i\}_{1 \leq i \leq N_\rho + 1} \subset \Lambda$ from $\ell$ to $\ell + \rho$, such that for each $1 \leq i \leq N_\rho$, $\ell_{i+1} \in N(\ell_i)$. Moreover, there exists $C > 0$, independent of $\ell$ and $\rho$, such that $N_\rho \leq C|\rho|$.

**Lemma A.3.** Let $\Lambda$ satisfy (RC). For $\ell \in \Lambda$ and $n \in \mathbb{N}$, define

$$\mathcal{B}_n(\ell) = \left\{ (\ell_1, \ell_2) \in \Lambda \times \Lambda \left| \begin{array}{c} n - 1 < |\ell_1 - \ell_2| \leq n, \ell \in \mathcal{P}(\ell_1, \ell_2) \end{array} \right. \right\}. \quad (A.6)$$

The paths $\mathcal{P}(\ell_1, \ell_2)$ in Lemma A.2 may be chosen such that the following statement is true: there exists $C > 0$ such that

$$|\mathcal{B}_n(\ell)| \leq Cn^d \quad \text{for all } \ell \in \Lambda. \quad (A.6)$$

**Proof of Lemma A.2.** Let $\Gamma$ denote the unit cell of the lattice $\Lambda$, centred at 0. Then consider fixed $k \in \mathbb{N}$ large enough such that $k\Gamma \supset B_{R_{\kappa_a}}(0)$. Then define $\Lambda_0 = \Lambda \cap k\Gamma$, which satisfies: $\Lambda_0$ is finite, $\Lambda_0^b := \Lambda \setminus \Lambda_0 = \Lambda^b \setminus \Lambda_0$, $\partial \Lambda_0 \subset \Lambda_0$ and $\partial \Lambda_0 \subset \Lambda^b$.

Case 1 First consider $\ell \in \Lambda_0^b, \rho \in \Lambda_0^b - \ell$, then $\rho \in \Lambda^b$ and can be expressed as $\rho = \sum_{j=1}^d n_j a_j$, where $(a_j)_{1 \leq j \leq d}$ are the lattice vectors and $(n_j) \in \mathbb{Z}^d$. As the lattice
vectors are independent, one can define a norm $|\rho|_1 = \sum_{j=1}^d |n_j|$, which is equivalent to the standard Euclidean norm $|\rho|$, hence $|\rho|_1 \leq C|\rho|$, where $C > 0$ is independent of $\rho \in \Lambda^h$. It is straightforward to construct a lattice path $(\ell_i)_{1 \leq i \leq N_\rho} \subset (\Lambda_0^c \cup \partial \Lambda_0)$, from $\ell$ to $\ell + \rho$ that avoids the defect core $\Lambda \cap B_{R_{\text{int}}(0)}$, such that $\ell_{i+1} \in \{\ell_i + A e_j\}_{1 \leq j \leq d} \subseteq N(\ell_i)$, such that $N_\rho \leq 2|\rho|_1 \leq C|\rho|$. 

**Figure 2.** Diagrams represented the arguments used to prove Lemmas A.2 and A.3.
Moreover, for $1 \leq i \leq d$, define the sets

$$Q_{1,i} = \left\{ \sum_{j=1}^{d} n_j A e_j \mid (n_j) \in \mathbb{Z}^d, n_i < -k \text{ and } n_j \in [-k, k] \text{ for all } j \neq i \right\},$$

$$Q_{2,i} = \left\{ \sum_{j=1}^{d} n_j A e_j \mid (n_j) \in \mathbb{Z}^d, n_i > k \text{ and } n_j \in [-k, k] \text{ for all } j \neq i \right\}.$$  

(A.7)  

(A.8)

It follows that $\Lambda_0 = \bigcup_{i=1}^{d} (Q_{1,i} \cup Q_{2,i})$. The paths can be chosen such that for $\ell_1, \ell_2 \in \Lambda_0$, then the path $(\ell_{i})_{1 \leq i \leq N_\rho} \subset (\Lambda_0 \cup \partial \Lambda_0)$ from $\ell_1$ to $\ell_2$ satisfies $(\ell_{i})_{1 \leq i \leq N_\rho} \cap \Lambda_0 \neq \emptyset$ if and only if

$$(\ell_1, \ell_2) \in \bigcup_{i=1}^{d} ((Q_{1,i} \times Q_{2,i}) \cup (Q_{2,i} \times Q_{1,i})).$$  

(A.9)

Case 2 Now consider $\ell \in \Lambda_0, \rho \in \Lambda_0 - \ell$. For $\ell' \in \Lambda, \rho' \in \Lambda - \ell'$, then define the Voronoi cell $\mathcal{V}(\ell')$ and its boundary $\partial \mathcal{V}(\ell')$ by

$$\mathcal{V}(\ell') = \left\{ x \in \mathbb{R}^d \mid |x - \ell'| \leq |x - k| \quad \forall k \in \Lambda \right\},$$

$$\partial \mathcal{V}(\ell') = \left\{ x \in \mathcal{V}(\ell') \mid |x - \ell'| = |x - m| \text{ for some } m \in \mathcal{N}(\ell') \right\}.$$  

(A.10)

Also, define the function $d_{\ell'} : \mathbb{R}^d \to \mathbb{R}_{\geq 0}$ by

$$d_{\ell'}(x) := \max_{k \in \Lambda \setminus \{\ell'\}} (|x - \ell'| - |x - k|).$$

Since $|\ell_1 - \ell_2| \geq \mu > 0$ for all $\ell_1, \ell_2 \in \Lambda$ such that $\ell_1 \neq \ell_2$, it follows that $d_{\ell'}$ is continuous and satisfies $d_{\ell'}(k) \leq -\mu < 0$ and $d_{\ell'}(k) \geq \mu > 0$ for all $k \in \Lambda \setminus \{\ell'\}$. Moreover, it follows that $\mathcal{V}(\ell') = \{x|d_{\ell'}(x) \leq 0\}$ and $\partial \mathcal{V}(\ell') = \{x|d_{\ell'}(x) = 0\}$. For $t \in [0, 1]$ define $f(t) = d_{\ell'}(\ell' + t \rho')$. As $f$ is continuous and satisfies $f(0) < 0, f(1) > 0$, by the Intermediate Value Theorem, there exists $t_0 \in (0, 1)$ such that $f(t_0) = d_{\ell'}(\ell' + t_0 \rho') = 0$, hence $\ell' + t_0 \rho' \in \partial \mathcal{V}(\ell')$, hence there exists $m = m(\ell', \ell' + \rho') \in \mathcal{N}(\ell')$ such that $t_0|\rho'| = |\ell' + t_0 \rho' - \ell'| = |\ell' + t_0 \rho' - m|$. By the triangle inequality, it follows that

$$|\ell' + \rho' - m| \leq |\ell' + t_0 \rho' - m| + |(1 - t_0)|\rho'| = t_0|\rho'| + (1 - t_0)|\rho'| = |\rho'|.$$  

(A.11)

The inequality in (A.11) is actually strict. Define the line $L = \{\ell' + t \rho'|t \in \mathbb{R}\}$ and the surface $S = \{x \in \mathbb{R}^d \mid |x - \ell'| = |x - m|\}$. Observe that $L$ and $S$ can intersect at most once and $\ell' + t_0 \rho' \in L \cap S$, where $t_0 \in (0, 1)$. It follows that as $\ell' + \rho' \in L, \ell' + \rho' \notin S$ so (A.11) ensures that

$$|\ell' + \rho' - m| < |\rho'|.$$  

(A.12)

We use (A.12) to construct a finite path of neighbouring lattice points from $\ell'$ to $\ell' + \rho'$. Let $\ell_i(\ell', \rho') = \ell'$, then for $i \in \mathbb{N}$, given $\ell_i(\ell', \rho')$, define $\ell_{i+1}(\ell', \rho') = m(\ell_i, \ell' + \rho') \in \mathcal{N}(\ell_i)$, which satisfies

$$|\ell' + \rho' - \ell_{i+1}| < |\rho'|.$$  

(A.13)

We now show that this path reaches $\ell' + \rho'$ after finitely many steps. Observe that $\ell_1 = \ell' \in \Lambda \cap B_{|\rho'|+1}(\ell' + \rho')$, which is a finite set. The estimate (A.13) implies that $\ell_2 \in \Lambda \cap B_{|\rho'|+1}(\ell' + \rho') \setminus \{\ell_1\}$, and arguing inductively it follows if $\ell_j \neq \ell' + \rho'$ for all $j \leq i$, then $\ell_{i+1} \in \Lambda \cap B_{|\rho'|+1}(\ell' + \rho') \setminus \{\ell_1, \ldots, \ell_i\}$. Let $N = N_{\ell', \rho'} = |\Lambda \cap B_{|\rho'|+1}(\ell' + \rho')|$, and suppose that after $N - 1$ steps, the path has not reached $\ell' + \rho'$, hence $\ell_N \in \Lambda \cap B_{|\rho'|+1}(\ell' + \rho') \setminus \{\ell_1, \ldots, \ell_{N-1}\} = \{\ell' + \rho'\}$, hence there exists a finite path of neighbouring lattice points for any $\ell', \ell' + \rho'$.
Now consider the set
\[ \{ \ell_i(\ell, \rho) \mid \ell \in \Lambda_0, \rho \in \Lambda_0 - \ell, 1 \leq i \leq N_{\ell, \rho} - 1 \}, \]
which is finite, hence there exists \( c_0 > 0 \) such that: for all \( \ell \in \Lambda_0, \rho \in \Lambda_0 - \ell, 1 \leq i \leq N_{\ell, \rho} - 1, \ell_i = \ell_i(\ell, \rho) \) and \( \ell_{i+1} = \ell_{i+1}(\ell, \rho) \) satisfy
\[ |\ell + \rho - \ell_{i+1}| \leq |\ell + \rho - \ell_i| - c_0. \]
As \( \ell_1 = \ell \) satisfies \( |\ell + \rho - \ell_1| = |\rho| \), by arguing inductively we deduce
\[ |\ell + \rho - \ell_{i+1}| \leq |\rho| - c_0i. \]  
(A.14)

Observe that for \( i \geq N_\rho := \lceil c_0^{-1}|\rho| \rceil, |\ell + \rho - \ell_{i+1}| \leq |\rho| - c_0i \leq 0 \), hence the path reaches \( \ell + \rho \) within \( N_\rho \leq c_0^{-1}|\rho| + 1 \leq (c_0^{-1} + \mu^{-1})|\rho| = C|\rho| \) steps.

**Case 3** It remains to consider the case \( \ell \in \Lambda_0, \rho \in \Lambda_0^c \setminus \{ \ell \} \), as the case \( \ell \in \Lambda_0 \setminus \{ \ell \} \) can be treated identically. We follow the procedure of Case 2, starting from \( \ell_1 = \ell \) and moving along neighbouring lattice points in \( \Lambda_0 \) until the boundary \( \partial \Lambda_0 \) is reached, hence there exist neighbouring lattice points \( \ell_1, \ldots, \ell_{i-1} \in \Lambda_0 \setminus \partial \Lambda_0 \) and \( \ell_i \in \partial \Lambda_0 \) satisfying \( |\ell + \rho - \ell_i| \leq |\rho| - c_0(i - 1) \). As \( \ell_i + \rho \in \Lambda_0^c \), there exists a lattice path \((\ell'_j)_{1 \leq j \leq N_{i, \rho} + 1} \) along neighbouring lattice points, from \( \ell_i \) to \( \ell + \rho \), satisfying \( N_{i, \rho} \leq C|\rho| + |\ell + \rho - \ell_i| \leq C(|\rho| - c_0(i - 1)) \), hence joining these paths creates a lattice path of length \( N_{i, \rho} + 1 \), where \( N_{i, \rho} = i + N_{i, \rho} \leq C(c_0i + N_{i, \rho}) \leq C|\rho| \).

**Proof of Lemma A.3.** We first recall the subset \( \Lambda_0 \subset \Lambda \) defined in the proof of Lemma A.2, then decompose \( \Lambda^2 \) into the following sets
\[
A_1 := \Lambda_0 \times \Lambda_0, \quad A_2 := (\Lambda_0^c \times \Lambda_0) \cup (\Lambda_0 \times \Lambda_0^c), \\
A_3 := \{ (\ell_1, \ell_2) \mid (\ell_1, \ell_2) \in (\Lambda_0^c)^2, (\ell_1, \ell_2) \cap \Lambda_0 = \emptyset \}, \\
A_4 := \{ (\ell_1, \ell_2) \in (\Lambda_0^c)^2 \mid (\ell_1, \ell_2) \cap \Lambda_0 \neq \emptyset \}. 
\]
It is clear to see that \( \Lambda^2 = \bigcup_{i=1}^4 A_i \), hence for all \( \ell \in \Lambda \) and \( n \in \mathbb{N} \), \( |\mathcal{B}_n(\ell)| = \sum_{i=1}^4 |\mathcal{B}_n(\ell) \cap A_i| \)

We first estimate \( |\mathcal{B}_n(\ell) \cap A_1| \). As \( \Lambda_0 \) is finite, it follows that
\[ |\mathcal{B}_n(\ell) \cap A_1| \leq |A_1| = |\Lambda_0 \times \Lambda_0| \leq |\Lambda_0|^2n^d. \]  
(A.15)

As \( \Lambda_0^c \subset \Lambda^h \), it follows that
\[
\mathcal{B}_n(\ell) \cap A_3 \subset \left\{ (\ell_1, \ell_1 + \rho) \mid \ell_1 \in \Lambda_0^c, \rho \in \Lambda_0^h, n - 1 \leq |\rho| < n, \ell \in (\ell_1, \ell_1 + \rho) \right\}.
\]
For each \( \rho \in \Lambda_0^h \cap B_n(0) \), there exist at most \( N_{\rho} + 1 \leq C|\rho| \leq Cn \) choices for \( \ell_1 \in \Lambda_0^c \) such that \( \ell \in (\ell_1, \ell_1 + \rho) \). Consequently,
\[ |\mathcal{B}_n(\ell) \cap A_3| \leq Cn|\Lambda_0^h \cap (B_n(0) \setminus B_{n-1}(0))| \leq Cn|B_n(0) \setminus B_{n-1}(0)| \leq Cn(n^d - (n - 1)^d) \leq Cn^d. \]  
(A.16)

In order to show the remaining estimates, we require the following estimate. Suppose that \( (\ell_1, \ell_2) \in \mathcal{B}_n(\ell) \), then using Lemma A.2, we deduce that
\[ |\ell - \ell_1| \leq C|\ell_1 - \ell_2| \max_{\ell' \in \Lambda, \ell' \in \Lambda(\ell')} |\ell' - m'| \leq C_0n. \]  
(A.17)

An identical argument also shows that \( |\ell - \ell_2| \leq C_0n \).
Applying (A.17), we now estimate
\[ |B_n(\ell) \cap A_2| \leq 2|A^h \cap B_{C_{0,n}}(\ell) \times \Lambda_0| = |\Lambda_0||A^h \cap B_{C_{0,n}}(\ell)| \leq C|\Lambda_0||B_{C_{0,n}}(\ell)| \leq CC_0^d d^d. \tag{A.18} \]
For the final estimate, recall the sets \( Q_{1,i}, Q_{2,i} \subset A^h \), for \( 1 \leq i \leq d \), defined by (A.7)–(A.8) in the proof of Lemma A.2. It follows from (A.9) that \( A_4 = \bigcup_{i=1}^d ((Q_{1,i} \times Q_{2,i}) \cup (Q_{2,i} \times Q_{1,i})) \). Now suppose \( \ell_1, \ell_2 \in B_n(\ell) \cap A_4 \), then without loss of generality suppose that \( \ell_1 \in Q_{1,i}, \ell_2 \in Q_{2,i} \), for some \( 1 \leq i \leq d \). By definition, for \( i' = 1, 2 \), \( \ell_{i'} = \sum_{j=1}^d n_{j,i'} A e_j \), where \( n_{i,1} < -k, n_{i,2} > k \) and \( n_{j,1}, n_{j,2} \in \mathbb{Z} \cap [-k, k] \) for \( j \neq i \). Let \( c_0 = \min_{1 \leq i \leq d} |A e_{i}| > 0 \) and observe that \( d(\ell_1, \Lambda_0) = n_{i,1} + k \leq |\ell_1 - \ell_2| \leq n \). Arguing by contradiction, it follows that \( n_{i,1} \geq -c_0^{-1} n - k \). An identical argument shows that \( n_{i,2} \leq c_0^{-1} n + k \), so define
\[
Q_{1, n, i} = \left\{ \sum_{j=1}^d n_{j,1} A e_j \mid (n_{j}) \in \mathbb{Z}^d, -c_0^{-1} n - k \leq n_{i} < -k \text{ and } n_{j} \in [-k, k] \text{ for all } j \neq i \right\},
\]
\[
Q_{2, n, i} = \left\{ \sum_{j=1}^d n_{j,2} A e_j \mid (n_{j}) \in \mathbb{Z}^d, k < n_{i} \leq c_0^{-1} n + k \text{ and } n_{j} \in [-k, k] \text{ for all } j \neq i \right\}.
\]
We then deduce that
\[
|B_n(\ell) \cap A_4| = \sum_{i=1}^d |B_n(\ell) \cap ((Q_{1,i} \times Q_{2,i}) \cup (Q_{2,i} \times Q_{1,i}))| \\
= 2 \sum_{i=1}^d |B_n(\ell) \cap (Q_{1,i} \times Q_{2,i})| \leq 2 \sum_{i=1}^d |Q_{1,n,i} \times Q_{2,n,i}| \\
\leq 2 \sum_{i=1}^d |Q_{1,n,i}| |Q_{2,n,i}| \leq C d k^{2d-2} n^2 \leq C n^d,
\]
where we have used that \( d \in \{2, 3\} \). Collecting the estimates (A.15),(A.16),(A.18) and (A.19) gives the desired estimate (A.6)
\[
|B_n(\ell)| = \sum_{i=1}^4 |B_n(\ell) \cap A_i| \leq C n^d.
\]

Proof of Lemma A.1. We show that for \( k = 1, 2 \)
\[
c_k \|Du\|_{\ell^2_N} \leq \|Du\|_{\ell^2_{\varphi, k}}.
\]
From the uniform lower bound on \( \varphi \), for any \( \ell \in \Lambda, \rho \in \mathcal{N}(\ell) - \ell \), \( \varphi(|\rho|)^{-1} \leq c_0^{-1} \). As \( k \leq 2 \), using the embedding \( \ell^k \subseteq \ell^2 \)
\[
|Du(\ell)|_{\mathcal{N}} = \left( \sum_{\rho \in \mathcal{N}(\ell) - \ell} |D_\rho u(\ell)|^2 \right)^{1/2} \leq \left( \sum_{\rho \in \mathcal{N}(\ell) - \ell} |D_\rho u(\ell)|^k \right)^{1/k} \leq \left( c_0^{-1} \sum_{\rho \in \mathcal{N}(\ell) - \ell} \varphi(|\rho|)^{-1} |D_\rho u(\ell)|^k \right)^{1/k} \leq c_0^{-1/k} |Du(\ell)|_{\varphi, k}.
\]
This implies (A.20) as
\[
\|Du\|_{\ell^2_N} = \left( \sum_{\ell \in \Lambda} |Du(\ell)|_{\mathcal{N}}^2 \right)^{1/2} \leq c_0^{-1/k} \left( \sum_{\ell \in \Lambda} |Du(\ell)|_{\varphi, k}^2 \right)^{1/2} = c_0^{-1/k} \|Du\|_{\ell^2_{\varphi, k}}.
\]
We now show (A.5). By Lemma A.2, for each \( \ell \in \Lambda \) and \( \rho \in \Lambda - \ell \), there exists a path \( \mathcal{P}(\ell, \ell + \rho) = \{ \ell_i \in \Lambda | 1 \leq i \leq N_\rho + 1 \} \) of neighbouring lattice points, such that \( N_\rho \leq C|\rho| \) and \( \rho_i := \ell_{i+1} - \ell_i \in \mathcal{N}(\ell_i) - \ell_i \) for all \( 1 \leq i \leq N_\rho \), satisfying

\[
|D_\rho u(\ell)| \leq \sum_{i=1}^{N_\rho} |D_{\rho_i} u(\ell_i)|.
\]

Applying Hölder’s inequality gives

\[
|D_\rho u(\ell)|^k \leq \left( \sum_{i=1}^{N_\rho} |D_{\rho_i} u(\ell_i)| \right)^k \leq |\rho|^{k-1} \sum_{i=1}^{N_\rho} |D_{\rho_i} u(\ell_i)|^k \leq C|\rho|^{k-1} \sum_{i=1}^{N_\rho} |D_{\rho_i} u(\ell_i)|^k.
\]

Now,

\[
\|Du\|_{L^k_{w,k}} = \left( \sum_{\ell \in \Lambda} |D u(\ell)|^k \right)^{1/k} = \left( \sum_{\ell \in \Lambda} \sum_{\rho \in \Lambda - \ell} w(|\rho|)|D_\rho u(\ell)|^k \right)^{1/k} \leq C \left( \sum_{\ell \in \Lambda} \sum_{\rho \in \Lambda - \ell} w(|\rho|)|\rho|^{k-1} \sum_{i=1}^{N_\rho} |D_{\rho_i} u(\ell_i)|^k \right)^{1/k} \leq C \left( \sum_{\ell \in \Lambda} \sum_{\rho \in \Lambda - \ell} w(|\rho|)|\rho|^{k-1} \sum_{i=1}^{N_\rho} \sum_{\rho' \in \mathcal{N}(\ell_i) - \ell_i} |D_{\rho'} u(\ell_i)|^k \right)^{1/k} = C \left( \sum_{\ell' \in \Lambda} \sum_{\rho' \in \mathcal{N}(\ell') - \ell'} |D_{\rho'} u(\ell')|^k \right)^{1/k} \sum_{\ell \in \Lambda} \sum_{\rho \in \Lambda - \ell} w(|\rho|)|\rho|^{k-1} \right)^{1/k} \tag{A.21}
\]

By Lemma A.3, for all \( \ell' \in \Lambda \) and \( n \in \mathbb{N} \), the set

\[
\mathcal{B}_n(\ell') = \left\{ (\ell_1, \ell_2) \in (\Lambda)^2 \mid n - 1 < |\ell_1 - \ell_2| \leq n, \ell' \in \mathcal{P}(\ell_1, \ell_2) \right\}
\]

satisfies \( |\mathcal{B}_n(\ell')| \leq Cn^d \). As \( w \) is a decreasing function, it follows that

\[
\sum_{\ell \in \Lambda} \sum_{\rho \in \Lambda - \ell} w(|\rho|)|\rho|^{k-1} = \sum_{n=1}^{\infty} \sum_{\ell_1, \ell_2 \in \mathcal{B}_n(\ell')} w(|\ell_1 - \ell_2|)|\ell_1 - \ell_2|^{k-1} \leq C \sum_{n=1}^{\infty} w(n-1)n^{k+d-1} \leq w(0) + 2^{k+d-1}w(1) + C \sum_{n=3}^{\infty} w(n-1)(n-2)^{k+d-1} \leq C \left( 1 + \sum_{n=1}^{\infty} w(n+1)n^{k+d-1} \right) \leq C \left( 1 + \int_1^{\infty} w(x)x^{k+d-1}dx \right) \leq C(1 + \|w\|_{L^k_{w,k}}).
\]

\[\tag{A.22}\]
Combining (A.21)–(A.22) and applying the embedding $\ell^k \subset \ell^2$ yields

$$
\|Du\|_{H_{m,k}} \leq C \left( \sum_{\ell' \in \Lambda} \sum_{\rho' \in \mathcal{N}(\ell')-\ell'} |D_{\rho'} u(\ell')|^k \sum_{\rho \in \Lambda-\ell} \sum_{\ell'' \in \mathcal{P}(\ell',\ell''+\rho)} w(|\rho|)|\rho|^{k-1} \right)^{1/k}
$$

$$
\leq C \left( \sum_{\ell' \in \Lambda} \sum_{\rho' \in \mathcal{N}(\ell')-\ell'} |D_{\rho'} u(\ell')|^k \right)^{1/k}
\leq C \left( \sum_{\ell' \in \Lambda} \sum_{\rho' \in \mathcal{N}(\ell')-\ell'} |D_{\rho'} u(\ell')|^2 \right)^{1/2} = C \|Du\|_{L_N^2}.
$$

It remains to show that for $w \in \mathcal{L}_1$, $\|Du\|_{l^2_{m,1}} \leq C \|Du\|_{l^2_N}$. Define for $x > 0$, $\tilde{w}(x) = w(x)|x|^{-1} \in \mathcal{L}_2$, which satisfies $\|\tilde{w}\|_{\mathcal{L}_2} = \|w\|_{\mathcal{L}_1}$. Applying Cauchy–Schwarz gives

$$
|Du(\ell)|_{m,1} = \sum_{\rho \in \Lambda-\ell} w(|\rho|)|D_{\rho} u(\ell)| = \sum_{\rho \in \Lambda-\ell} (w(|\rho|)^{1/2}|\rho|^{1/2}) (w(|\rho|)^{1/2}|\rho|^{-1/2}|D_{\rho} u(\ell)|)
\leq \left( \sum_{\rho \in \Lambda-\ell} w(|\rho|)|\rho| \right)^{1/2} \left( \sum_{\rho \in \Lambda-\ell} w(|\rho|)|\rho|^{-1} |D_{\rho} u(\ell)|^2 \right)^{1/2} = \|w\|^{1/2}_{L_1} \|Du(\ell)\|_{l^2_{m,2}}.
$$

The desired estimate follows from applying (A.5)

$$
\|Du\|_{l^2_{m,1}} \left( \sum_{\ell \in \Lambda} |Du(\ell)|^2_{l^2_{m,1}} \right)^{1/2} \leq \|w\|^{1/2}_{L_1} \left( \sum_{\ell \in \Lambda} |Du(\ell)|^2_{l^2_{m,2}} \right)^{1/2} = \|w\|^{1/2}_{L_1} \|Du\|_{l^2_{m,2}}
\leq C \|w\|^{1/2}_{L_1} \|\tilde{w}\|^{1/2}_{L_{\infty}} \|Du\|_{l^2_N} = C \|w\|_{L_1} \|Du\|_{l^2_N}.
$$

This completes the proof. \(\square\)

**APPENDIX B. PROOFS: INTERPOLATIONS BETWEEN DEFECTIVE AND HOMOGENEOUS LATTICE**

We now introduce three interpolation operators that map displacements from a defective reference configuration to the corresponding homogeneous lattice and vice versa. These operators will be used to prove our main results.

**Lemma B.1.** There exists an operator $I^h_1 : \mathcal{W}^{1,2}(\Lambda) \to \mathcal{W}^{1,2}(\Lambda^h)$ and $C_* > 0$ such that for all $u \in \mathcal{W}^{1,2}(\Lambda)$

$$
\|DI^h_1 u\|_{H^2(\Lambda^h)} \leq C_* \|Du\|_{H^2(\Lambda)},
$$

and there exists $R_0 = R_0(u) > 0$ such that $I^h_1 u(\ell) = u(\ell)$ for all $|\ell| > R_0$. Moreover, suppose $u \in \mathcal{H}_{m,\Lambda}(\Lambda)$, where $0 < m < 1$, then $I^h_1 u \in \mathcal{H}_{m,C_*,\Lambda}(\Lambda^h)$.

The key property of the interpolation $I^h_1$ is that it maps $\mathcal{H}(\Lambda)$ to $\mathcal{H}(\Lambda^h)$, hence for any $u \in \mathcal{H}(\Lambda)$, the locality and homogeneity estimates (2.13), (2.16) continue to hold for $I^h_1 u$.

We also define the following pair of linear interpolations.

**Lemma B.2.** There exists a bounded linear operator $I^h_2 : \mathcal{W}^{1,2}(\Lambda) \to \mathcal{W}^{1,2}(\Lambda^h)$ and $C > 0$ such that for all $u \in \mathcal{W}^{1,2}(\Lambda)$

$$
\|DI^h_2 u\|_{H^2(\Lambda^h)} \leq C \|Du\|_{H^2(\Lambda)},
$$

and $I^h_2 u(\ell) = u(\ell)$ for all $|\ell| > R_{\text{def}}$, $u \in \mathcal{W}^{1,2}(\Lambda)$. 
Moreover, there exists $c_0 \in (0, 1]$ such that for all $r > 0$, there exists $R \geq r$ satisfying: for all $w \in \mathcal{L}_1$

$$\sum_{\ell \in \Lambda \cap B_r} |D I^h u(\ell)|_{m,1} \leq C \sum_{\ell \in \Lambda \cap B_R} |D u(\ell)|_{m,1},$$

where $\tilde{w}(r) := w(c_0 r) \in \mathcal{L}_1$.

The main differences between $I^h_1, I^h_2$ is that $I^h_2$ is linear and in general $I^h_2$ does not map $\mathcal{H}(\Lambda)$ to $\mathcal{H}(\Lambda^h)$ and that $I^h_2 u(\ell) = u(\ell)$ for all $|\ell| > R_{\text{def}}$, where the constant $R_{\text{def}}$ is fixed, hence is independent of $u \in \mathcal{H}^{1,2}(\Lambda)$. In comparison, the constant $R_0$ appearing in Lemma B.1 is dependent on $u \in \mathcal{H}^{1,2}(\Lambda)$, in particular it is straightforward to define a sequence $\{u_n\} \subset \mathcal{H}^{1,2}(\Lambda)$ with $\|Du_n\|_{\mathcal{H}_2(\Lambda)} = 1$ satisfying $R_0(u_n) \to \infty$ as $n \to \infty$.

One can also define interpolations from $\mathcal{H}^{1,2}(\Lambda^h)$ to $\mathcal{H}^{1,2}(\Lambda)$, analogously to Lemmas B.1 and B.2. However, for the purpose of our analysis, we only require the following interpolation.

**Lemma B.3.** There exists a bounded linear operator $I^d : \mathcal{H}^{1,2}(\Lambda^h) \to \mathcal{H}^{1,2}(\Lambda)$ and $C > 0$ such that for all $v^h \in \mathcal{H}^{1,2}(\Lambda^h)$

$$\|D I^d v^h\|_{\mathcal{H}^2(\Lambda)} \leq C \|D v^h\|_{\mathcal{H}^2(\Lambda^h)},$$

and $I^d v^h(\ell) = v^h(\ell)$ for all $|\ell| > R_{\text{def}}$, $v^h \in \mathcal{H}^{1,2}(\Lambda^h)$.

Moreover, there exists $c_0 \in (0, 1]$ such that for all $r > 0$, there exists $R \geq r$ satisfying: for all $w \in \mathcal{L}_1$

$$\sum_{\ell \in \Lambda \cap B_r} |D I^d v^h(\ell)|_{m,1} \leq C \sum_{\ell \in \Lambda \cap B_R} |D v(\ell)|_{m,1},$$

Proof of Lemma B.1. Let $u \in \mathcal{H}(\Lambda)$, hence there exist $\lambda > 0$ and $0 < m < 1$ such that $y_0 + u \in \mathcal{A}_{m,\lambda}(\Lambda)$. Alternatively, when $u \in \mathcal{H}^{1,2}(\Lambda) \setminus \mathcal{H}(\Lambda)$, we simply choose $m = 1/2$. As $\|Du\|_{\mathcal{H}^2(\Lambda)} < \infty$, for all $\varepsilon > 0$, there exists $R_1 = R_1(\varepsilon) > R_{\text{def}}$ such that for all $R \geq R_1$

$$\|Du\|_{\mathcal{H}^2(\Lambda \setminus B_R)} = \left( \sum_{|\ell| > R, \rho \in \mathcal{N}(\ell) - \ell} |D\rho u(\ell)|^2 \right)^{1/2} < \varepsilon. \tag{B.1}$$

Using that $\Lambda \setminus B_{R_{\text{def}}} = \Lambda^h \setminus B_{R_{\text{def}}}$ and $R_1 > R_{\text{def}}$, we define $u_1 \in \mathcal{H}^{1,2}(\Lambda^h)$ by

$$u_1(\ell) := \begin{cases} u(\ell) & \text{if } |\ell| > R_1, \\ 0 & \text{otherwise.} \end{cases}$$

Due to the boundary terms introduced by the truncation, it is not in general possible to estimate the norm $\|Du_1\|_{\mathcal{H}^2(\Lambda^h)}$ in terms of $\|Du\|_{\mathcal{H}^2(\Lambda)}$, however, there exists $R_2 = R_2(\varepsilon) > R_1$ such that choosing $|\ell| > R_2$ ensures that $D\rho u_1(\ell) = D\rho u(\ell)$ for all $\rho \in \mathcal{N}(\ell) - \ell$, hence for any subset $A \subset B_{R_2(\varepsilon)}$, we have $\|Du_1\|_{\mathcal{H}^2(\Lambda^h \setminus A)} = \|Du\|_{\mathcal{H}^2(\Lambda \setminus A)}$.

For any $v \in \mathcal{H}^{1,2}(\Lambda^h)$, it is possible to define a triangulation of $\Lambda^h$ and construct an interpolant [13, 30]

$$\tilde{v} \in \tilde{W}^{1,2} := \{ w : \mathbb{R}^d \to \mathbb{R}^d \mid w \in W^{1,2}_\text{loc}, \nabla w \in L^2 \},$$

satisfying $\tilde{v}(\ell) = v(\ell)$ for all $\ell \in \Lambda^h$ and there exist constants $C, R_3 > 0$ such that for all $v \in \mathcal{H}^{1,2}(\Lambda^h)$ and $R \geq R_3$,

$$\|\nabla \tilde{v}\|_{L^2(B_{R/2}(0)^c)} \leq C \|Dv\|_{\mathcal{H}^2(\Lambda^h \setminus B_{R/4}(0))}. \tag{B.2}$$
Additionally, by [30, Lemma 3] there exists \( C', R_4 > 0 \) such that for all \( v \in \dot{W}^{1,2}(\Lambda^h) \) and \( \ell \in \Lambda^h \)

\[
|v(\ell)| = |\tilde{v}(\ell)| \leq C'\|\tilde{v}\|_{L^2(B_{R_4}(\ell))}.
\]

Suppose that \( R \geq 2R_4 \) and define \( A_R = B_{5R/2}(0) \setminus B_{R/2}(0) \), then we deduce that for all \( v \in \dot{W}^{1,2}(\Lambda^h) \)

\[
\sum_{\ell \in \Lambda^h, R<|\ell|<2R} |v(\ell)|^2 \leq C C_0\|\tilde{v}\|^2_{L^2(A_R)} = C\|\tilde{v}\|^2_{L^2(A_R)},
\]

where the final constant is independent of \( R > 0 \). We remark that the constants \( R_3, R_4 \) are independent of \( \varepsilon > 0 \).

Choose \( \eta \in C^\infty(\mathbb{R}^d) \) satisfying \( 0 \leq \eta \leq 1 \), \( \eta = 0 \) on \( B_1(0) \), \( \eta = 1 \) over \( B_2(0)^c \) and \( \|\eta\|_{W^{1,\infty}(\mathbb{R}^d)} \leq C_\eta \), then for \( R \geq R_5 = R_5(\varepsilon) := \max\{4R_2, R_3, 2R_4\} \), define \( \eta_R(x) := \eta(x/R) \). Observe that \( \eta_R \) satisfies \( |\nabla \eta_R(x)| \leq C_\eta R^{-1} \) for all \( x \in \mathbb{R}^d \). Now define \( \tilde{u}_R \in \dot{W}^{1,2} \) by

\[
\tilde{u}_R(x) = \eta_R(x) (\tilde{u}_1(x) - \langle \tilde{u}_1 \rangle_{A_R}) + \langle \tilde{u}_1 \rangle_{A_R},
\]

where \( \langle \tilde{u}_1 \rangle_{A_R} = |A_R|^{-1} \int_{A_R} \tilde{u}_1 \) denotes the average integral of \( \tilde{u}_1 \) over \( A_R \). We now define \( u_R \in \dot{W}^{1,2}(\Lambda^h) \) by \( u_R(\ell) = \tilde{u}_R(\ell) \) for all \( \ell \in \Lambda^h \). We now estimate the norm

\[
\|D u_R\|^2_{\dot{W}^2(\Lambda^h)} = \sum_{\ell \in \Lambda^h, \rho \in N(\ell) - \ell} |D_\rho u_R(\ell)|^2.
\]

We remark that while similar estimates have been performed in [13], we additionally require that our construction satisfies \( I_1^h u \in \mathcal{H}(\Lambda^h) \). In particular, this prevents the accumulation of atoms, which is necessary to treat the models given in Section 4. Hence, we need to establish more careful estimates.

We can decompose the above sum into the following terms

\[
\|D u_R\|^2_{\dot{W}^2(\Lambda^h)} \leq \sum_{|\ell|<R, \rho \in N(\ell) - \ell} |D_\rho u_R(\ell)|^2 + \sum_{|\ell|>2R, \rho \in N(\ell) - \ell} |D_\rho u_R(\ell)|^2 \quad (B.5)
\]

\[
+ 3 \sum_{R<|\ell|<2R, \rho \in N(\ell) - \ell} |D_\rho u_R(\ell)|^2. \quad (B.6)
\]

As \( \eta_R = 0 \) over \( B_R(0) \), it follows that \( D_\rho u_R(\ell) = 0 \) whenever \( |\ell|, |\ell + \rho| < R \), therefore the first term in (B.5) vanishes

\[
\sum_{|\ell|<R, \rho \in N(\ell) - \ell} |D_\rho u_R(\ell)|^2 = 0. \quad (B.7)
\]

Similarly, using that \( \eta_R = 1 \) on \( B_{2R}(0)^c \), it follows that \( D_\rho u_R(\ell) = D_\rho \tilde{u}_1(\ell) = D_\rho u_1(\ell) \) for all \( |\ell|, |\ell + \rho| > 2R \), hence the second term of (B.5) can be estimated by

\[
\sum_{|\ell|>2R, \rho \in N(\ell) - \ell} |D_\rho u_R(\ell)|^2 = \sum_{|\ell|>2R, \rho \in N(\ell) - \ell} |D_\rho u_1(\ell)|^2 \leq \sum_{|\ell|>2R, \rho \in N(\ell) - \ell} |D_\rho u_1(\ell)|^2 = \|D u_1\|^2_{\dot{W}^2(\Lambda^h(B_{2R}(0)))}. \quad (B.8)
\]

It remains to estimate the term (B.6), we first express

\[
D_\rho u_R(\ell) = (\eta_R(\ell + \rho) - \eta_R(\ell)) (\tilde{u}_1(\ell) - \langle \tilde{u}_1 \rangle_{A_R}) + \eta_R(\ell + \rho) D_\rho \tilde{u}_1(\ell),
\]
which can be estimated by
\[ |D_\rho u_R(\ell)| = |\eta_R(\ell + \rho) - \eta_R(\ell)||\tilde{u}_1(\ell) - \langle \tilde{u}_1 \rangle_{A_R}| + |D_\rho \tilde{u}_1(\ell)| \]
\[ \leq \left| \int_0^1 \nabla \eta_R(\ell + t\rho) \, dt \right| |\tilde{u}_1(\ell) - \langle \tilde{u}_1 \rangle_{A_R}| + |D_\rho u_1(\ell)| \]
\[ \leq CR^{-1}\rho||\tilde{u}_1(\ell) - \langle \tilde{u}_1 \rangle_{A_R}| + |D_\rho u_1(\ell)| \]
\[ \leq CR^{-1}|\tilde{u}_1(\ell) - \langle \tilde{u}_1 \rangle_{A_R}| + |D_\rho u_1(\ell)|. \] (B.9)

Applying (B.9) to (B.6) yields
\[ \sum_{R<|\ell|<2R} \sum_{\rho \in N(\ell)-\ell} |D_\rho u_R(\ell)|^2 \]
\[ \leq CR^{-2} \sum_{R<|\ell|<2R} \sum_{\rho \in N(\ell)-\ell} |\tilde{u}_1(\ell) - \langle \tilde{u}_1 \rangle_{A_R}|^2 + C \sum_{R<|\ell|<2R} \sum_{\rho \in N(\ell)-\ell} |D_\rho u_1(\ell)|^2 \]
\[ \leq CR^{-2} \sum_{R<|\ell|<2R} |\tilde{u}_1(\ell) - \langle \tilde{u}_1 \rangle_{A_R}|^2 + C\|Du_1\|_{L^2(A_R)}^2 \] (B.10)

We observe that applying (B.3) to \( v = u_1 - \langle \tilde{u}_1 \rangle_{A_R} \), which satisfies \( \bar{v} = \tilde{u}_1 - \langle \tilde{u}_1 \rangle_{A_R} \), gives
\[ CR^{-2} \sum_{R<|\ell|<2R} |\tilde{u}_1(\ell) - \langle \tilde{u}_1 \rangle_{A_R}|^2 \leq CR^{-2}\|\tilde{u}_1 - \langle \tilde{u}_1 \rangle_{A_R}\|_{L^2(A_R)}^2. \] (B.11)

By applying Poincaré’s inequality on \( A_1 \) and using a standard scaling argument, we deduce that
\[ CR^{-2}\|\tilde{u}_1 - \langle \tilde{u}_1 \rangle_{A_R}\|_{L^2(A_R)}^2 \leq (CR^{-2})(CPR^2)\|\nabla \tilde{u}_1\|_{L^2(A_R)}^2 \]
\[ \leq C\|\nabla \tilde{u}_1\|_{L^2(B_{R/2}(0)^c)}^2. \] (B.12)

hence by inserting (B.11)–(B.12) into (B.10) and applying (B.2), we infer that
\[ \sum_{R<|\ell|<2R} \sum_{\rho \in N(\ell)-\ell} |D_\rho u_R(\ell)|^2 \leq C\|\nabla \tilde{u}_1\|_{L^2(B_{R/2}(0)^c)}^2 \leq C\|Du_1\|_{L^2(A_R)}^2, \] (B.13)

where the final constant is independent of \( R > 0 \).

Combining the estimates (B.7), (B.8) and (B.13) with (B.5)–(B.6), we deduce that
\[ \|Du_R\|_{L^2(A_R)} \leq C\|Du_1\|_{L^2(A_R)} \leq C\|Du\|_{L^2(A_R)} \leq C_*\|Du\|_{L^2(A_R)}. \] (B.14)

We remark that collecting the estimates (B.11)–(B.13) and applying (B.1) with \( R/4 \geq R > R_1 \), we infer that
\[ \|u_1 - \langle \tilde{u}_1 \rangle_{A_R}\|_{L^2(B_{R/2}(0)^c)} \leq CR\|Du\|_{L^2(A_R)} \leq CR \varepsilon. \] (B.15)

It remains to show that we can choose \( R > 0 \) sufficiently large to ensure that for all \( \ell, m \in \Lambda^h \),
\[ |\ell - m + u_R(\ell) - u_R(m)| \geq m|\ell - m|. \] (B.16)

Once (B.16) has been shown, it follows that \( y_0^h + u_R \in \mathcal{H}_{m,C_*}(\Lambda^h) \) for sufficiently large \( R > 0 \).

We prove (B.16) by consider four distinct cases.

**Case 1** Suppose that \( \ell, m \in B_R(0) \), then as \( \eta_R = 0 \) on \( B_R(0) \), it follows that \( u_R(\ell) = u_R(m) \), hence
\[ |\ell - m + u_R(\ell) - u_R(m)| = |\ell - m| \geq m|\ell - m|. \] (B.17)

**Case 2** Suppose that \( |\ell| > 2R \) and \( |m| < R \), which implies that \( |\ell - m| > R \), then by Lemma A.2, there exists a path \( \mathbf{P}(\ell,m) = \{\ell_i \in \Lambda |1 \leq i \leq N_{\ell,m} + 1\} \) of neighbouring
lattice points, such that \( N_{\ell, m} \leq C|\ell - m| \) and \( \rho_i := \ell_{i+1} - \ell_i \in N(\ell_i) - \ell_i \) for all \( 1 \leq i \leq N_{\ell, m} \), satisfying \( |u_R(\ell) - u_R(m)| \leq \sum_{i=1}^{N_{\ell, m}} |D_{\rho_i}u_R(\ell_i)| \). Applying Cauchy-Schwarz gives

\[
|u_R(\ell) - u_R(m)| \leq N_{\ell, m}^{1/2} \left( \sum_{i=1}^{N_{\ell, m}} |D_{\rho_i}u_R(\ell_i)|^2 \right)^{1/2} \leq C|\ell - m|^{1/2} \|Du_R\|_{L^2(\Lambda)}.
\]  

Choosing \( R \geq R_6 = (C\Lambda(1-\lambda/m)^2 \) ensures that \( (1 - m)|\ell - m|^{1/2} \geq (1 - m)R^{1/2} \geq C_1 \lambda \), hence

\[
|\ell + m + u_R(\ell) - u_R(m)| \geq |\ell - m| - |u_R(\ell) - u_R(m)| \geq |\ell - m| - C_1 \lambda |\ell - m|^{1/2}
\]

\[
= |\ell - m|^{1/2}(|\ell - m|^{1/2} - C_1 \lambda) \geq |m| - |\ell - m|.
\]  

Case 3 Now suppose \( \ell, m \in B_R(0)^c \), then applying the estimate (B.9) gives

\[
|u_R(\ell) - u_R(m)| \leq |\eta_R(\ell) - \eta_R(m)||u_1(\ell) - \langle \tilde{u}_1 \rangle_{A_R}| + |\eta_R(m)||u_1(\ell) - u_1(m)| \\
\leq CR^{-1}|\ell - m|u_1(\ell) - \langle \tilde{u}_1 \rangle_{A_R}| + |u_1(\ell) - u_1(m)|.
\]  

In order to estimate the first term of (B.20), we apply (B.15) and the embedding \( \ell^2 \subset \ell^\infty \) to deduce

\[
CR^{-1}\|u_1(\ell) - \langle \tilde{u}_1 \rangle_{A_R}\| \leq CR^{-1}\|u_1 - \langle \tilde{u}_1 \rangle_{A_R}\|_{\ell^\infty(\Lambda \cap (B_{2R}(0) \setminus B_R(0)))} \\
\leq CR^{-1}\|u_1 - \langle \tilde{u}_1 \rangle_{A_R}\|_{\ell^2(\Lambda \cap (B_{2R}(0) \setminus B_R(0)))} \\
\leq (CR^{-1})(CR\varepsilon) = C_1\varepsilon,
\]  

where the constant \( C_1 \) is independent of \( R > 0 \).

We estimate the second term appearing in (B.20) using the argument of (B.18). By Lemma A.2, there exists a path \( \mathcal{P}(\ell, m) = \{\ell_i \in \Lambda | 1 \leq i \leq N_{\ell, m} + 1\} \) of neighbouring lattice points, such that \( N_{\ell, m} \leq C|\ell - m| \) and \( \rho_i := \ell_{i+1} - \ell_i \in N(\ell_i) - \ell_i \) for all \( 1 \leq i \leq N_{\ell, m} \), satisfying \( |u_1(\ell) - u_1(m)| \leq \sum_{i=1}^{N_{\ell, m}} |D_{\rho_i}u_1(\ell_i)| \). Moreover, the path \( \mathcal{P}(\ell, m) \) can be chosen to ensure that \( |\ell_i| > R \) for all \( 1 \leq i \leq N_{\ell, m} + 1 \). Applying Cauchy-Schwarz gives

\[
|u_1(\ell) - u_1(m)| \leq N_{\ell, m}^{1/2} \left( \sum_{i=1}^{N_{\ell, m}} |D_{\rho_i}u_1(\ell_i)|^2 \right)^{1/2} \leq C|\ell - m|^{1/2} \|Du_1\|_{L^2(\Lambda \setminus B_R(0))},
\]  

Using (B.1) and that \( \varepsilon_0 = \inf_{\ell \neq m} |\ell - m| > 0 \), we deduce that

\[
|u_1(\ell) - u_1(m)| \leq C|\ell - m|^{1/2}\|Du_1\|_{L^2(\Lambda \setminus B_R(0))} \\
\leq C\varepsilon_0^{-1/2}\|\ell - m| = C_2\varepsilon|\ell - m|.
\]  

Now let \( \varepsilon_0 = (C_1 + C_2)^{-1}(1 - m) \), then for \( R \geq \max\{R_5(\varepsilon_0), R_6\} \), collecting the estimates (B.20)–(B.22) gives

\[
|u_R(\ell) - u_R(m)| \leq (C_1 + C_2)\varepsilon|\ell - m| \leq (1 - m)|\ell - m|,
\]  

hence we obtain the desired estimate

\[
|\ell - m + u_R(\ell) - u_R(m)| \geq |\ell - m| - |u_R(\ell) - u_R(m)| \geq m|\ell - m|.
\]  

(B.23)
Case 4 In our final case, we consider \( \ell \in B_{2R}(0) \setminus B_R(0) \) and \( m \in B_R(0) \). We follow the argument of Case 3, while observing that as \( \eta_R(m) = 0 \), we obtain
\[
|u_R(\ell) - u_R(m)| \leq |\eta_R(\ell) - \eta_R(m)||u_1(\ell) - \langle \tilde{u}_1 \rangle_{A_R}| + |\eta_R(m)||u_1(\ell) - u_1(m)| \\
\leq |\eta_R(\ell) - \eta_R(m)||u_1(\ell) - \langle \tilde{u}_1 \rangle_{A_R}| \\
\leq CR^{-1}|\ell - m||u_1(\ell) - \langle \tilde{u}_1 \rangle_{A_R}| \\
\leq C_1\epsilon_0|\ell - m| \leq (1 - m)|\ell - m|.
\]
hence we obtain the desired estimate
\[
|\ell - m + u_R(\ell) - u_R(m)| \geq |\ell - m| - |u_R(\ell) - u_R(m)| \geq m|\ell - m|. \quad (B.24)
\]
Collecting the estimates (B.17)–(B.24) implies (B.16).

Finally, we define \( I_1^h u := u_R \in \mathcal{W}^{1,2}(A^h) \), where \( R = \max\{\tau_0(\epsilon_0), R_0\} \), which satisfies
\[
y_0^h + I_1^h u \in \mathcal{A}_{\mathfrak{m},\mathfrak{c},\Lambda} \text{ and } I_1^h u(\ell) = u(\ell).
\]
Due to the periodicity of \( \Lambda^h \), for each \( \ell \in \Lambda^h \) there exists a bounded Voronoi cell \( \mathcal{V}^h(\ell) \subset B_R(\ell) \), where \( \overline{R} = \frac{1}{2} \sum_{i=1}^{3} |\mathcal{A}_W| > 0 \), satisfying
\[
\mathcal{V}^h(\ell) = \left\{ x \in \mathbb{R}^3 \mid |x - \ell| \leq |x - k| \forall k \in \Lambda^h \right\}, \quad (B.25)
\]
and \( \mathcal{V}^h(\ell) = \mathcal{V}^h(0) + \ell \), due to the translation-invariance of \( \Lambda^h \). Using the definition (A.10), one may also define the Voronoi cell \( \mathcal{V}(\ell) \) for \( \ell \in \Lambda \). As \( \Lambda \setminus B_{R_0} = \Lambda^h \setminus B_{R_0} \), there exists \( R' > 0 \) such that \( \ell \in \Lambda \setminus B_{R'} \) guarantees \( \mathcal{V}(\ell) = \mathcal{V}^h(\ell) \subset B_{R_0}(\ell) \), which is bounded. As \( \{\mathcal{V}(\ell) | \ell \in \Lambda \} \) cover \( \mathbb{R}^3 \), it follows from the definition (A.10) that for \( \ell \in \Lambda \cap B_{R_1} \)
\[
\mathcal{V}(\ell) \subset \bigcup_{\ell' \in \Lambda \cap B_{R'}} \mathcal{V}(\ell') \subset \left( \left( \bigcup_{\ell' \in \Lambda \setminus B_{R'}} \mathcal{V}(\ell') \right)^{c} \right)^{c}, \quad (B.26)
\]
where \( X^{c} \) denotes the interior of the set \( X \). As the right-hand side of (B.26) is a bounded set, there exists \( R_0 > 0 \) such that \( \mathcal{V}(\ell) \subset B_{R_0}(\ell) \) for all \( \ell \in \Lambda \). In addition, there exists \( R_1 > 0 \) such that
\[
\Lambda^h \cap B_{R_0} \subset \bigcup_{\ell' \in \Lambda \cap B_{R_1}} \mathcal{V}(\ell'), \quad (B.27)
\]
hence for each \( \ell \in \Lambda^h \cap B_{R_0} \), there exists \( \ell' \in \Lambda \cap B_{R_1} \) such that \( \ell \in \mathcal{V}(\ell') \subset B_{R_0}(\ell'). \) Note that the choice of \( \ell' \) is in general not unique. Then define \( I_2^h u(\ell) = u(\ell') \). It follows from the construction that \( I_2^h \) is linear.

Consider distinct \( \ell_1, \ell_2 \in \Lambda^h \cap B_{R_0} \), then for \( i = 1, 2 \) there exist \( \ell_i' \in \Lambda \cap B_{R_1} \) such that \( I_2^h u(\ell_i) = u(\ell_i') \) and \( |\ell_i' - \ell_i| \leq R_0 \). It holds that
\[
|\ell_1 - \ell_2| \geq \min_{\ell' \in \Lambda, \ell' \neq \ell} |\ell - \ell'| := c_1 > 0 \text{ and similarly that}
\]
\[
|\ell_1' - \ell_2'| \leq \max_{\ell, \ell' \in \Lambda^h, \ell \neq \ell'} |\ell - \ell'| =: c_2 > 0, \text{ hence } |\ell_1 - \ell_2| \geq \frac{c_1}{c_2} |\ell_1' - \ell_2'| =: c_0 |\ell_1' - \ell_2'|, \text{ where}
\]
\( c_0 \in (0, 1] \). Using that \( w \in \mathcal{H}^{1} \), it follows that \( w \) is decreasing, hence
\[
w(|\ell_1 - \ell_2|) |I_2^h u(\ell_1) - I_2^h u(\ell_2)| \leq w(c_0 |\ell_1' - \ell_2'|) |u(\ell_1') - u(\ell_2')| \leq \sum_{\ell' \in \Lambda \cap B_{R_1}} w(c_0 |\ell_1' - \ell'|) |u(\ell_1') - u(\ell'|). \quad (B.28)
\]
We then define \( \tilde{w}(r) := w(c_0 r) \), and observe that \( \tilde{w} \in \mathcal{H}^{1} \). In the case \( \ell_1 \in \Lambda^h \cap B_{R_0} \) and \( \ell_2 \in \Lambda^h \setminus B_{R_0} \), then \( I_2^h u(\ell_2) = u(\ell_2) \), then a similar argument shows
\[
w(|\ell_1 - \ell_2|) |I_2^h u(\ell_1) - I_2^h u(\ell_2)| \leq w(c_0 |\ell_1' - \ell_2'|) |u(\ell_1') - u(\ell_2'|. \quad (B.29)
\]
Now, we decompose

\[ |D^h_2 u(\ell_1)|_{m,1} = \sum_{\ell_2 \in \Lambda^h} w(|\ell_1 - \ell_2|) |I^h_2 u(\ell_1) - I^h_2 u(\ell_2)| \]

\[ = \sum_{\ell_2 \in \Lambda^h \cap B_{ref}} w(|\ell_1 - \ell_2|) |I^h_2 u(\ell_1) - I^h_2 u(\ell_2)| + \sum_{\ell_2 \in \Lambda^h \setminus B_{ref}} w(|\ell_1 - \ell_2|) |I^h_2 u(\ell_1) - I^h_2 u(\ell_2)|, \]

then apply (B.28)–(B.29) to deduce

\[ |D^h_2 u(\ell_1)|_{m,1} \leq C|\Lambda^h \cap B_{ref}| \sum_{\ell' \in \Lambda \setminus B_{R_1}} w(c_0 |\ell_1 - \ell_2|) |u(\ell') - u(\ell')| \]

\[ + C \sum_{\rho' \in \Lambda - \ell_1} \tilde{w}(\rho') |D_{\rho'} u(\ell_1')| \]

\[ \leq C \sum_{\ell' \in \Lambda \setminus \ell_1} \tilde{w}(|\ell_1 - \ell_2|) |u(\ell_1') - u(\ell_2')| = C \sum_{\rho' \in \Lambda - \ell_1} \tilde{w}(|\rho|) |D_{\rho'} u(\ell_1')| \]

\[ = C |Du(\ell_1')|_{m,1} \leq C \sum_{\ell' \in \Lambda \setminus B_{R_1}} |Du(\ell')|_{m,1}. \] (B.30)

An identical argument shows that for \( \ell_1 \in \Lambda^h \setminus B_{R_{def}} \)

\[ |D^h_2 u(\ell_1)|_{m,1} \leq C |Du(\ell_1)|_{m,1}. \] (B.31)

Let \( r > 0 \) and choose \( R = \max\{R_1, r\} \), then combining (B.30)–(B.31) yields the desired estimate

\[ \sum_{\ell \in \Lambda^h \cap B_r} |D^h_2 u(\ell)|_{m,1} \leq C \sum_{\ell \in \Lambda^h \setminus B_R} |Du(\ell)|_{m,1}. \]

We now estimate \( \|D^h_2 u\|_{L^2(\Lambda^h)} \) using (B.30)–(B.31) and Cauchy–Schwarz

\[ \|D^h_2 u\|^2_{L^2(\Lambda^h)} = \sum_{\ell \in \Lambda^h} |D^h_2 u(\ell)|^2_{m,1} \]

\[ = \sum_{\ell \in \Lambda^h \cap B_{ref}} |D^h_2 u(\ell)|^2_{m,1} + \sum_{\ell \in \Lambda^h \setminus B_{ref}} |D^h_2 u(\ell)|^2_{m,1} \]

\[ \leq C \sum_{\ell \in \Lambda^h \cap B_{ref}} \left( \sum_{\ell' \in \Lambda \setminus B_{R_1}} |Du(\ell')|_{m,1} \right)^2 + C \sum_{\ell \in \Lambda \setminus B_{ref}} |Du(\ell)|^2_{m,1} \]

\[ \leq C |B_{R_1}| \sum_{\ell \in \Lambda^h \cap B_{ref}} \sum_{\ell' \in \Lambda \setminus B_{R_1}} |Du(\ell')|^2_{m,1} + C \sum_{\ell \in \Lambda \setminus B_{ref}} |Du(\ell)|^2_{m,1} \]

\[ \leq C |\Lambda^h \cap B_{R_{def}}| \sum_{\ell' \in \Lambda^h \setminus B_{R_1}} |Du(\ell')|^2_{m,1} + C \sum_{\ell' \in \Lambda \setminus B_{R_{def}}} |Du(\ell')|^2_{m,1} \]

\[ \leq C \sum_{\ell' \in \Lambda} |Du(\ell')|^2_{m,1} = C \|Du\|^2_{L^2_{m,1}(\Lambda)}. \]

The desired estimate then follows by an application of Lemma A.1

\[ \|D^h_2 u\|_{L^2(\Lambda^h)} \leq C \|D^h_2 u\|_{L^2_{m,1}(\Lambda^h)} \leq C \|Du\|^2_{L^2_{m,1}(\Lambda)} \leq C \|Du\|^2_{L^2_{m,1}(\Lambda)}. \]

**Proof of Lemma B.3.** This holds from following the proof of Lemma B.2 verbatim. \( \square \)
C.1. Proof of Lemma 2.2.

Proof of Lemma 2.2. Suppose that $u \in \mathcal{H}(\Lambda)$, then as $y := y_0 + u \in \mathcal{A}$, there exists $m > 0$ such that $|y(\ell) - y(m)| \geq m|\ell - m|$ for all $\ell, m \in \Lambda$. Moreover, as $u \in \mathcal{H}(\Lambda) \subset \mathcal{H}^{1,2}(\Lambda)$, Lemma 2.1 implies that there exists a sequence $u_n \in \mathcal{H}^c(\Lambda)$ such that $\|D(u_n - u)\|_{\mathcal{E}(\Lambda)} \to 0$ as $n \to \infty$. We now show that for sufficiently large $n$, we can ensure that $u_n \in \mathcal{H}^c(\Lambda)$.

Consider $\ell, m \in \Lambda$ and let $\rho = m - \ell$. By Lemma A.2, there exists a path $P(\ell, \ell + \rho) = \{\ell_i \in \Lambda|1 \leq i \leq N_\rho + 1\}$ of neighbouring lattice points, such that $N_\rho \leq C|\rho|$ and $\rho_i := \ell_{i+1} - \ell_i \in \mathcal{N}(\ell_i) - \ell_i$ for all $1 \leq i \leq N_\rho$, satisfying

$$|D_\rho(u_n - u)(\ell)| \leq \sum_{i=1}^{N_\rho} |D_{\rho_i}(u_n - u)(\ell_i)|.$$ 

Applying Cauchy-Schwarz gives

$$|D_\rho(u_n - u)(\ell)| \leq N_\rho^{1/2} \left( \sum_{i=1}^{N_\rho} |D_{\rho_i}(u_n - u)(\ell_i)| \right)^{1/2} \leq C|\rho|^{1/2} \|D(u_n - u)\|_{\mathcal{E}(\Lambda)} = C|\ell - m|^{1/2} \|D(u_n - u)\|_{\mathcal{E}(\Lambda)}.$$ 

Let $y_n = y_0 + u_n$, then rearranging gives

$$|y_n(\ell) - y_n(m)| = |\ell - m + u_n(\ell) - u_n(m)|$$
$$\geq |\ell - m + u(\ell) - u(m)| - |(u_n - u)(\ell) - (u_n - u)(m)|$$
$$= |y(\ell) - y(m)| - |D_\rho(u_n - u)(\ell)|$$
$$\geq m|\ell - m| - C_0 \|D(u_n - u)\|_{\mathcal{E}(\Lambda)} |\ell - m|^{1/2}.$$ 

As $c_1 := \inf_{\ell, m \in \Lambda} |\ell - m| > 0$, there exists $N > 0$, independent of $\ell, m$, such that $\|D(u_n - u)\|_{\mathcal{E}(\Lambda)} \leq c_1^{-1/2} m$ for all $n \geq N$, which ensures that

$$|y_n(\ell) - y_n(m)| \geq m|\ell - m| - C_0 \|D(u_n - u)\|_{\mathcal{E}(\Lambda)} |\ell - m|^{1/2}$$
$$\geq m|\ell - m| - \frac{m}{2} |\ell - m| \geq \frac{m}{2} |\ell - m|,$$

for all $\ell, m \in \Lambda$, hence for all $n \geq N$, $y_n = y_0 + u_n \in \mathcal{A}$ and thus $u_n \in \mathcal{H}^c(\Lambda)$, which completes the proof.

C.2. Proof of Theorem 2.7. In the following proof, we consider $u \in \mathcal{H}_{m,\lambda}$ for some $m, \lambda > 0$. For convenience, we assume that for all $t \in [0, 1]$, $y_0 + tu \in \mathcal{A}_{m/2,\lambda}$.

We remark that this condition does not hold in general, for example when $y_0 + u$ is a permutation of the initial configuration $y_0$. In this case, it is possible to construct a piecewise-linear path $y'_t \in \mathcal{A}_{m/2,\lambda}$ for $t \in [0, 1]$, satisfying $y'_0 = y_0$ and $y'_1 = y_0 + u$. Treating this case requires adapting the estimate (C.2) due to the fact that $\frac{1}{dt}Dy'_t(\ell) \neq Du(\ell)$ for some $\ell \in \Lambda$. We omit this argument for the sake of brevity.

Proof of Theorem 2.7. We remark that $\mathcal{L}_{k+2} \subset \mathcal{L}_k$ for all $k > 0$, hence it suffices to assume (S.L) holds under the perfect lattice and point defects condition, as the proof under the dislocations condition is identical.
Applying the estimate (C.2) and Lemma A.1 to (C.1) yields

\[
\left| V_t(Du_0(\ell) + Du(\ell)) - V_t(Du_0(\ell)) - \langle \delta V_t(Du_0(\ell)), Du(\ell) \rangle \right| 
\]

\[
\leq C \left( \sum_{\rho, \sigma \in \Lambda - \ell} \left| \omega_1(\rho) \right| \left| \omega_1(\sigma) \right| D_\rho u(\ell) D_\sigma u(\ell) \right) \leq C \left( \sum_{\rho \in \Lambda - \ell} \left| \omega_2(\rho) \right| D_\rho u(\ell) \right)^2 \]

\[
\leq C \left( \| D_\rho u \|_{\ell_{A,2}}^2 + \| D_\rho u \|_{\ell_{A,2}}^2 \right) \leq C \| D_\rho u \|_{\ell_{N}}^2. \tag{C.3}
\]

This implies that \( \mathcal{E}(u) - \langle T, u \rangle \) is well-defined for \( u \in \mathcal{H}_c \), hence as \( T \) is a bounded linear functional on \( (\mathcal{H}_c, \| D \cdot \|_{\ell_{N}}) \), it follows that \( \mathcal{E}(u) \) is well-defined for all \( u \in \mathcal{H}_c \) and that \( \delta \mathcal{E}(0) = T \).

(ii) Moreover, as \( \mathcal{E}(u) - \langle T, u \rangle = \mathcal{E}(u) - \mathcal{E}(0) - \langle \delta \mathcal{E}(0), u \rangle \), the estimate (C.3) implies that both \( \mathcal{E}(u) - \mathcal{E}(0) - \langle \delta \mathcal{E}(0), u \rangle \) is continuous on \( (\mathcal{H}_c, \| D \cdot \|_{\ell_{N}}) \). As \( \mathcal{E}(0) \) is a bounded linear functional, it also follows that \( \delta \mathcal{E}(u) \) is also continuous on \( (\mathcal{H}_c, \| D \cdot \|_{\ell_{N}}) \).

(iii) For \( u \in \mathcal{H}_c \) and \( j = 1 \), we have from (S.L) and Lemma A.1 that for any \( v \in \mathcal{H}_c \), there exists \( \theta \in (0, 1) \) such that

\[
\left| \langle \delta \mathcal{E}(u), v \rangle - \langle \delta \mathcal{E}(0), v \rangle \right| \leq \sum_{\ell \in \Lambda} \sum_{\rho, \sigma \in \Lambda - \ell} V_{\ell, \rho}(Dv_0(\ell) + \theta Du(\ell)) D_\rho v(\ell) D_\sigma v(\ell) \]

\[
\leq \sum_{\ell \in \Lambda} \sum_{\rho, \sigma \in \Lambda - \ell} \left| \omega_1(\rho) \right| \left| \omega_1(\sigma) \right| D_\rho u(\ell) D_\sigma v(\ell) + \sum_{\rho \in \Lambda - \ell} \left| \omega_2(\rho) \right| D_\rho u(\ell) D_\rho v(\ell) \]

\[
\leq C \left( \| D_\rho u \|_{\ell_{A,2}} \| Dv \|_{\ell_{A,2}} + \| D_\rho u \|_{\ell_{A,2}} \| Dv \|_{\ell_{A,2}} \right) \leq C \| D_\rho u \|_{\ell_{N}} \| Dv \|_{\ell_{N}}. \]

Since \( \delta \mathcal{E}(u_0) \) is a bounded linear functional on \( (\mathcal{H}_c, \| D \cdot \|_{\ell_{N}}) \), there exists a constant \( C \) such that

\[
\left| \langle \delta \mathcal{E}(u), v \rangle \right| \leq C \| Dv \|_{\ell_{N}} \quad \forall v \in \mathcal{H}_c,
\]

which implies that \( \mathcal{E} \) is differentiable. The case \( j = 2 \) in the following implies \( \mathcal{E} \) is continuously differentiable.
For \( u \in \mathcal{H}^c \) and \( 2 \leq j \leq n \), \( \mathbf{v} = (v_1, \ldots, v_j) \in (\mathcal{W}^c)^j \) and \( \mathbf{\rho} = (\rho_1, \ldots, \rho_j) \in (\Lambda - \ell)^j \), we have from (S.L) that there exist \( \mathbf{w}_k \in \mathcal{Z}_k \) for \( k = 1, \ldots, j \) such that

\[
|\langle \delta^j \mathbf{E}(u), \mathbf{v} \rangle| \leq \sum_{\ell \in \Lambda} \sum_{\mathbf{\rho} \in (\Lambda - \ell)} |\langle V_{\ell, \mathbf{\rho}}(Du(\ell)), D_{\mathbf{\rho}} \otimes \mathbf{v}(\ell) \rangle| \leq \sum_{\ell \in \Lambda} \sum_{\mathbf{\rho}_1, \ldots, \mathbf{\rho}_j} |V_{\ell, \mathbf{\rho}_1, \ldots, \mathbf{\rho}_j}(Du(\ell))| \prod_{1 \leq m \leq j} |D_{\rho_m} v_m(\ell)|.
\]

Applying (2.13) gives

\[
|\langle \delta^j \mathbf{E}(u), \mathbf{v} \rangle| \leq C \sum_{\ell \in \Lambda} \sum_{\mathbf{\rho}_1, \ldots, \mathbf{\rho}_j} \sum_{\{A_1, \ldots, A_k\} \in \mathcal{P}(j)} \left( \prod_{1 \leq i \leq k} \mathbf{w}_{|A_i|}(\rho_1^{\ell}) \prod_{m \in A_i} \delta_{\rho_i, \rho_m} \right) \prod_{1 \leq m \leq j} |D_{\rho_m} v_m(\ell)|.
\]

First fix \( \{A_1, \ldots, A_k\} \in \mathcal{P}(j) \) and consider

\[
\sum_{\ell \in \Lambda} \sum_{\mathbf{\rho}_1, \ldots, \mathbf{\rho}_j} \left( \prod_{1 \leq i \leq k} \mathbf{w}_{|A_i|}(\rho_1^{\ell}) \prod_{m \in A_i} \delta_{\rho_i, \rho_m} \right) \prod_{1 \leq m \leq j} |D_{\rho_m} v_m(\ell)|
= \sum_{\ell \in \Lambda} \sum_{\rho_{\mathbf{\rho}}} \left( \prod_{1 \leq i \leq k} \mathbf{w}_{|A_i|}(\rho_i^{\ell}) \prod_{m \in A_i} |D_{\rho_i} v_m(\ell)| \right)
= \sum_{\ell \in \Lambda} \prod_{1 \leq i \leq k} \left( \sum_{\rho_{\mathbf{\rho}}} \mathbf{w}_{|A_i|}(\rho_i^{\ell}) \prod_{m \in A_i} |D_{\rho_i} v_m(\ell)| \right)
= \sum_{\ell \in \Lambda} \prod_{1 \leq i \leq k} \left( \sum_{\rho_{\mathbf{\rho}}} \mathbf{w}_{|A_i|}(\rho_i^{\ell}) \prod_{m \in A_i} |D_{\rho_i} v_m(\ell)| \right).
\]

Then applying the generalised Hölder’s inequality and (A.1) yields

\[
\sum_{\ell \in \Lambda} \prod_{1 \leq i \leq k} \left( \sum_{\rho_{\mathbf{\rho}}} \mathbf{w}_{|A_i|}(\rho_i^{\ell}) \prod_{m \in A_i} |D_{\rho_i} v_m(\ell)| \right)
\leq \sum_{\ell \in \Lambda} \prod_{1 \leq i \leq k} \prod_{m \in A_i} \left( \sum_{\rho_{\mathbf{\rho}}} |D_{\rho_i} v_m(\ell)|^{1/|A_i|} \right)^{1/|A_i|}
= \sum_{\ell \in \Lambda} \prod_{1 \leq i \leq k} \prod_{m \in A_i} |Dv_m(\ell)|_{w_{|A_i|},|A_i|}.
\]

We will now show that for each \( 1 \leq i \leq k \) and \( m \in A_i \)

\[
\left( \sum_{\ell \in \Lambda} |Dv_m(\ell)|_{w_{|A_i|},|A_i|}^2 \right)^{1/j} \leq C \|Du\|_{L^\frac{C}{j}}.
\]

To prove (C.7), first consider the case \( |A_i| = 1 \). Recall that \( j \geq 2 \), hence \( \ell^2 \subset \ell^j \) and applying Lemma A.1 yields

\[
\left( \sum_{\ell \in \Lambda} |Dv_m(\ell)|_{w_{|A_i|},|A_i|}^2 \right)^{1/j} \leq \left( \sum_{\ell \in \Lambda} |Dv_m(\ell)|_{w_{|A_i|},|A_i|}^2 \right)^{1/2} \leq \|Dv_m\|_{L^2_{w_{|A_i|},|A_i|}} \leq C \|Dv_m\|_{L^2_{N}}.
\]
For the remaining case, observe that $2 \leq |A_i| \leq j$, the argument above follows using the embedding $\ell^{|A_i|} \subset \ell^j$

$$
\left( \sum_{\ell \in \Lambda} |Dv_m(\ell)|_m^{2|A_i|} \right)^{1/j} \leq \left( \sum_{\ell \in \Lambda} |Dv_m(\ell)|_m^{|A_i|} \right)^{1/|A_i|} \leq \|Dv_m\|_{m|A_i|, |A_i|} \leq C\|Dv_m\|_{\ell^j}. 
$$

Lemma D.1. The lattice Green’s function

First, we have a more general form of the homogeneous difference equation (3.3) as in the following lemma. It can be proved by using (S.PS) and we refer to the preprint [8] for details (see also [20, Lemma 3.4]).
Moreover, \( h \) satisfies \( h(-\rho) = h(\rho) \) and \( h(0) = -\sum_{\rho \in \Lambda^h} h(\rho) \).

Using (D.2) and a direct calculation, we have

\[
\langle Hu, v \rangle = -2 \sum_{\ell \in \Lambda^h} \sum_{\rho \in \Lambda^h} h(\rho) u(\ell - \rho)v(\ell),
\]

and hence

\[
Hu = -2h \ast_d u := -2 \sum_{\rho \in \Lambda^h} h(\rho) u(\ell - \rho),
\]

where \( \ast_d \) denotes the discrete convolution. From (D.3), one can alternatively write \( h(\rho) := -\frac{1}{2} \frac{\partial^2 (Hu, v)}{\partial u(0) \partial v(0)} \) (see also [20, Lemma 3.4]). The following lemma defines a lattice Green’s function of the homogeneous difference equation and gives a decay estimate.

**Lemma D.2.** If (LS) is satisfied, then

(i) there exists \( G : \Lambda^h \to \mathbb{R}^{d \times d} \) such that for any \( f : \Lambda^h \to \mathbb{R}^d \), which is compactly supported,

\[
H(G \ast_d f) = f;
\]

(ii) for all \( j \in \mathbb{N} \), there exist constants \( C_j \) such that

\[
|D_{\rho} G(\ell)| \leq C_j (1 + |\ell|)^{2-d-j} \prod_{i=1}^j |\rho_i| \quad \forall \ \rho = (\rho_1, \cdots, \rho_j) \in (\Lambda^h)^J;
\]

(iii) \( G \) can be chosen in such a way that there exists \( C_0 > 0 \) such that

\[
|G(\ell)| \leq \begin{cases} 
C_0 (1 + |\ell|)^{2-d} & \text{if } d = 3, \\
C_0 \log (2 + |\ell|) & \text{if } d = 2.
\end{cases}
\]

**Proof.** The proof is similar to that of [13, Lemma 6.2], with extensions from finite-range potential to infinite-range potential. We refer to the preprint [8] for details. \( \square \)

With the definition and decay estimates of the lattice Green’s function, we are now able to prove decay estimates for the linearised lattice elasticity problem

\[
\langle Hu, v \rangle = \langle g, Dv \rangle \quad \forall \ v \in \mathcal{W}^{1,2}(\Lambda^h), \tag{D.4}
\]

where \( g \in \mathcal{W}^{-1,2}(\Lambda^h) \). The canonical form of \( \langle g, Dv \rangle \) is

\[
\langle g, Dv \rangle := \sum_{\ell \in \Lambda^h} \sum_{\rho \in \Lambda^h} g(\ell) \cdot D_{\rho} v(\ell), \tag{D.5}
\]

with \( g = \{g(\ell)\}_{\ell \in \Lambda^h} \) and \( g(\ell) \in (\mathbb{R}^d)^{\Lambda^h} \).

**Lemma D.3.** Let (LS) be satisfied and \( u \in \mathcal{W}^{1,2}(\Lambda^h) \) be the solution of (D.4). If there exist \( s > d/2 \) and \( w_k \in \mathcal{L}_k \) for \( k = 1, 2, 3 \), such that

\[
|\langle g, Dv \rangle| \leq C \sum_{\ell \in \Lambda^h} \sum_{k=1}^3 \tilde{g}_k(\ell) |Dv(\ell)|_{w_k, k} \quad \forall \ v \in \mathcal{W}^{1,2}(\Lambda^h) \tag{D.6}
\]
 Then using the definition (A.1) and (D.8), it follows that

\[ |D_\rho u(\ell)| \leq C|\rho| \left\{ \begin{array}{ll}
(1 + |\ell|)^{-d} & \text{if } s > d, \\
(1 + |\ell|)^{-s} \log(2 + |\ell|) & \text{if } \frac{d}{2} < s \leq d.
\end{array} \right. \quad (D.7) \]

**Proof.** We adapt the argument used to show [13, Lemma 6.3]. For \( \ell \in \Lambda^h \), testing (D.4) with \( v(m) := D_\rho G(\ell - m) \) and \( \rho \in \Lambda^h \) yields

\[ D_\rho u(\ell) = -\langle Hu, D_\rho G(\ell - \cdot) \rangle = -\langle g, DD_\rho G(\ell - \cdot) \rangle, \]

and together with Lemma D.2 (ii), (D.6) and the fact that \( \sum_{\sigma \in \Lambda^h} w_k(|\sigma|)|\sigma|^k < \infty \) for \( k = 1, 2, 3 \), this implies

\[
|D_\rho u(\ell)| \leq C \sum_{m \in \Lambda^h} \left( 1 + |m| \right)^{-s} + \sum_{k=1}^{3} \left| Du(m) \right|^2_{w_k,k} \left( 1 + |m - \ell| \right)^{-d}. \quad (D.8)
\]

Then using the definition (A.1) and (D.8), it follows that

\[
\sum_{j=1}^{3} |Du(\ell)|_{m_{j},j} = \sum_{j=1}^{3} \left( \sum_{\rho \in \Lambda^h} w_j(|\rho|) \left| D_\rho u(\ell) \right|^2 \right)^{1/j} \leq C \sum_{m \in \Lambda^h} \left( 1 + |m| \right)^{-s} + \sum_{k=1}^{3} \left| Du(m) \right|^2_{w_k,k} \left( 1 + |m - \ell| \right)^{-d}. \quad (D.9)
\]

We first estimate the linear part in (D.9). For \( s > d \), we have

\[
\sum_{m \in \Lambda^h} (1 + |m|)^{-s} (1 + |m - \ell|)^{-d} \leq C(1 + |\ell|)^{-d} \sum_{|m - \ell| \geq |\ell|/2} (1 + |m|)^{-s} + C(1 + |\ell|)^{-s} \sum_{|m - \ell| \leq |\ell|/2} (1 + |m - \ell|)^{-d} \leq C \left( (1 + |\ell|)^{-d} + (1 + |\ell|)^{-s} \log(2 + |\ell|) \right) \leq C(1 + |\ell|)^{-d}. \quad (D.10)
\]

For \( 0 < s \leq d \), we introduce an exponent \( \delta > 0 \) and estimate

\[
\sum_{|m - \ell| \geq |\ell|/2} (1 + |m|)^{-s} (1 + |m - \ell|)^{-d} \leq C(1 + |\ell|)^{-s + \delta} \sum_{|m - \ell| \geq |\ell|/2} (1 + |m|)^{-s} (1 + |m - \ell|)^{-d + \delta} \leq C(1 + |\ell|)^{-s + \delta} \sum_{|m - \ell| \geq |\ell|/2} (1 + |m|)^{-(d + \delta)} \sum_{|m - \ell| \geq |\ell|/2} \left( \sum_{|m - \ell| \geq |\ell|/2} (1 + |m - \ell|)^{-(d + \delta)} \right)^{\frac{s + \delta}{d + \delta}} \leq C(1 + ||\ell|)^{-s + \delta} \sum_{m \in \Lambda^h} (1 + |m|)^{-(d + \delta)}. \quad (D.11)
\]
Applying the bound $\sum_{m \in \Lambda^b} (1 + |m|)^{-(d+\delta)} \leq C\delta^{-1}$, we deduce
\[
\sum_{|m - \ell| \geq |\ell|/2} (1 + |m|)^{-s} (1 + |m - \ell|)^{-d} \leq C (1 + |\ell|)^{-s} \frac{(2 + |\ell|)^{\delta}}{\delta}
\]
\[
\leq C (1 + |\ell|)^{-s} \log(2 + |\ell|),
\] (D.12)
where $\delta = 1/\log(2 + |\ell|)$ is chosen for the second inequality. Therefore, combining (D.10)–(D.12) gives
\[
\sum_{m \in \Lambda^b} (1 + |m|)^{-s} (1 + |m - \ell|)^{-d} \leq C (1 + |\ell|)^{-s} \log(2 + |\ell|),
\] (D.13)
Collecting the estimates (D.9) and (D.13), we obtain
\[
\sum_{k=1}^{3} |Du(\ell)|_{w_k,k} \leq C \left( z(|\ell|) + \sum_{m \in \Lambda^b} (1 + |m - \ell|)^{-d} \left( \sum_{k=1}^{3} |Du(m)|_{w_k,k}^{2} \right) \right),
\] (D.14)
where $z(r) = (1 + r)^{-d}$ if $s > d$ and $z(r) = (1 + r)^{-s} \log(2 + r)$ if $0 < s \leq d$. It remains to estimate the nonlinear residual term appearing in (D.9). For $r > 0$, define
\[
w(r) := \sup_{\ell \in \Lambda^b, |\ell| \geq r} \left( \sum_{k=1}^{3} |Du(\ell)|_{w_k,k} \right).
\]
Our aim is to show that there exists constant $C > 0$ such that for all $r > 0$
\[
w(r) \leq C (1 + r)^{-t},
\] (D.15)
where $t = \min\{s, \frac{2d}{3}\} > 0$. For any $|m| \geq 2r$, by applying Lemma A.1, we deduce
\[
\sum_{m \in \Lambda^b} (1 + |m - \ell|)^{-d} \left( \sum_{k=1}^{3} |Du(m)|_{w_k,k}^{2} \right)
\]
\[
= \sum_{|m| < r} (1 + |m|)^{-d} \left( \sum_{k=1}^{3} |Du(m + \ell)|_{w_k,k}^{2} \right) + \sum_{|m| \geq r} (1 + |m|)^{-d} \left( \sum_{k=1}^{3} |Du(m + \ell)|_{w_k,k}^{2} \right)
\]
\[
\leq C w(r)^{3/2} \left( \|1 + |m|\|^{-d}_{\ell^{\delta/3}} \left( \sum_{k=1}^{2} \|Du(m + \ell)_{m_k,k}^{1/2} \|_{\ell^{\delta/3}} \right) + \|1 + |m|\|^{-d}_{\ell^{\delta/5}} \|Du(m + \ell)_{m_k,k}^{1/2} \|_{\ell^{\delta/3}} \right)
\]
\[
+ C(1 + r)^{-d} \left( \sum_{k=1}^{2} \|Du(m + \ell)_{m_k,k}^{1/2} \|_{\ell^{\delta/3}} \right) + C(1 + r)^{-2d/3} \|Du(m + \ell)_{m_k,k}^{1/2} \|_{\ell^{\delta/3}}
\]
\[
\leq C \left( (1 + r)^{-2d/3} + w(r)^{3/2} \right).
\] (D.16)
Collecting the estimates (D.14) and (D.16) yields
\[
w(2r) \leq C(1 + r)^{-t} + \eta(r) w(r),
\] (D.17)
where $\eta(r) = w(r)^{1/2}$ and $\eta(r) \to 0$ as $r \to \infty$, as $Du(\ell) \in \ell^{2}(\Lambda^b)$. From here on, we follow [13, Lemma 6.3] verbatim, but show the argument for the sake of completeness. For $r > 0$, let $v(r) := \frac{w(r)}{z(r)}$. Multiplying (D.17) with $\frac{2d}{z(2r)}$, we obtain
\[
v(2r) \leq C \left( 1 + \eta(r) v(r) \right).
\]
Since $\eta(r) \to 0$ as $r \to \infty$, there exists $r_0 > 0$ such that for all $r > r_0$
\[
v(2r) \leq C + \frac{1}{2} v(r) \quad \forall \ r > r_0.
\]
Arguing by induction, (c.f. [13, Lemma 6.3]), we infer that $v$ is bounded on $\mathbb{R}_+$, which implies (D.15) holds.

$$w(r) \leq C(1 + r)^{-t} \quad \forall \ r > 0,$$

and thus implies

$$|D u(\ell)| w_k \leq C(1 + |\ell|)^{-t},$$

for $k = 1, 2, 3$. \hspace{1cm} (D.18)

Substituting (D.18) into (D.8) gives

$$|D_{\rho} u(\ell)| \leq C|\rho| \sum_{m \in \Lambda^h} \left( (1 + |m|)^{-s} + \sum_{k=1}^3 |D u(m)|_{\mathbb{R}_+}^{2} \right) (1 + |m - \ell|)^{-d}, \hspace{1cm} (D.19)$$

then repeating the argument (D.10)–(D.13) with (D.19) and $s' = \min\{s, \frac{4d}{3}\} > d/2$, we obtain the desired estimate (D.7). This completes the proof. \hfill \Box

**Remark D.4.** From (D.5), we can write

$$\langle g, Dv \rangle = \sum_{\ell \in \Lambda^h} f(\ell) \cdot v(\ell) \quad \text{with} \quad f(\ell) = \sum_{\rho \in \Lambda^h} D_{-\rho} g_{\rho}(\ell).$$

If there is an extra decay assumption on $f$ as $|f(\ell)| \leq (1 + |\ell|)^{-(s+1)}$, then we can drop the log term in (D.7) for the case $d/2 < s < d$. However, it is not clear whether this assumption can be true (for e.g. point defects case in Lemma E.5) from our existing assumptions in (S). \hfill \Box

**APPENDIX E. PROOFS: POINT DEFECTS**

The purpose of this section is to prove Theorems 3.2 and 3.3. First, we establish results for the homogeneous lattice that will be used in our proofs.

**E.1. Proof of Lemma 3.1.**

Proof of Lemma 3.1. As we have remarked in Appendix B.1 on Page 30, it is sufficient to consider that (S.L) holds under the homogeneous lattice and point defects condition.

The result follows directly from [31, Lemma 2.12], once we establish that for any $u \in \mathcal{W}^{c}(\Lambda^h)$, the sum

$$\sum_{\ell \in \Lambda^h} \sum_{\rho \in \Lambda^h} v^h(0) \cdot D_{\rho} u(\ell) \hspace{1cm} (E.1)$$

converges absolutely. As $u \in \mathcal{W}^{c}(\Lambda^h)$, $u$ is constant outside $B_R(0)$, for some $R > 0$. Then, for fixed $\rho \in \Lambda^h$, applying Lemma A.2 yields

$$\sum_{\ell \in \Lambda^h} |D_{\rho} u(\ell)| \leq C|\rho| \sum_{\ell \in \Lambda^h} \sum_{\rho' \in N(\ell) - \ell} |D_{\rho'} u(\ell)|.$$
Moreover, there exists $R' > 0$ such that $N(\ell) - \ell \subset B_{R'}(0)$ for all $\ell \in \Lambda^h$, hence for $\ell \in \Lambda^h \cap B_{R+R'}(0)^c$ and $\rho' \in N(\ell) - \ell$, $D_{\rho'} u(\ell) = 0$. Consequently, applying Cauchy–Schwarz twice, we deduce

$$
\sum_{\ell \in \Lambda^h} |D_{\rho} u(\ell)| \leq C|\rho| \sum_{\ell \in \Lambda^h \cap B_{R+R'}(0)} \left( \sum_{\rho' \in N(\ell) - \ell} |D_{\rho'} u(\ell)| \right) \leq C|\rho|(R + R')^{d/2} \left( \sum_{\ell \in \Lambda^h \cap B_{R+R'}(0)} \left( \sum_{\rho' \in N(\ell) - \ell} |D_{\rho'} u(\ell)| \right) \right)^{1/2} \leq C|\rho|(R + R')^{d/2} \left( \sum_{\ell \in \Lambda^h \cap B_{R+R'}(0)} \sum_{\rho' \in N(\ell) - \ell} |D_{\rho'} u(\ell)|^2 \right)^{1/2}
$$

$$
= C|\rho|(R + R')^{d/2} \left| Du \right|_{\ell^2_2(\Lambda^h)}.
$$

(E.2)

where the constant $C$ is independent of $\rho$. Applying (2.13), (E.2) and using that $w_1 \in L_1$, we deduce

$$
\sum_{\rho \in \Lambda^h} \sum_{\ell \in \Lambda^h} |V_{\rho}^h(0) \cdot D_{\rho} u(\ell)| \leq C \sum_{\rho \in \Lambda^h} w_1(|\rho|) \sum_{\ell \in \Lambda^h} |D_{\rho} u(\ell)| \leq C(R + R')^{d/2} \left| Du \right|_{\ell^2_2(\Lambda^h)} \sum_{\rho \in \Lambda^h} w_1(|\rho|)|\rho| < \infty.
$$

(E.3)

As the sum (E.3) converges, changing the order of summation of (E.1) is allowed and the sum is well-defined. Then as $u \in W^c(\Lambda^h)$, it follows that for all $\rho \in \Lambda^h$, $\sum_{\ell \in \Lambda^h} D_{\rho} u(\ell) = 0$, hence the desired result holds

$$
\sum_{\ell \in \Lambda^h} \sum_{\rho \in \Lambda^h} V_{\rho}^h(0) \cdot D_{\rho} u(\ell) = \left( \sum_{\rho \in \Lambda^h} V_{\rho}^h(0) \right) \cdot \left( \sum_{\ell \in \Lambda^h} D_{\rho} u(\ell) \right) = 0.
$$

This completes the proof.

\[ \square \]

E.2. Proof of Theorem 3.2. To show the boundedness of the functional $F$, defined in the statement of Theorem 3.2, we shall use the interpolation functions introduced in Section 3.1 to compare displacements on $\Lambda$ to those on $\Lambda^h$ in the following result.

Lemma E.1. Suppose that the assumptions of Theorem 3.2 hold. Let $I_1^h, I_2^h : W^{1,2}(\Lambda) \rightarrow W^{1,2}(\Lambda^h)$ and $I^d : W^{1,2}(\Lambda^h) \rightarrow W^{1,2}(\Lambda)$ be the interpolation operators defined in Lemmas B.1, B.2 and B.3. Then, for $u \in H(\Lambda)$, define the functionals $T_u : W^c(\Lambda) \rightarrow \mathbb{R}$ and $T_u^h : W^c(\Lambda^h) \rightarrow \mathbb{R}$ by

$$
\langle T_u, v \rangle = \sum_{\ell_1 \in \Lambda^h} \sum_{\rho_1 \in \Lambda^h - \ell_1} V_{\ell_1, \rho_1}^h(Du(\ell_1)) \cdot D_{\rho_1} v(\ell_1) - \sum_{\ell_2 \in \Lambda^h \cap B_{R+R'}(0)} \sum_{\rho_2 \in \Lambda^h} V_{\ell_2, \rho_2}^h(DI_1^h u(\ell_2)) \cdot D_{\rho_2} v(\ell_2),
$$

(E.4)

$$
\langle T_u^h, v^h \rangle = \sum_{\ell_1 \in \Lambda^h} \sum_{\rho_1 \in \Lambda^h - \ell_1} V_{\ell_1, \rho_1}^h(Du(\ell_1)) \cdot D_{\rho_1} I^d v^h(\ell_1) - \sum_{\ell_2 \in \Lambda^h \cap B_{R+R'}(0)} \sum_{\rho_2 \in \Lambda^h} V_{\ell_2, \rho_2}^h(DI_1^h u(\ell_2)) \cdot D_{\rho_2} v^h(\ell_2).
$$

(E.5)
There exists a constant \( C > 0 \), depending on \( s \) and \( u \in \mathcal{H}(\Lambda) \), such that for all \( v \in \mathcal{H}^c(\Lambda) \) and \( v^h \in \mathcal{H}^c(\Lambda^h) \)

\[
\left| \langle T^h_u, v \rangle \right| \leq C \| Dv \|_{L^2_v(\Lambda^h)}, \quad (E.6)
\]

\[
\left| \langle T^h_u, v^h \rangle \right| \leq C \| Dv^h \|_{L^2_v(\Lambda^h)}. \quad (E.7)
\]

Using Lemma E.1, we define unique continuous extensions of \( T_u, T^h_u \) to \( \mathcal{H}^{1,2}(\Lambda), \mathcal{H}^{1,2}(\Lambda^h) \), respectively. For convenience, we choose to denote these extensions by \( T_u, T^h_u \) and remark that they satisfy (E.4)–(E.7) for all \( v \in \mathcal{H}^{1,2}(\Lambda) \) and \( v^h \in \mathcal{H}^{1,2}(\Lambda^h) \), respectively.

**Remark E.2.** For each \( u \in \mathcal{H}(\Lambda) \) such that \( y_0 + u \in \mathscr{A}_{m, \lambda} \), the constant \( C > 0 \) appearing in the estimates (E.6)–(E.7) has the form \( C'(1 + R_0^{3/2}) \), where \( C' \) depends only on \( m \) and \( R_0 \) is the constant appearing in Lemma B.1, which depends on \( u \in \mathcal{H}^{1,2}(\Lambda) \).

**Proof.** We first observe from (RC) and Lemmas B.1 and B.3 that for each \( u \in \mathcal{H}(\Lambda) \) and \( v^h \in \mathcal{H}^c(\Lambda^h) \), there exists \( R_0 > R_{\text{def}} > 0 \) such that

\[
D_{\rho}l^h_1(u(\ell)) = D_{\rho}u(\ell), \quad \forall \ \ell \in \Lambda \setminus B_{2R_0}, \rho \in \Lambda^h \cap B_{R_0} \text{ or } \rho \in (\Lambda^h \setminus B_{R_0}) - \ell, \quad (E.8)
\]

\[
D_{\rho}l^d v^h(\ell) = D_{\rho}v^h(\ell), \quad \forall \ \ell \in \Lambda \setminus B_{2R_{\text{def}}}, \rho \in \Lambda^h \cap B_{R_{\text{def}}} \text{ or } \rho \in (\Lambda^h \setminus B_{R_{\text{def}}}) - \ell. \quad (E.9)
\]

We then decompose the right-hand side of (E.5) into four terms:

\[
\langle T^h_u, v^h \rangle = \sum_{\ell_1 \in \Lambda} \sum_{\rho_1 \in \Lambda \setminus \ell_1} V_{\ell_1, \rho_1}(Du(\ell_1)) \cdot D_{\rho_1}l^d v^h(\ell_1) - \sum_{\ell_2 \in \Lambda^h} \sum_{\rho_2 \in \Lambda^h} V_{\rho_2}(Dl^h_1 u(\ell_2)) \cdot D_{\rho_2} v^h(\ell_2)
\]

\[
= \sum_{\ell \in \Lambda^h} \sum_{\rho \in \Lambda^h} \left( V_{\ell, \rho}(Du(\ell)) - V_{\rho, \rho}(Dl^h_1 u(\ell)) \right) \cdot D_{\rho} v^h(\ell)
\]

\[
+ \sum_{\ell \in \Lambda^h} \sum_{\rho \in \Lambda^h \cap B_{R_0} - \ell} \left( V_{\ell, \rho}(Du(\ell)) - V_{\rho, \rho}(Dl^h_1 u(\ell)) \right) \cdot D_{\rho} v^h(\ell)
\]

\[
+ \sum_{\ell \in \Lambda^h} \sum_{\rho \in \Lambda^h \cap B_{R_{\text{def}}}} \left( V_{\ell, \rho}(Du(\ell)) - V_{\rho, \rho}(Dl^h_1 u(\ell)) \right) \cdot D_{\rho} v^h(\ell)
\]

\[
+ \sum_{\ell_1 \in \Lambda} \sum_{\rho_1 \in \Lambda \setminus \ell_1} V_{\ell_1, \rho_1}(Du(\ell_1)) \cdot D_{\rho_1}l^d v^h(\ell_1)
\]

\[
- \sum_{\ell_2 \in \Lambda^h} \sum_{\rho_2 \in \Lambda^h \setminus \ell_2} V_{\rho_2}(Dl^h_1 u(\ell_2)) \cdot D_{\rho_2} v^h(\ell_2).
\]

Let \( w_1(r) := (1 + r)^{s/2} \), where \( s \) is given in (S.H) then \( s > d/2 \) implies that \( w_1 \in L^2(\mathbb{R}^d) \).

Note that for \( |\ell| \geq 2R_0 \) and \( |\rho| < R_0 \), we have \( |\rho| \leq |\ell| - R_0 \), then (E.10) can be estimated.
using (E.9), (2.16) and Lemma A.1

\[
\begin{align*}
&\sum_{\ell \in \Lambda^h} \sum_{\rho \in \Lambda^h \setminus \{0\}} (V_{\ell,\rho}(Du(\ell)) - V_{\rho,\ell}(DI^1_h u(\ell))) \cdot D_\rho v^h(\ell) \\
&\leq C \sum_{\ell \in \Lambda^h} \sum_{\rho \in \Lambda^h \setminus \{0\}} w_h(|\ell| - R_0) w_1(|\rho|) |D_\rho v^h(\ell)| \leq C \sum_{\ell \in \Lambda^h} w_h(|\ell|/2) |Dv^h(\ell)|_{\Theta_1} \\
&\leq C \|w_h(|\ell|/2)\|_{\ell^2(\Lambda^h)} \|Dv^h\|_{\ell^2_{\Theta_1} (\Lambda^h)} \leq C \|w_h\|_{L^2(\mathbb{R}^d)} \|Dv^h\|_{\ell^2_{\Theta_1} (\Lambda^h)}. \quad (E.14)
\end{align*}
\]

An identical argument gives the following estimate for (E.11)

\[
\begin{align*}
&\sum_{\ell \in \Lambda^h} \sum_{\rho \in (\Lambda^h \setminus B_{R_0}) - \ell} (V_{\ell,\rho}(Du(\ell)) - V_{\rho,\ell}(DI^1_h u(\ell))) \cdot D_\rho v^h(\ell) \\
&\leq C \sum_{\ell \in \Lambda^h} \sum_{\rho \in (\Lambda^h \setminus B_{R_0}) - \ell} w_h(|\ell|/2) w_1(|\rho|) |D_\rho v^h(\ell)| \leq C \sum_{\ell \in \Lambda^h} w_h(|\ell|/2) |Dv^h(\ell)|_{\Theta_1} \\
&\leq C \|w_h\|_{L^2(\mathbb{R}^d)} \|Dv^h\|_{\ell^2_{\Theta_1} (\Lambda^h)} \leq C \|w_h\|_{L^2(\mathbb{R}^d)} \|Dv^h\|_{\ell^2_{\Theta_1} (\Lambda^h)}. \quad (E.15)
\end{align*}
\]

For (E.12), we first consider the following part by using (2.13), Lemmas A.1 and B.3, together with the Cauchy–Schwarz inequality

\[
\begin{align*}
&\sum_{\ell \in \Lambda^h} \sum_{\rho \in (\Lambda \cap B_{R_0}) - \ell} V_{\ell,\rho}(Du(\ell)) \cdot D_\rho I^d v^h(\ell) \\
&= \sum_{\ell' \in \Lambda \setminus B_{R_0}} \sum_{\rho' \in (\Lambda^h \setminus B_{2R_0}) - \ell'} V_{\ell,\rho'}(Du(\ell')) \cdot D_\rho I^d v^h(\ell') \\
&\leq C \sum_{\ell' \in \Lambda \setminus B_{R_0}} \sum_{\rho' \in (\Lambda^h \setminus B_{2R_0}) - \ell'} w_1(|\rho|) |D_\rho I^d v^h(\ell')| \leq C \sum_{\ell' \in \Lambda \setminus B_{R_0}} |DI^d v^h(\ell')|_{\Theta_1} \\
&\leq C |\Lambda \cap B_{R_0}|^{1/2} \|DI^d v^h\|_{\ell^2_{\Theta_1} (\Lambda)} \leq C \|DI^d v^h\|_{\ell^2_{\Theta_1} (\Lambda)} \leq C \|Dv^h\|_{\ell^2_{\Theta_1} (\Lambda)}, \quad (E.16)
\end{align*}
\]

where we have used the substitutions \( \ell' = \ell + \rho, \rho' = -\rho \) to obtain the estimate above. The remaining term in (E.12) can be estimated by an identical argument

\[
\begin{align*}
&\sum_{\ell \in \Lambda^h} \sum_{\rho \in (\Lambda \cap B_{R_0}) - \ell} V_{\rho,\ell}(D_I^h u(\ell)) \cdot D_\rho v^h(\ell) \\
&\leq C \sum_{\ell \in \Lambda \setminus B_{2R_0}} \sum_{\rho \in \Lambda - \ell} w_1(|\rho|) |D_\rho I^d v^h(\ell)| \leq C \sum_{\ell \in \Lambda \setminus B_{2R_0}} |DI^d v^h(\ell)|_{\Theta_1} \\
&\leq C |\Lambda \cap B_{2R_0}|^{1/2} \|DI^d v^h\|_{\ell^2_{\Theta_1} (\Lambda)} \leq C \|Dv^h\|_{\ell^2_{\Theta_1} (\Lambda)}. \quad (E.17)
\end{align*}
\]

For (E.13), we can estimate the following part

\[
\begin{align*}
&\sum_{\ell \in \Lambda \cap B_{2R_0}} \sum_{\rho \in \Lambda - \ell} V_{\rho,\ell}(Du(\ell)) \cdot D_\rho I^d v^h(\ell) \\
&\leq C \sum_{\ell \in \Lambda \cap B_{2R_0}} \sum_{\rho \in \Lambda - \ell} w_1(|\rho|) |D_\rho I^d v^h(\ell)| \leq C \sum_{\ell \in \Lambda \cap B_{2R_0}} |DI^d v^h(\ell)|_{\Theta_1} \\
&\leq C |\Lambda \cap B_{2R_0}|^{1/2} \|DI^d v^h\|_{\ell^2_{\Theta_1} (\Lambda)} \leq C \|Dv^h\|_{\ell^2_{\Theta_1} (\Lambda)}. \quad (E.18)
\end{align*}
\]
and similarly for the remaining term
\[
\left| \sum_{\ell \in \Lambda \setminus B_{2r_0}, \rho \in \Lambda - \ell} V^h_{\rho} (D^l I^h_{\rho} u (\ell)) \cdot D_{\rho} v^h (\ell) \right| \leq C \| D v^h \|_{L^2(\Lambda^h)}.
\] (E.19)

We obtain the desired estimate (E.7) by combining the estimates (E.14)--(E.19) and remark that the final constant depends on \( R_0 \) and hence on \( u \in \mathcal{W}^{1,2}(\Lambda) \), but is independent of \( v^h \in \mathcal{W}^c(\Lambda^h) \).

The proof of (E.6) follows immediately by the same arguments. \( \square \)

**Proof of Theorem 3.2.** Recall the definition of the functional \( F : \mathcal{W}^{1,2}(\Lambda) \to \mathbb{R} \) given in (3.4), then we similarly define \( F^h : \mathcal{W}^{1,2}(\Lambda^h) \to \mathbb{R} \) using (3.2), so for \( v \in \mathcal{W}^{1,2}(\Lambda) \) and \( v^h \in \mathcal{W}^{1,2}(\Lambda^h) \)
\[
\langle F, v \rangle = \sum_{\ell_1 \in \Lambda, \rho_1 \in \Lambda - \ell_1} V_{\ell_1, \rho_1}(0) \cdot D_{\rho_1} v(\ell_1),
\]
\[
\langle F^h, v^h \rangle := \sum_{\ell_2 \in \Lambda^h, \rho_2 \in \Lambda^h} V^h_{\rho_2}(0) \cdot D_{\rho_2} v^h(\ell_2) = 0.
\]

Recall that we have shown in Lemma 3.1 that \( F^h \equiv 0 \). Lemma B.1 implies that for \( 0 \in \mathcal{W}^{1,2}(\Lambda) \), we have \( I^h u = 0^h \in \mathcal{W}^{1,2}(\Lambda^h) \), which together with (E.4) implies that for all \( v \in \mathcal{W}^{1,2}(\Lambda) \)
\[
\langle F, v \rangle = \langle F, v \rangle - \langle F^h, I^h_2 v \rangle = \langle T_0, v \rangle,
\]
where \( T_0 \) denotes the operator \( T_u \) defined in (E.4) with \( u = 0 \). The desired estimate then follows from the estimate (E.6) appearing in Lemma E.1
\[
\left| \langle F, v \rangle \right| = \left| \langle T_0, v \rangle \right| \leq C \| D v \|_{L^2(\Lambda)}.
\] \( \square \)

Now that we have proved that Lemma 3.1, Theorem 3.2 and Theorem 2.7 all hold, the following result holds immediately.

**Corollary E.3.** For each \( u \in \mathcal{H}(\Lambda) \), the functionals \( T_u, T^h_u \) defined in (E.4)--(E.5) can be expressed as
\[
\langle T_u, v \rangle = \langle \delta \mathcal{E}(u), v \rangle - \langle \delta \mathcal{E}^h(I^h u), I^h_2 v \rangle,
\]
\[
\langle T^h_u, v^h \rangle = \langle \delta \mathcal{E}(u), I^h v^h \rangle - \langle \delta \mathcal{E}^h(I^h u), v^h \rangle.
\]
Moreover, there exists a constant \( C > 0 \), depending on \( u \in \mathcal{H}(\Lambda) \), such that for all \( v \in \mathcal{W}^{1,2}(\Lambda) \) and \( v^h \in \mathcal{W}^{1,2}(\Lambda^h) \)
\[
\left| \langle \delta \mathcal{E}(u), v \rangle - \langle \delta \mathcal{E}^h(I^h u), I^h_2 v \rangle \right| \leq C \| D v \|_{L^2(\Lambda)}, \quad (E.20)
\]
\[
\left| \langle \delta \mathcal{E}(u), I^h v^h \rangle - \langle \delta \mathcal{E}^h(I^h u), v^h \rangle \right| \leq C \| D v^h \|_{L^2(\Lambda^h)}. \quad (E.21)
\]

**Remark E.4.** In the proof of (E.7) in Lemma E.1, we obtain the following estimate by collecting (E.14)--(E.19) and using that \( m_\theta (r) = (1 + r)^{-\alpha} \): for all \( u \in \mathcal{W}^{1,2}(\Lambda) \), there
exist constants \( C, R_0 > 0 \) such that for all \( v^h \in \mathcal{W}^{1,2}(\Lambda^h) \)
\[
\left| \langle \delta \mathcal{E}^h(I_1^h u), v^h \rangle - \langle \delta \mathcal{E}(u), I^d v^h \rangle \right|
\leq C \left( \sum_{\ell \in \Lambda^h} (1 + |\ell|/2)^{-s} |DV^h(\ell)|_{W^{1,1}} + \sum_{\ell \in \Lambda^h \cap B_{2R_0}} |DV^h(\ell)|_{W^{1,1}} + \sum_{\ell \in \Lambda^h \cap B_{2R_0}} |DI^d v^h(\ell)|_{W^{1,1}} \right)
\leq C \left( \sum_{\ell \in \Lambda^h} (1 + |\ell|/2)^{-s} |DV^h(\ell)|_{\tilde{w}_{1,1}} + \sum_{\ell \in \Lambda^h \cap B_{2R_0}} |DV^h(\ell)|_{\tilde{w}_{1,1}} \right),
\] (E.22)

where \( \tilde{w}(r) := w(c_0 r) \in \mathcal{H}^1 \), for a fixed constant \( c_0 \in (0,1) \). We remark that we have applied Lemma B.1 to obtain the final estimate. We also note that \( R_0 > 0 \) is a constant depending only on \( u \in \mathcal{W}^{1,2}(\Lambda) \), so is independent of \( v^h \in \mathcal{W}^{1,2}(\Lambda^h) \). This estimate will be used in the proof of Lemma E.5. □

E.3. Proof of Theorem 3.3. We shall use the following result in order to prove Theorem 3.3.

**Lemma E.5.** If the conditions of Theorem 3.3 are satisfied, then for any \( \tilde{u} \) solving (2.21), there exists \( g \in (\mathcal{W}^{1,2}(\Lambda^h))^* \) such that
\[
\langle HI_1^h \tilde{u}, v^h \rangle = \langle g, DV^h \rangle \quad \forall \ v^h \in \mathcal{W}^{1,2}(\Lambda^h),
\]
where \( I_1^h : \mathcal{W}^{1,2}(\Lambda) \to \mathcal{W}^{1,2}(\Lambda^h) \) is defined in Lemma B.1 and \( g \) satisfies
\[
\left| \langle g, DV^h \rangle \right| \leq C \sum_{\ell \in \Lambda^h} \sum_{j=1}^3 \tilde{g}_j(\ell) |DV^h(\ell)|_{w_{j,j}},
\]
with some constant \( C > 0 \), \( w_j \in \mathcal{L}_j \) for \( 1 \leq j \leq 3 \) and
\[
\tilde{g}_1(\ell) = \tilde{g}_2(\ell) = (1 + |\ell|)^{-s} + \left( \sum_{k=1}^2 |DI_1^h \tilde{u}(\ell)|_{w_{k,k}} \right)^2, \quad \tilde{g}_3(\ell) = |DI_1^h \tilde{u}(\ell)|^2_{w_{3,3}}.
\]

**Proof.** For \( \tilde{u} \) solving (2.21) and \( v^h \in \mathcal{W}^{1,2}(\Lambda^h) \), we denote by \( \tilde{v} := (\tilde{v}_1, \tilde{v}_2, \tilde{v}_3) := (I_1^h \tilde{u}, I_1^h \tilde{u}, v^h) \in (\mathcal{W}^{1,2}(\Lambda^h))^3 \). Using that \( \delta \mathcal{E}^h(0) = \delta \mathcal{E}(\tilde{u}) = 0 \), we can rewrite the residual \( \langle HI_1^h \tilde{u}, v^h \rangle \) by
\[
\langle HI_1^h \tilde{u}, v^h \rangle = \langle \delta^2 \mathcal{E}^h(0)I_1^h \tilde{u}, v^h \rangle
\]
\[
= \langle \delta \mathcal{E}^h(0) + \delta^2 \mathcal{E}^h(0)I_1^h \tilde{u} - \delta \mathcal{E}^h(I_1^h \tilde{u}), v^h \rangle \quad \text{(E.23)}
\]
\[
+ \langle \delta \mathcal{E}^h(I_1^h \tilde{u}), v^h \rangle - \langle \delta \mathcal{E}(\tilde{u}), I^d v^h \rangle. \quad \text{(E.24)}
\]
For (E.23), by following a similar argument to (C.4)–(C.10), we deduce by Taylor’s theorem that
\[
\left| \langle \delta \mathcal{E}^h(0) + \delta^2 \mathcal{E}^h(0)I_1^h \tilde{u} - \delta \mathcal{E}^h(I_1^h \tilde{u}), v^h \rangle \right| \leq \int_0^1 \left| \langle \delta^3 \mathcal{E}(tI_1^h \tilde{u}), \tilde{v} \rangle \right| dt
\]
\[
\leq C \sum_{\{A_1, \ldots, A_k\} \in \mathcal{P}(3)} \sum_{\ell \in \Lambda} \sum_{\rho_1, \ldots, \rho_j} \prod_{m \in A_i} |DV_{m,\rho}(\ell)|_{w_{A_i,\rho^i}} \quad \text{(E.25)}
\]
Recall the definition (2.14), \( \mathcal{P}(3) \) is the set of partitions of \( \{1, 2, 3\} \) as
\[
\mathcal{P}(3) = \left\{ \{1\}, \{2\}, \{3\}, \{1, 2\}, \{1, 3\}, \{2, 3\}, \{1, 2, 3\} \right\}. \quad \text{(E.26)}
\]
which together with (E.25) implies
\[
\left| \langle \delta \varepsilon^h(0) + \delta^2 \varepsilon^h(0) I_1^h \tilde{u} - \delta \varepsilon^h(I_1^h \tilde{u}), v^h \rangle \right|
\leq C \sum_{\ell \in \Lambda} \left( |D I_1^h \tilde{u}(\ell)|^2_{\text{m}_1,1} |D v^h(\ell)|_{\text{m}_1,1} + |D I_1^h \tilde{u}(\ell)|^2_{\text{m}_2,2} |D v^h(\ell)|_{\text{m}_1,1} \right.
\left. + |D I_1^h \tilde{u}(\ell)|_{\text{m}_1,1} |D I_1^h \tilde{u}(\ell)|_{\text{m}_2,2} |D v^h(\ell)|_{\text{m}_2,2} + |D I_1^h \tilde{u}(\ell)|^2_{\text{m}_3,3} |D v^h(\ell)|_{\text{m}_3,3} \right)
\leq C \sum_{\ell \in \Lambda} \left( \sum_{k=1}^2 |D I_1^h \tilde{u}(\ell)|_{\text{m}_k,1} \right)^2 \left( \sum_{k'=1}^2 |D v^h(\ell)|_{\text{m}_{k',k'}} \right) + |D I_1^h \tilde{u}(\ell)|^2_{\text{m}_3,3} |D v^h(\ell)|_{\text{m}_3,3} .
\] (E.27)

To estimate (E.24), we obtain from (S.H) and (E.22) that
\[
\left| \langle \delta \varepsilon^h(I_1^h \tilde{u}), v^h \rangle - \langle \delta \varepsilon^h(\tilde{u}), I^d v^h \rangle \right|
\leq C \sum_{\ell \in \Lambda^b} (1 + |\ell|/2)^{-s} |D v^h(\ell)|_{\text{m}_1,1} + \sum_{\ell \in \Lambda^b \cap B_R^i \text{def}} |D v^h(\ell)|_{\text{m}_1,1}
\leq C \sum_{\ell \in \Lambda^b} (1 + |\ell|)^{-s} |D v^h(\ell)|_{\text{m}_1,1} \leq C \sum_{\ell \in \Lambda^b} (1 + |\ell|)^{-s} \left( \sum_{k'=1}^2 |D v^h(\ell)|_{\text{m}_{k',k'}} \right),
\] (E.28)

where we define \( \tilde{w}_k(r) := w_k(c_0 r) \in \mathcal{L}_k \), where \( c_0 \in (0, 1) \) is a fixed constant given in the proof of Lemma B.2. Combining the estimates (E.27) and (E.28) and using that \( w_k(r) \leq \tilde{w}_k(r) \) for all \( r > 0 \), we obtain the desired result
\[
\left| \langle g, D v \rangle \right| \leq C \sum_{\ell \in \Lambda^b} \left( (1 + |\ell|)^{-s} + \left( \sum_{k=1}^2 |D I_1^h \tilde{u}(\ell)|_{\text{m}_k,1} \right)^2 \left( \sum_{k'=1}^2 |D v^h(\ell)|_{\text{m}_{k',k'}} \right) \right)
+ C \sum_{\ell \in \Lambda} |D I_1^h \tilde{u}(\ell)|^2_{\text{m}_3,3} |D v^h(\ell)|_{\text{m}_3,3},
\]
which completes the proof. \( \Box \)

**Proof of Theorem 3.3.** By Lemma E.5, we have that \( I_1^h \tilde{u} \) satisfies the conditions of Lemma D.3. Hence applying Lemma D.3 gives the desired decay estimate (3.5). \( \Box \)

**Appendix F. Proofs: Dislocations**

The purpose of this section is to prove Theorems 3.6 and 3.7. First, we introduce the elastic strain and describe its decay properties.

**F.1. Elastic strain.** The following setting for dislocations can be found in [13]. We first recall the far-field predictor for dislocations defined in Section 3.3:
\[
u_0(\ell) := u^{\text{in}}(\xi^{-1}(\ell)) + u^{\text{c}}(\ell), \quad \text{for all } \ell \in \Lambda.
\]
The role of \( \xi \) in the definition of \( u_0 \) is that applying a plastic slip across the plane \( \{x_2 = \hat{x}_2\} \) via the definition
\[
y^S(\ell) := \begin{cases} y(\ell), & \ell_2 > \hat{x}_2, \\
y(\ell - b_1), & \ell_2 < \hat{x}_2 \end{cases},
\]
achieves exactly this transfer: it leaves the configuration invariant, while generating a new predictor \( y_0^S \in C^\infty(\Omega_\Gamma) \), where \( \Omega_\Gamma = \{x_1 > \hat{x}_1 + r + b_1\} \) with a sufficiently large \( r \). Since
the map $y \mapsto y^S$ represents a relabelling of the atom indices and an integer shift in the
out-of-plane direction, we can apply (3.7) and (S.P) to obtain
\[ \Phi_L(y) = \Phi_{S^*L}(y^S), \]  
where $S$ is the $\ell^2$-orthogonal operator with inverse $S^* = S^{-1}$ defined by
\[ Su(\ell) := \begin{cases} u(\ell), & \ell_2 > \hat{x}_2, \\ u(\ell - b_{12}), & \ell_2 < \hat{x}_2. \end{cases} \quad \text{and} \quad S^* u(\ell) := \begin{cases} u(\ell), & \ell_2 > \hat{x}_2, \\ u(\ell + b_{12}), & \ell_2 < \hat{x}_2. \end{cases} \]

We can translate (F.1) to a statement about $u_0$ and the corresponding site strain
potential $V_\ell$. Let $S_0 w(x) = w(x)$, for $x_2 > \hat{x}_2$ and $S_0 w(x) = w(x - b_{12}) - b$, when $x_2 < \hat{x}_2$. We then obtain that $y_0^S(x) = x + S_0 u_0(x)$, $S_0 u_0 \in C^\infty(\Omega \Gamma)$ and $S_0(u_0 + u) = S_0 u_0 + Su$. The permutation invariance (F.1) can now be rewritten as an invariance of $V_\ell$ under the
slip $S_0$:
\[ V_\ell(D(u_0 + u)(\ell)) = e(\ell) + \tilde{Du}(\ell) \quad \forall u \in \mathcal{A}(\Lambda), \ell \in \Lambda \] (F.2)
where
\[ e(\ell) := (e_\rho(\ell))_{\rho \in \Lambda - \ell} \quad \text{with} \quad e_\rho(\ell) := \begin{cases} S^* D_\rho S_0 u_0(\ell), & \ell \in \Omega \Gamma, \\ D_\rho u_0(\ell), & \text{otherwise}, \end{cases} \] (F.3)
and
\[ \tilde{Du}(\ell) := (\tilde{D}_\rho u(\ell))_{\rho \in \Lambda - \ell} \quad \text{with} \quad \tilde{D}_\rho u(\ell) := \begin{cases} S^* D_\rho Su(\ell), & \ell \in \Omega \Gamma, \\ D_\rho u(\ell), & \text{otherwise}. \end{cases} \] (F.4)

We remark that as $\Lambda = \Lambda^h$ is a Bravais lattice, it also follows that $V_\ell$ is independent of $\ell \in \Lambda$, hence we use $V$ to denote $V_\ell$ from this point onwards. Additionally, in this section, we assume that (S.L) holds with the dislocations condition.

We remark that the expression (F.2) implicitly assumes that the predictor $y_0 \in \mathcal{A}(\Lambda)$, which we now verify.

**Lemma F.1.** There exists $u^c \in C^\infty_c(\mathbb{R}^2; \mathbb{R}^3)$ such that the dislocation predictor configuration satisfies $y_0 \in \mathcal{A}(\Lambda)$, where $y_0(\ell) := \ell + u_0(\ell)$ and $u_0(\ell) := u^\text{lin}(\xi^{-1}(\ell)) + u^c(\ell)$, for $\ell \in \Lambda$.

For $x = (x_1, x_2, x_3) \in \mathbb{R}^3$, let $x_{12} := (x_1, x_2) \in \mathbb{R}^2$. We consider $\tilde{y}_0 : (\mathbb{R}^2 \setminus \Gamma) \times \mathbb{R} \to \mathbb{R}^3$ defined by $\tilde{y}_0(x) = x + u_0(x_{12})$, where $u_0$ is given above. Due to the definition of the admissible space $\mathcal{A}(\Lambda)$ in (2.9), we remark that showing $y_0 \in \mathcal{A}(\Lambda)$ is equivalent to showing $\tilde{y}_0 \in \mathcal{A}^0(\Lambda_0)$, where $\tilde{y}_0(\ell_1, \ell_2, \ell_3) = y_0(\ell_1, \ell_2) + (0, 0, \ell_3)$ for $(\ell_1, \ell_2, \ell_3) \in \Lambda_0$. That is to show: there exists $m, \lambda > 0$ such that
\[ B_\lambda(x) \cap \tilde{y}_0(\Lambda_0) \neq \emptyset \quad \forall x \in \mathbb{R}^3, \] (F.5)
\[ |\tilde{y}_0(\ell) - \tilde{y}_0(m)| \geq m|\ell - m| \quad \forall \ell, m \in \Lambda_0. \] (F.6)

We now state an intermediate result, which will be used to prove Lemma F.1.

For $R > 0$, define the two-dimensional disc
\[ D_R := \{(x_1, x_2) \in \mathbb{R}^2 \mid (x_1^2 + x_2^2)^{1/2} < R\}. \]
Additionally, let $u_1 := u^\text{lin} \circ \xi^{-1}$ and define $\tilde{y}_1 : (\mathbb{R}^2 \setminus \Gamma) \times \mathbb{R} \to \mathbb{R}^3$ by $\tilde{y}_1(x) = x + u_1(x_{12})$, which is analogous to $\tilde{y}_0(\ell)$ without a compactly supported term. Also, let $\Gamma_S := \{(x_1, \hat{x}_2) \mid x_1 \leq \hat{x}_1\}$ denotes the reflected branch cut, then define $\tilde{y}_1^S : (\mathbb{R}^2 \setminus \Gamma_S) \times \mathbb{R} \to \mathbb{R}^3$ by $\tilde{y}_1^S(x) = x + S_0 u_1(x_{12})$, where $S_0 u_1 \in C^\infty(\Omega \Gamma)$.

As $\Lambda \cap \Gamma = \emptyset$, so there exists $\varepsilon > 0$ such that $\Lambda \cap \Gamma_\varepsilon = \emptyset$, where
\[ \Gamma_\varepsilon := \{(x_1, x_2) \mid x_1 \geq \hat{x}_1, |x_2 - \hat{x}_2| \leq \varepsilon\}. \]
Now choose $\eta \in C^\infty(\mathbb{R}, \mathbb{R})$ satisfying $0 \leq \eta \leq 1$, $\eta(t) = 0$ for $t \geq \varepsilon$, $\eta(t) = 1$ for $t \leq -\varepsilon$ and $|\eta'(t)| \leq C\varepsilon^{-1}$ for all $t \in [-\varepsilon, \varepsilon]$. Then define $Iy_1 : \mathbb{R}^3 \to \mathbb{R}^3$ by

$$Iy_1(x) := \begin{cases} \tilde{y}_1(x), & x_{12} \notin \Gamma_\varepsilon, \\ \tilde{y}_1^S(x + b\eta(x_2 - \hat{x}_2)), & x_{12} \in \Gamma_\varepsilon. \end{cases}$$

It follows from the definition that $Iy_1(\ell) = \tilde{y}_1(\ell)$ for all $\ell \in \Lambda_0$.

**Lemma F.2.** There exist $R_0 > 0$, $m', M > 0$ such that for all $x_1, x_2 \in (\mathbb{R}^2 \setminus D_{R_0}) \times \mathbb{R}$

$$|x_1 - x_2| \leq |Iy_1(x_1) - Iy_1(x_2)| \leq M|x_1 - x_2|, \quad (F.7)$$

hence the restriction $Iy_1 : (\mathbb{R}^2 \setminus D_{R_0}) \times \mathbb{R} \to \mathbb{R}^3$ is smooth, injective and is also a homeomorphism onto its image. Moreover there exists open, bounded $\Omega \subset \mathbb{R}^2$ such that

$$Iy_1((\mathbb{R}^2 \setminus D_{R_0}) \times \mathbb{R}) \subset (\mathbb{R}^2 \setminus \Omega) \times \mathbb{R}. \quad (F.8)$$

**Proof of Lemma F.2.** By [13, Lemma 3.1] there exists $C > 0$ such that $|\nabla u_1(z)| \leq C|z|^{-1}$ for all $z \in \mathbb{R}^2 \setminus (D_r \cup \Gamma)$, where $r > 0$ has been introduced in the definition of $\Omega_\Gamma$. Consequently, there exists $R_0 \geq r > 0$ such that $D_{R_0} \cap \Gamma \supseteq \Omega_\Gamma \cap \Gamma$ and additionally satisfying $|\nabla u_1(z)| \leq 1/4$ for all $z \in \mathbb{R}^2 \setminus (D_{R_0} \cup \Gamma)$ and $|\nabla S_0 u_1(z)| \leq 1/4$ for all $z \in \mathbb{R}^2 \setminus (D_{R_0} \cup \Gamma \setminus S)$.

We now justify that $Iy_1$ is smooth over $(\mathbb{R}^2 \setminus D_{R_0}) \times \mathbb{R}$. As $y_1 \in C^\infty((\mathbb{R}^2 \setminus \Gamma) \times \mathbb{R})$, $\tilde{y}_1^S \in C^\infty(\Omega_\Gamma \times \mathbb{R})$, it only remains to show that $Iy_1$ is smooth over $(\mathbb{R}^2 \setminus D_{R_0} \cap \partial \Gamma) \times \mathbb{R}$. Consider $x \in (\mathbb{R}^2 \setminus D_{R_0}) \times \mathbb{R}$ such that $x_1 \geq \hat{x}_1$ and $x_2 = \tilde{x}_2 - \varepsilon$, then taking the derivative from below in the $x_2$-direction gives $\nabla \tilde{y}_1(x^-) = \nabla \tilde{y}_1(x)$. Then, using that $\tilde{y}_1^S(x + b) = \tilde{y}_1(x)$, we deduce that

$$\nabla Iy_1(x^+) = \nabla \tilde{y}_1^S(x + b\eta(-\varepsilon))(I + b\eta'(\varepsilon)) = \nabla \tilde{y}_1^S(x + b) = \nabla \tilde{y}_1(x),$$

hence $Iy_1$ is differentiable at $x$. Repeating this argument also shows that $Iy_1$ is smooth at $x$. An analogous argument shows that $Iy_1$ is smooth at $x \in (\mathbb{R}^2 \setminus D_{R_0}) \times \mathbb{R}$ satisfying $x_1 \geq \hat{x}_1$ and $x_2 = \hat{x}_2 + \varepsilon$.

We now show (F.7). Let $x, x' \in (\mathbb{R}^2 \setminus D_{R_0}) \times \mathbb{R}$, so that $x_{12}, x'_{12} \in \mathbb{R}^2 \setminus D_{R_0}$, then define the path

$$P_{x_{12},x'_{12}} := \{ x_{12} + t(x'_{12} - x_{12}) | t \in [0, 1] \}. \quad \text{Now suppose } P_{x_{12},x'_{12}} \cap (D_{R_0} \cup \Gamma_\varepsilon) = \emptyset, \text{ then}$$

$$|u_1(x_{12}) - u_1(x'_{12})| \leq \int_0^1 |\nabla u_1(x_{12} + t(x'_{12} - x_{12}))||x_{12} - x'_{12}| dt \leq \frac{1}{4}|x_{12} - x'_{12}|. \quad (F.8)$$

Alternatively, suppose that $P_{x_{12},x'_{12}} \cap D_{R_0} \neq \emptyset$, then it is straightforward to construct a piecewise smooth path $P'_{x_{12},x'_{12}} \subset \mathbb{R}^2 \setminus D_{R_0}$ from $x_{12}$ to $x'_{12}$, by following $\partial D_{R_0}$ instead of intersecting $D_{R_0}$, satisfying $|P'_{x_{12},x'_{12}}| \leq 2|x_{12} - x'_{12}|$. We additionally suppose that $P'_{x_{12},x'_{12}} \subset \mathbb{R}^2 \setminus (D_{R_0} \cup \Gamma_\varepsilon)$, hence it follows that

$$|u_1(x_{12}) - u_1(x'_{12})| \leq |P'_{x_{12},x'_{12}}| \sup_{z \in P'_{x_{12},x'_{12}}} |\nabla u_1(z)| \leq \frac{1}{2}|x_{12} - x'_{12}|. \quad (F.9)$$

As $x_{12}, x'_{12} \notin \Gamma_\varepsilon$, we have $I\tilde{y}_1(x) = \tilde{y}_1(x), Iy_1(x') = \tilde{y}_1(x')$, hence (F.8)–(F.9) imply

$$|Iy_1(x) - I\tilde{y}_1(x')| = |\tilde{y}_1(x) - \tilde{y}_1(x')| \geq |x - x'| - |u_1(x_{12}) - u_1(x'_{12})| \geq \frac{1}{2}|x - x'|. \quad (F.10)$$

Similarly, we also obtain

$$|Iy_1(x) - I\tilde{y}_1(x')| \leq |x - x'| - |u_1(x_{12}) - u_1(x'_{12})| \leq \frac{3}{2}|x - x'|. \quad (F.11)$$
Now suppose that $P_{x_{12},x_{12}'} \cap \Gamma \neq \emptyset$, then define $\tilde{x} = x + b\eta(x_2 - \hat{x}_2)$, $\tilde{x}' = x' + b\eta(x_2' - \hat{x}_2)$, then there exists a path $P_{\tilde{x}_{12},\tilde{x}_{12}'}$ joining $\tilde{x}_{12},\tilde{x}_{12}'$ such that $P_{\tilde{x}_{12},\tilde{x}_{12}'} \cap D_{\Gamma} = \emptyset$, $P_{\tilde{x}_{12},\tilde{x}_{12}'} \cap \Gamma \neq \emptyset$ and $|P_{\tilde{x}_{12},\tilde{x}_{12}'}| \leq 2|\tilde{x}_{12} - \tilde{x}_{12}'|$. Following the argument (F.9)–(F.10) gives

$$|I\tilde{y}_1(x) - I\tilde{y}_1(x')| = |\tilde{y}_1^S(x + b\eta(x_2 - \hat{x}_2)) - \tilde{y}_1^S(x' + b\eta(x_2' - \hat{x}_2))| = |\tilde{y}_1^S(\tilde{x}) - \tilde{y}_1^S(\tilde{x}')|$$

$$\geq |\tilde{x} - \tilde{x}'| - |S_0u_1(\tilde{x}_{12}) - S_0u_1(\tilde{x}_{12}')| \geq \frac{1}{2}|\tilde{x} - \tilde{x}'|. \quad (F.12)$$

By the Mean Value Theorem, there exists $\theta = \theta(x_2, x_2') \in \mathbb{R}$ such that $\tilde{x} - \tilde{x}' = x - x' + b(\eta(x_2 - \hat{x}_2) - \eta(x_2' - \hat{x}_2)) = x - x' + b\eta'(\theta)(x_2 - x_2') =: A_\theta(x - x')$, where the matrix $A_\theta \in \mathbb{R}^{3 \times 3}$ is invertible with inverse $A_\theta^{-1}$,

$$A_\theta = \begin{pmatrix} 1 & b_1\eta'(\theta) & 0 \\ 0 & 1 & 0 \\ 0 & b_3\eta'(\theta) & 1 \end{pmatrix}, \quad A_\theta^{-1} = \begin{pmatrix} 1 & -b_1\eta'(\theta) & 0 \\ 0 & 1 & 0 \\ 0 & -b_3\eta'(\theta) & 1 \end{pmatrix}.$$  

Consequently,

$$|x - x'| = |A_\theta^{-1}(\tilde{x} - \tilde{x}')| \leq |A_\theta^{-1}||\tilde{x} - \tilde{x}'| \leq C_0|\tilde{x} - \tilde{x}'|, \quad (F.13)$$

where the constant $C_0 > 0$ is independent of $\theta, x, x'$ and depends only on $C_\eta$. We also obtain $|\tilde{x} - \tilde{x}'| \leq C_0|x - x'|$. Combining (F.12)–(F.13) yields

$$|I\tilde{y}_1(x) - I\tilde{y}_1(x')| \geq \frac{1}{2}|\tilde{x} - \tilde{x}'| \geq \frac{1}{2C_0}|x - x'|, \quad (F.14)$$

and also

$$|I\tilde{y}_1(x) - I\tilde{y}_1(x')| \leq \frac{3}{2}|\tilde{x} - \tilde{x}'| \leq \frac{3C_0}{2}|x - x'|, \quad (F.15)$$

Collecting the estimates (F.10)–(F.15), we obtain the desired estimate (F.7)

$$m'|x - x'| \leq |I\tilde{y}_1(x) - I\tilde{y}_1(x')| \leq M|x - x'|,$$

for all $x, x' \in (\mathbb{R}^2 \setminus D_{R_0}) \times \mathbb{R}$, where $m' = (2C_0)^{-1}, M = \frac{3C_0}{2} > 0$. It follows immediately from (F.7) that $I\tilde{y}_1 : (\mathbb{R}^2 \setminus D_{R_0}) \times \mathbb{R} \to \mathbb{R}^3$ is both injective and a closed map, thus is a homeomorphism onto its image.

It follows from the definition of $I\tilde{y}_1$ that $x = (x_1, x_2, x_3) \in I\tilde{y}_1((\mathbb{R}^2 \setminus D_{R_0}) \times \mathbb{R})$ and only if $(x_1, x_2, x_3') \in I\tilde{y}_1((\mathbb{R}^2 \setminus D_{R_0}) \times \mathbb{R})$ for all $x_3' \in \mathbb{R}$, hence $I\tilde{y}_1((\mathbb{R}^2 \setminus D_{R_0}) \times \mathbb{R}) = A \times \mathbb{R}$ for some $A \subset \mathbb{R}^2$. Define $Iy_1 : \mathbb{R}^2 \setminus D_{R_0} \to \mathbb{R}^2$ by $Iy_1(z_1, z_2) = (I\tilde{y}_1, I\tilde{y}_1, 0)(z_1, z_2, 0)$, so $A = Iy_1(\mathbb{R}^2 \setminus D_{R_0})$. The arguments (F.8)–(F.14) can be applied verbatim to also show: there exists $m_{12} > 0$ such that for all $z, z' \in \mathbb{R}^2 \setminus D_{R_0}$

$$|Iy_1(z) - Iy_1(z')| \geq m_{12}|z - z'|, \quad (F.16)$$

so we also deduce that $Iy_1$ is a homeomorphism onto its image. In particular, this implies $Iy_1(\partial D_{R_0}) = \partial Iy_1(\mathbb{R}^2 \setminus D_{R_0})$, hence $Iy_1(\partial D_{R_0})$ is a closed loop that encloses an open, bounded region $\Omega \subset \mathbb{R}^2$. The estimate (F.16) together with the fact that $Iy_1$ is a homeomorphism onto its image implies $Iy_1(\mathbb{R}^2 \setminus D_{R_0}) = \mathbb{R}^2 \setminus \Omega$, which concludes the proof. \[\square\]

**Proof of Lemma F.1.** We first show (F.6), by considering several cases. In the following, we consider $\ell, m \in A_0$. To begin, recall the constants $m', R_0 > 0$ introduced in Lemma F.2. Suppose $\ell, m \in (\mathbb{R}^2 \setminus D_{R_0}) \times \mathbb{R}$, then by (F.7)

$$|\tilde{y}_1(\ell) - \tilde{y}_1(m)| = |I\tilde{y}_1(\ell) - I\tilde{y}_1(m)| \geq m'|\ell - m|. \quad (F.17)$$

Consider the case $\ell \in (\mathbb{R}^2 \setminus D_{R_0 + R_1}) \times \mathbb{R}$, $m \in D_{R_0} \times \mathbb{R}$, where $R_1 > 0$ is a constant whose value will be specified shortly. Let $c_0 := \min\{|n_{12}| : n \in A_0 \cap ((\mathbb{R}^2 \setminus D_{R_0}) \times \mathbb{R})\}$ and fix
\( \ell' \) to be one such minimiser. As \( \Lambda_0 \) is periodic in the \( e_3 \)-direction, for all \( j \in \mathbb{Z} \), we have \( \ell'_j := \ell' + je_3 \in \Lambda_0 \), hence we may choose \( k \in \mathbb{Z} \) such that \( |(\ell'_k - m)| \leq 1 \). Now define \( C_1 := \max \{ |y_1(n_{12})| \mid n_{12} \in \Lambda \cap (D_{R_0} \cup \{ \ell'_{12} \}) \} \) and \( R_1 := \max \{ c_0 + 4(m')^{-1}(C_1 + 1), R_0 + 2(2c_0 + 1) \} \). We first estimate
\[
|\tilde{y}_1(\ell'_k) - \tilde{y}_1(m)| = |y_1(\ell'_{12}) - y_1(m_{12}) + (\ell'_k - m)| \\
\leq |y_1(\ell'_{12}) - y_1(m_{12})| + 1 \leq 2C_1 + 1,
\]
Using the choice of \( R_1 \), Lemma F.2 and the triangle inequality imply
\[
|\tilde{y}_1(\ell) - \tilde{y}_1(m)| \geq |\tilde{y}_1(\ell) - \tilde{y}_1(\ell'_k)| - |y_1(\ell'_k) - y_1(m)| \\
\geq m'||\ell - \ell'_k| - (2C_1 + 1) \geq \frac{m'}{2}|\ell - \ell'_k| \geq \frac{m'}{4}|\ell - m|. \tag{F.18}
\]
Next, we consider the case \( \ell \in D_{R_0+R_1} \times \mathbb{R}, m \in D_{R_0} \times \mathbb{R} \), which additionally satisfy \( |(\ell - m)| \geq R_2 > 0 \), where the value of \( R_2 \) will be given shortly. Also, define \( C_2 := \max \{ |y_1(n_{12})| \mid n_{12} \in \Lambda \cap D_{R_0+R_1} \} \) and \( R_2 := \max \{ 2(C_1 + C_2 + 1), 2R_0 + R_1 \} \). Then,
\[
|\tilde{y}_1(\ell) - \tilde{y}_1(m)| = |y_1(\ell_{12}) - y_1(m_{12}) + (\ell - m)| \geq |(\ell - m)| - (C_1 + C_2) \\
\geq |(\ell - m)| - 2C_1 - 2R_0 - R_1 \geq |(\ell - m)| - 2C_1 - 2R_0 - R_1 \geq |(\ell - m)| \geq \frac{m'}{4}|\ell - m|. \tag{F.19}
\]
We now consider the remaining case, where \( \ell \in D_{R_0+R_1} \times \mathbb{R}, m \in D_{R_0} \times \mathbb{R} \) satisfy \( |(\ell - m)| \leq R_2 \). Due to the periodicity of \( \tilde{y}_1 \) in the \( e_3 \)-direction, it suffices to consider \( m \in D_{R_0} \times [0,1) \) and \( \ell \in D_{R_0+R_1} \times [-R_2, R_2 + 1) \).

Define \( c_1 := \min \{ |\tilde{y}_1(\ell') - \tilde{y}_1(m')| \mid m' \in D_{R_0} \times [0,1), \ell' \in D_{R_0+R_1} \times [-R_2, R_2 + 1) \} \), then if \( c_1 > 0 \), then using that \( |\ell - m| \leq 2(R_0 + 1) + R_1 + R_2 \), we deduce
\[
|\tilde{y}_1(\ell) - \tilde{y}_1(m)| \geq c_1 \geq \frac{c_1|\ell - m|}{2(R_0 + 1) + R_1 + R_2} :=: m_1|\ell - m|. \tag{F.20}
\]
In this case, we may simply define \( u^c \in C^\infty_c(\mathbb{R}^2; \mathbb{R}^3) \) by \( u^c \equiv 0 \), in which case we let \( \tilde{y}_0 := \tilde{y}_1 \). Collecting the estimates (F.17)–(F.20) then yields the desired estimate (F.6):
\[
|\tilde{y}_0(\ell) - \tilde{y}_0(m)| = |\tilde{y}_1(\ell) - \tilde{y}_1(m)| \geq m|\ell - m| \quad \text{for all } \ell, m \in \Lambda_0,
\]
where \( m := \min \{ \frac{m'}{4}, m_1 \} > 0 \).

Otherwise, if \( c_1 = 0 \), in order to guarantee that no collisions occur, we add a small perturbation to \( \tilde{y}_1 \) within \( D_{R_0+1} \). For each \( m_{12}' \in \Lambda \cap D_{R_0} \), choose \( a_{m_{12}'} \in D_1 \) such that \( c_2 := \min \{ |y_1(\ell'_{12}) - y_1(m_{12}')| \mid m_{12} \in \Lambda \cap D_{R_0}, \ell_{12}' \in \Lambda \cap D_{R_0+1} \} > 0 \).

For \( \delta > 0 \), choose \( \eta_0 \in C^\infty_c(D_0; \mathbb{R}^2) \) satisfying \( 0 \leq \eta_0 \leq 1 \) and \( \eta_0(0) = 1 \), then define \( \eta_0 \in C^\infty_c(D_0; \mathbb{R}^3) \). We then construct \( u^c \in C^\infty_c(\mathbb{R}^2; \mathbb{R}^3) \), given by \( u^c(z) := \sum_{m_{12}' \in \Lambda \cap D_{R_0}} a_{m_{12}'} \eta_0(z - m_{12}') \), where \( \delta \in (0,1) \) is chosen to be sufficiently small to ensure that \( u^c(\ell_{12}') = (a_{\ell_{12}'}, 0) \) when \( \ell_{12}' \in \Lambda \cap D_{R_0} \) and \( u^c(\ell_{12}') = 0 \) for all \( \ell_{12}' \in \Lambda \setminus D_{R_0} \).

Now define \( u_0(z) := u_1(z) + u^c(z) \), \( y_0(z) := y_1(z) + u^c(z) \) for \( z \in \mathbb{R}^2 \) and also \( \tilde{y}_0(z) := \tilde{y}_1(z) + u^c(x_{12}) \) for \( x \in \mathbb{R}^3 \). From the construction of \( u^c \), we obtain the following: for all \( m \in D_{R_0} \times [0,1] \), \( \ell \in D_{R_0+R_1} \times [-R_2, R_2 + 1) \),
\[
|\tilde{y}_0(\ell) - \tilde{y}_0(m)| \geq |y_0(\ell_{12}) - y_0(m_{12})| \geq \frac{c_2|\ell - m|}{2(R_0 + 1) + R_1 + R_2} =: m_2|\ell - m|. \tag{F.21}
\]
We remark that as \( u^c(\ell_{12}') = 0 \) for all \( \ell_{12}' \in \Lambda \setminus D_{R_0} \) and that \( |u^c(z)| \leq 1 \) for all \( z \in \mathbb{R}^2 \), we observe that the estimates (F.17)–(F.19) continue to hold after substituting \( \tilde{y}_1 \) and \( \tilde{y}_0 \).

Combining these estimates with (F.21) gives (F.6), for \( m := \min \{ \frac{m'}{4}, m_2 \} > 0 \).

It remains to show (F.5). We first observe that for any \( \ell \in \Lambda_0 \cap ((\mathbb{R}^2 \setminus D_{R_0+1}) \times \mathbb{R}) \), we have \( \tilde{y}_0(\ell) = \tilde{y}_1(\ell) = I \tilde{y}_0(\ell) \). By Lemma F.2, there exists open, bounded \( \Omega_1 \subset \mathbb{R}^2 \) such
that \( I\tilde{y}_1 : (\mathbb{R}^2 \setminus D_{R_0+1}) \times \mathbb{R} \rightarrow (\mathbb{R}^2 \setminus \Omega_1) \times \mathbb{R} \) is a homeomorphism. Moreover, as \( \Omega_1 \) is bounded, there exists \( R_3 > 0 \) such that \( \Omega_1 \subset D_{R_3} \).

Consider \( x \in (\mathbb{R}^2 \setminus \Omega_1) \times \mathbb{R} \), then there exists unique \( x' \in (\mathbb{R}^2 \setminus D_{R_0+1}) \times \mathbb{R} \) satisfying \( I\tilde{y}_1(x') = x \). Additionally, there exists \( \ell \in \Lambda_0 \cap ((\mathbb{R}^2 \setminus D_{R_0+1}) \times \mathbb{R}) \) satisfying \( |\ell - x'| \leq c_3 \), where \( c_3 > 0 \) is independent of \( \ell, x' \) and only depends on \( \Lambda_0 \). We now apply (F.7) to deduce

\[
|\tilde{y}_0(\ell) - x| = |I\tilde{y}_1(\ell) - I\tilde{y}_1(x')| \leq M|\ell - x'| \leq c_3M =: \lambda_1.
\]

Now consider \( x \in \Omega_1 \times \mathbb{R} \), then choosing \( \ell = 0 \in \Lambda_0 \) yields

\[
|\tilde{y}_0(0) - x| = |\tilde{y}_0(0)| + |x| \leq |\tilde{y}_0(0)| + R_3 =: \lambda_2.
\]

Let \( \lambda := \max\{\lambda_1, \lambda_2\} > 0 \), then the desired estimate (F.5) follows from the preceding estimates, that is \( B_\lambda(x) \cap \tilde{y}_0(\Lambda_0) \neq \emptyset \) for all \( x \in \mathbb{R}^3 \). This concludes the proof.

We shall first give the following far-field decay estimate of the dislocation predictor on the left half-plane.

**Lemma F.3.** If the setting for dislocations hold and \( \ell \in \Lambda \) with \( \ell_1 < \hat{x}_1 \), then there exist constants \( C_j \) for \( j \in \mathbb{N} \), such that for \( \rho = (\rho_1, \ldots, \rho_j) \in (\Lambda^h)^j \),

\[
|D_{\rho}u_0(\ell)| \leq C_j|\ell|^{-j} \max_{1 \leq i \leq j} \{|\rho_i|^j \log |\rho_i|\}.
\]

**Remark F.4.** It may be possible to sharpen the decay estimates (F.22). If so, then the decay assumptions (S.L) for dislocations may be weakened. However, consider the case that \( |\rho_2| = O(1) \), \( m \in \Lambda^h \) fixed, \( \ell = m - \rho_1 \) with \( |\ell| \to \infty \). In this case \( |D_{\rho}u_0(\ell)| = |u(m + \rho_2) - u(m) - u(\ell + \rho_2) + u(\ell)| \approx |m|^{-1} \leq |\ell|^{-3}|\rho_1|^2 \), but the factor \( |\rho_1|^2 \) cannot be improved upon in an obvious way.

**Proof.** Let \( j \in \mathbb{N} \), \( \rho = (\rho_1, \ldots, \rho_j) \in (\Lambda^h)^j \) and we consider \( \ell \in \Lambda \) sufficiently large.

For the case \( \max_{1 \leq i \leq j} |\rho_i| \leq \frac{|\ell|}{2j} \), using (3.11) and Taylor’s theorem, we deduce that

\[
|D_{\rho}u_0(\ell)| \leq \sum_{i=1}^j |\rho_i| \int_0^1 \cdots \int_0^1 \left| \nabla^i u_0 \left( \ell + \sum_{i=1}^j t_i \rho_i \right) \right| dt_1 \cdots dt_j
\]

\[
\leq C \sum_{i=1}^j |\rho_i| \int_0^1 \cdots \int_0^1 |\ell + \sum_{i=1}^j t_i \rho_i|^{-j} dt_1 \cdots dt_j
\]

\[
\leq C2^j|\ell|^{-j} \sum_{i=1}^j |\rho_i| \leq C_j|\ell|^{-j} \max_{1 \leq i \leq j} \{|\rho_i|^j \log |\rho_i|\}.
\]

Now suppose that \( \max_{1 \leq i \leq j} |\rho_i| > \frac{|\ell|}{2j} \), then we expand the finite-difference stencil to obtain

\[
D_{\rho}u_0(\ell) = \sum_{k=0}^j (-1)^{j-k} \sum_{1 \leq i_1 < \ldots < i_k \leq j} u_0 \left( \ell + \sum_{n=1}^k \rho_{i_n} \right).
\]
Then, as (3.9) implies $|u_0(x)| \leq C \log(2 + |x|)$, for all $x \in \mathbb{R}^2 \setminus \Gamma$, it follows that

$$|D_\rho u_0(\ell)| \leq C \sum_{k=0}^j \sum_{1 \leq i_1 < \cdots < i_k \leq j} \log \left(2 + \sum_{n=1}^k |\rho_{i_n}| \right)$$

$$\leq C 2^j \log \left(2 + |\ell| + \sum_{i=1}^j |\rho_i| \right) \leq \tilde{C}_j \log \left(1 + \max_{1 \leq i \leq j} |\rho_i| \right)$$

$$\leq \tilde{C}_j (2j)^j \left(\max_{1 \leq i \leq j} |\rho_i| \right)^j j \log \left(1 + \max_{1 \leq i \leq j} |\rho_i| \right)$$

$$\leq C_j |\ell|^{-j} \max_{1 \leq i \leq j} \{ |\rho_i|^j \log(1 + |\rho_i|) \}.$$  

This completes the proof. □

**Remark F.5.** For finite-difference stencils with finite interaction range, Lemma F.3 implies that if $\ell \in \Lambda$ with $\ell_2 < \tilde{x}_2 |\rho_i| \leq R_c$ $\forall$ $1 \leq i \leq j$ with some cut-off radius $R_c$, then $|D_\rho u_0(\ell)| \leq C_j |\ell|^{-j}$.

Lemma F.3 together with definition (F.3) and the fact that $S_0 u_0 \in C^\infty(\Omega_\Gamma)$ give us the decay of the elastic strain: for $\ell \in \Lambda$ and $|\ell|$ sufficiently large, there exist constants $C_j > 0$ for $j \in \mathbb{N}_0$, such that

$$|e_\sigma(\ell)| \leq C_1 |\ell|^{-1} |\sigma| \log(1 + |\sigma|) \quad \text{and} \quad |D_\rho e_\sigma(\ell)| \leq C_{j+1} |\ell|^{-j-1} \max \left\{ |\sigma|^j \log(1 + |\sigma|), \max_{1 \leq i \leq j} |\rho_i|^j \log(1 + |\rho_i|) \right\}, \quad (F.23)$$

with $\sigma \in \Lambda^h$ and $\rho \in (\Lambda^h) \cap$, when $j \geq 1$. The estimate (F.23) holds by the same argument used to prove Lemma F.3. □

**F.2. Proof of Theorem 3.6.** Recall the operator $F : \mathbb{W}^c(\Lambda) \to \mathbb{R}$, defined in Theorem 3.6 by

$$\langle F, u \rangle := \sum_{\ell \in \Lambda} \langle \delta V(\ell) (Du_0(\ell)), Du(\ell) \rangle = \sum_{\ell \in \Lambda} \sum_{\rho \in \Lambda - \ell} V_{\ell, \rho} (Du_0(\ell)) \cdot D_\rho u(\ell).$$

To show that $F$ is defined, it is convenient for us to rewrite

$$\langle F, u \rangle = \sum_{\ell \in \Lambda} \langle \delta V(\ell) (Du_0(\ell)), Du(\ell) \rangle = \sum_{\ell \in \Lambda} \langle \delta V(e(\ell)), Du(\ell) \rangle$$

$$(F.24)$$

in force-displacement form

$$\langle F, u \rangle = \sum_{\ell \in \Lambda} f(\ell) \cdot u(\ell), \quad (F.25)$$

where $f : \Lambda \to \mathbb{R}^d_s$ describes the residual forces. The detailed expression of $f$ will be discussed in the proof of next lemma. The following lemma gives the far-field decay of the residual force $f(\ell)$.

**Lemma F.6.** Under the conditions of Theorem 3.6, there exists $C > 0$ such that

$$|f(\ell)| \leq C |\ell|^{-3}. \quad (F.26)$$
Proof. Case 1: left half-plane: We first consider the simplified situation when $\ell_1 < \hat{x}_1$, and will see below that a generalisation to $\ell_1 > \hat{x}_1$ is straightforward.

Let us assume $\ell_2 > \hat{x}_2$ first. Using (F.24), (F.25) and the definition of $\tilde{D}$, we obtain from a direct calculation that

$$
f(\ell) = \sum_{\rho \in A^b} D_{-\rho} V_{\rho}(e(\ell)) + \left( \sum_{\rho \in A^b} \frac{\rho}{\ell-\rho-b_{12} \in \Omega} V_{\rho}(e(\ell - \rho - b_{12})) - \sum_{\rho \in A^b} \frac{\rho}{\ell-\rho \in \Omega} V_{\rho}(e(\ell - \rho)) \right) = \tilde{f}(\ell) + f^c(\ell). \tag{F.27}
$$

Note that $\ell_1 < \hat{x}_1$, $\ell_2 > \hat{x}_2$ and $\ell - \rho \in \Omega$, $\ell_2 - \rho_2 < \hat{x}_2$ implies $|\rho| \geq |\ell|$. Then by (S.L) there exists $w_3 \in \mathcal{L}^3_{\infty}$ such that

$$
|f^c(\ell)| \leq C \sum_{\rho \in A^b \atop |\rho| \geq |\ell|} w_3(|\rho|) \leq C \sum_{\rho \in A^b \atop |\rho| \geq |\ell|} w_3(|\rho|) \left( \frac{|\rho|}{|\ell|} \right)^3 \leq C |\ell|^{-3} \|w_3\|_{\mathcal{L}^3_{\infty}} \leq C |\ell|^{-3}. \tag{F.28}
$$

We now estimate $|\tilde{f}(\ell)|$ by first expanding $V_{\rho}$ to second order,

$$
V_{\rho}(e(\ell)) = V_{\rho}(0) + \langle \delta V_{\rho}(0), e(\ell) \rangle + \int_0^1 (1-t) \langle \delta^2 V_{\rho}(te(\ell)) e(\ell), e(\ell) \rangle \, dt. \tag{F.29}
$$

The symmetry assumption (S.PS) implies that $\sum_{\rho} V_{\rho}(0) = 0$. Hence, we obtain

$$
\tilde{f}(\ell) = \sum_{\rho \in A^b} \int_0^1 \sigma \tilde{D}_{-\rho} \sigma(\ell) + \sum_{\rho \in A^b} \int_0^1 (1-t) \tilde{D}_{-\rho} \delta^2 V_{\rho}(te(\ell)) e(\ell), e(\ell) \rangle \, dt 
=: f^{(1)}(\ell) + f^{(2)}(\ell). \tag{F.30}
$$

To estimate $f^{(1)}(\ell)$, we observe that $\tilde{D}_{-\rho} \sigma(\ell) = D_{-\rho} D_{\sigma} u_0(\ell)$ as $\ell_1 < \hat{x}_1$, then using as $u_0(x)$ is smooth for $x < \hat{x}_1$, for $|\rho|, |\sigma| \leq |\ell|/4$, applying (3.11) and a Taylor expansion gives

$$
|D_{-\rho} D_{\sigma} u_0(\ell) + \nabla_{\rho} \nabla_{\sigma} u_0(\ell)| = |D_{\sigma} u_0(\ell - \rho) - D_{\sigma} u_0(\ell) + \nabla_{\rho} \nabla_{\sigma} u_0(\ell)|

\leq |\nabla_{\sigma} u_0(\ell - \rho) - \nabla_{\sigma} u_0(\ell) + \frac{1}{2} \int_0^1 \nabla_{\sigma}^2 u_0(\ell - \rho - t(1-t) \sigma - u_0(\ell - t(1-t) \sigma) | dt + \nabla_{\rho} \nabla_{\sigma} u_0(\ell)|

\leq \int_0^1 |\nabla_{\sigma}^2 u_0(\ell - \rho - t(1-t) \sigma - t(1-t) \sigma) - u_0(\ell - t(1-t) \sigma)| dt_1

\leq C |\ell|^{-3} \|\rho\|^2 \|\sigma\| \leq C |\ell|^{-3} \max \{|\rho|^3 \log(1 + |\rho|), |\sigma|^3 \log(1 + |\sigma|)\}. \tag{F.31}
$$

For the remaining case $\max\{|\rho|, |\sigma|\} > |\ell|/4$, we apply the triangle inequality together with Lemma F.3 and (3.11) to obtain

$$
|D_{-\rho} D_{\sigma} u_0(\ell) + \nabla_{\rho} \nabla_{\sigma} u_0(\ell)| \leq |D_{-\rho} D_{\sigma} u_0(\ell)| + |\nabla_{\rho} \nabla_{\sigma} u_0(\ell)|

\leq C |\ell|^{-2} \max \{|\rho|^2 \log(1 + |\rho|), |\sigma|^2 \log(1 + |\sigma|)\}

\leq C |\ell|^{-3} \max \{|\rho|^3 \log(1 + |\rho|), |\sigma|^3 \log(1 + |\sigma|)\}. \tag{F.32}
$$
Combining (F.31)–(F.32) and applying (S.L), there exist \(w_3 \in \mathcal{L}_3^{\text{log}}, w_4 \in \mathcal{L}_4^{\text{log}}\) such that

\[
\left| \sum_{\rho, \sigma \in \Lambda_h^b} V_{\rho\sigma}(0)(D_{-\rho}e_{\sigma}(\ell) + \nabla_{\rho} \nabla_{\sigma} u_0(\ell)) \right|
\leq C|\ell|^{-3} \sum_{\rho, \sigma \in \Lambda_h^b} |w_3(\rho)||w_3(\sigma)|(|\rho|^3 \log(1 + |\rho|) + |\sigma|^3 \log(1 + |\sigma|))
+ C|\ell|^{-3} \sum_{\rho \in \Lambda_h^b} |w_4(\rho)||\rho|^3 \log(1 + |\rho|)
\leq C|\ell|^{-3}(\|w_3\|_{\mathcal{L}_3^{\text{log}}}^2 + \|w_4\|_{\mathcal{L}_4^{\text{log}}}^2) \leq C|\ell|^{-3}. \tag{F.33}
\]

For the remaining term, we have from (3.11) that \(\nabla^2 u_0 = \nabla^2 u_{\text{lin}} + O(|x|^{-3})\), which together with the fact \(\sum_{\rho, \sigma \in \Lambda_h^b} V_{\rho\sigma}(0)\nabla_{\rho} \nabla_{\sigma} u_{\text{lin}}(x) = 0\) and (F.33) leads to

\[
|f^{(1)}(\ell)| \leq C|\ell|^{-3}. \tag{F.34}
\]

To estimate \(f^{(2)}(\ell)\) in (F.30), we decompose \(f^{(2)}\) into two parts

\[
f^{(2)}(\ell) = \sum_{\rho \in \Lambda_h^b, |\rho| \leq |\ell|/2} \int_0^1 (1 - t)\widetilde{D}_{-\rho}\langle \delta^2 V_{\rho}(te(\ell))e(\ell), e(\ell) \rangle \, dt
+ \sum_{\rho \in \Lambda_h^b, |\rho| \geq |\ell|/2} \int_0^1 (1 - t)\widetilde{D}_{-\rho}\langle \delta^2 V_{\rho}(te(\ell))e(\ell), e(\ell) \rangle \, dt =: f^{(2)}_A(\ell) + f^{(2)}_B(\ell). \tag{F.35}
\]

We first express

\[
\widetilde{D}_{-\rho}\langle \delta^2 V_{\rho}(t_1e(\ell))e(\ell), e(\ell) \rangle = D_{-\rho}\langle \delta^2 V_{\rho}(t_1e(\ell))e(\ell), e(\ell) \rangle
= \langle \delta^2 V_{\rho}(t_1e(\ell - \rho))e(\ell - \rho), e(\ell - \rho) \rangle - \langle \delta^2 V_{\rho}(t_1e(\ell))e(\ell), e(\ell) \rangle
= \langle \delta^2 V_{\rho}(t_1e(\ell))e(\ell - \rho) + e(\ell), D_{-\rho}e(\ell) \rangle + \langle D_{-\rho}\delta^2 V_{\rho}(t_1e(\ell))e(\ell), e(\ell) \rangle
= \langle \delta^2 V_{\rho}(t_1e(\ell))e(\ell - \rho) + e(\ell), D_{-\rho}e(\ell) \rangle
- t_1 \int_0^1 \langle \delta^3 V_{\rho}(t_1e(\ell - t_2\rho))\nabla_{\rho}e(\ell - t_2\rho), e(\ell), e(\ell) \rangle \, dt_2,
\]

hence using (F.23) and (S.L) together with (3.11) to eventually deduce

\[
|f^{(2)}_A(\ell)| \leq C \left( \int_0^1 \sum_{\rho, \sigma, \xi \in \Lambda_h^b \atop |\rho| \leq |\ell|/2} \left| V_{\rho\sigma\xi}(t_1e(\ell - \rho)) \right| e_\sigma(\ell - \rho) + e_\sigma(\ell) \right| D_{-\rho}e_\xi(\ell) \, dt_1
+ \int_0^1 \int_0^1 \sum_{\rho, \sigma, \xi \in \Lambda_h^b \atop |\rho| \geq |\ell|/2} \left| V_{\rho\sigma\xi}(t_1e(\ell - t_2\rho)) \right| \nabla_{\rho}e_\sigma(\ell - t_2\rho) \left| e_\ell(\ell) \right| e_\xi(\ell) \, dt_1 \, dt_2
\leq C|\ell|^{-3}, \tag{F.36}
\]

by considering the various partition cases in (2.13).

For the remaining case, recall that

\[
\widetilde{D}_{-\rho}\langle \delta^2 V_{\rho}(t_1e(\ell))e(\ell), e(\ell) \rangle
= \langle \delta^2 V_{\rho}(t_1e(\ell - \rho))e(\ell - \rho), e(\ell - \rho) \rangle - \langle \delta^2 V_{\rho}(t_1e(\ell))e(\ell), e(\ell) \rangle,
\]
then using (S.L), there exist \( w_3 \in \mathcal{L}^3, w_4 \in \mathcal{L}^4, w_5 \in \mathcal{L}^5 \) such that

\[
\sum_{\rho \in \Lambda^b} \left| \langle \delta^2 V_{\rho}(t_1 e(\ell)) e(\ell), e(\ell) \rangle \right| \leq C|\ell|^{-3} \sum_{\rho \in \Lambda^b} w_5(|\rho|)|\rho|^3 \log^2(1 + |\rho|)
\]

\[
+ C|\ell|^{-3} \left( \left( \sum_{\rho \in \Lambda^b} w_3(|\rho|)|\rho| \log(1 + |\rho|) \right)^3 + \left( \sum_{\rho \in \Lambda^b} w_4(|\rho|)|\rho|^2 \log^2(1 + |\rho|) \right)^{3/2} \right)
\]

\[
\leq C|\ell|^{-3} \left( \|w_3\|_{\mathcal{L}^3}^3 + \|w_4\|_{\mathcal{L}^4}^{3/2} + \|w_5\|_{\mathcal{L}^5} \right) \leq C|\ell|^{-3}. \tag{F.37}
\]

For \( |\rho| \geq |\ell|/2 \) and \( \sigma \in \Lambda^b \), we have from (F.3) that

\[
|e_\sigma(\ell - \rho)| = |D_\sigma u_0(\ell - \rho)| \leq |u_0(\ell - \rho + \sigma)| + |u_0(\ell - \rho)| \leq C(\log(2 + |\ell - \rho|) + |\sigma|) \leq C(\log(1 + |\rho|) + |\sigma|),
\]

hence we deduce

\[
\sum_{\rho \in \Lambda^b} \left| \langle \delta^2 V_{\rho}(t_1 e(\ell - \rho)) e(\ell - \rho), e(\ell - \rho) \rangle \right| \leq C|\ell|^{-3} \sum_{\rho \in \Lambda^b} w_5(|\rho|)|\rho|^5
\]

\[
+ C|\ell|^{-3} \left( \left( \sum_{\rho \in \Lambda^b} w_3(|\rho|)|\rho|^3 \log^2(1 + |\rho|) \right)^3 + \left( \sum_{\rho \in \Lambda^b} w_4(|\rho|)|\rho|^4 \log^2(1 + |\rho|) \right)^{3/2} \right)
\]

\[
\leq C|\ell|^{-3} \left( \|w_3\|_{\mathcal{L}^3}^3 + \|w_4\|_{\mathcal{L}^4}^{3/2} + \|w_5\|_{\mathcal{L}^5} \right) \leq C|\ell|^{-3}. \tag{F.38}
\]

Collecting the estimates (F.35)–(F.38) yields

\[
|f^{(2)}(\ell)| \leq C|\ell|^{-3}, \tag{F.39}
\]

hence \( |f(\ell)| \leq C|\ell|^{-3} \) whenever \( \ell_2 > \tilde{x}_2 \).

Combining (F.27), (F.28), (F.30), (F.34) and (F.39), we can show (F.26) when \( \ell \) lies in the left half-plane and \( \ell_2 > \tilde{x}_2 \). The case \( \ell_2 < \tilde{x}_2 \) follows verbatim by rewriting (F.27) as

\[
f(\ell) = \sum_{\rho \in \Lambda^b} D_{-\rho} V_{\rho}(e(\ell)) + \left( \sum_{\rho \in \Lambda^b} V_{\rho}(e(\ell - \rho + b_{12})) - \sum_{\rho \in \Lambda^b} V_{\rho}(e(\ell - \rho)) \right).
\]

**Case 2: right half-space:** To treat the case \( \ell_1 > \tilde{x}_1 \), we first observe that the definition of the reference solution with branch-cut \( \Gamma = \{(x_1, \tilde{x}_2) \mid x_1 \geq \tilde{x}_1\} \) was somewhat arbitrary, in that we could have equally chosen \( \Gamma_S := \{(x_1, \tilde{x}_2) \mid x_1 \leq \tilde{x}_1\} \). In this case the predictor solution \( u_0 \) would be replaced with \( S_0 u_0 \). Let the resulting energy functional be denoted by

\[
\mathcal{E}_S(u) := \sum_{\ell \in \Lambda^b} V(DS_0 u_0(\ell) +Du(\ell)) - V(DS_0 u_0(\ell)).
\]

It is straightforward to see that if \( \delta \mathcal{E}(\bar{u}) = 0 \), then \( \delta \mathcal{E}_S(S\bar{u}) = 0 \) as well.

With this observation, we can rewrite

\[
f = \tilde{D}_{-\rho} V_{\rho}(\tilde{D}_0 u_0) = [RD_{-\rho} S] V_{\rho}([RD_S] u_0) = RD_{-\rho} V_{\rho} DS_0 u_0.
\]

Since \( S_0 u_0 \) is smooth in a neighbourhood of \( |\ell| \) even if that neighbourhood crosses the branch-cut, we can now repeat the foregoing argument in Case 1 to deduce again that \( |S f(\ell)| \leq C|\ell|^{-3} \) as well. But since \( S \) represents an \( O(1) \) shift, this immediately implies also that \( |f(\ell)| \leq C|\ell|^{-3} \). This completes the proof of (F.26). \( \square \)
We also need the following result to convert pointwise forces into divergence form. Define $D_N u(\ell) := \{D_p u(\ell)\}_{p \in \mathcal{N}(\ell) - \ell}$, we have the following result inherited from [13, Lemma 5.1 and Corollary 5.2].

**Lemma F.7.** Let $p > d$, $f : \mathbb{A}^d \to \mathbb{R}^d$, such that $|f(\ell)| \leq C_{f} |\ell|^{-p}$ for all $\ell \in \mathbb{A}^d$, and $\sum_{\ell \in \mathbb{A}^d} f(\ell) = 0$. Then there exists $g : \mathbb{A}^d \to (\mathbb{R}^d)^{N(\ell) - \ell}$ and a constant $C > 0$ depending on $p$ such that

$$
\sum_{\ell \in \mathbb{A}^d} f(\ell) \cdot v(\ell) = \sum_{\ell \in \mathbb{A}^d} \langle g(\ell), D_N v(\ell) \rangle \quad \text{and} \quad |g(\ell)| \leq C|\ell|^{-p+1} \quad \forall \, \ell \in \mathbb{A}^d.
$$

**Proof.** This is an immediate consequence of in [13, Lemma 5.1] and the fact that $\mathcal{N}(\ell) \supset \{\ell \pm A \varepsilon_i\}$. □

**Proof of Theorem 3.6.** We have from Lemma F.6 that $|f(\ell)| \leq C|\ell|^{-3}$, which together with Lemma F.7 yields a map $g$ such that $|g(\ell)| \leq C|\ell|^{-2}$ and

$$
\langle F, v \rangle \leq C\|g\|_{L^2} \|Dv\|_{L^2}^2 \quad \forall \, v \in \dot{W}^{1,2}(\Lambda).
$$

Therefore $F$ is bounded and this completes the proof. □

**F.3. Proof of Theorem 3.7.** We will extend the arguments of Appendix E.3 to the dislocation case. We shall modify the homogeneous difference operator (3.3) in the analysis for dislocations by defining $\tilde{H} : \dot{W}^{1,2}(\Lambda^h) \to \dot{W}^{-1,2}(\Lambda^h)$ as

$$
\langle \tilde{H}u, v \rangle := \sum_{\ell \in \Lambda^h} \langle \delta^2 V(0) \tilde{D}u(\ell), \tilde{D}v(\ell) \rangle \quad \forall \, v \in \dot{W}^{1,2}(\Lambda^h). \tag{F.40}
$$

The following lemma is analogous to Lemma E.5, which gives the first-order residual estimate for dislocations.

**Lemma F.8.** If the conditions of Theorem 3.7 are satisfied, then for any $\tilde{u}$ solving (2.21), there exists $g : \Lambda^h \to (\mathbb{R}^d)^{\Lambda^h}$ such that

$$
\langle \tilde{H} \tilde{u}, v \rangle = \langle g, \tilde{D}v \rangle \quad \forall v \in \dot{W}^c,
$$

where $g$ satisfies

$$
\left| \langle g, \tilde{D}v \rangle \right| \leq C \sum_{\ell \in \Lambda^h} \sum_{j=1}^{3} \tilde{g}_j(\ell) |\tilde{D}v(\ell)|_{W_{j,1}},
$$

with some constant $C > 0$, $w_j \in L^\infty_{j+2}$ for $1 \leq j \leq 3$ and

$$
\tilde{g}_1(\ell) = \tilde{g}_2(\ell) = (1 + |\ell|)^{-2} + \left( \sum_{k=1}^{2} |\tilde{D} \tilde{u}(\ell)|_{W_{3,k}} \right)^2, \quad \tilde{g}_3(\ell) = (1 + |\ell|)^{-2} + |\tilde{D} \tilde{u}(\ell)|_{W_{3,3}}^2.
$$

**Proof.** By the definition of $\tilde{H}$, we can write

$$
\langle \tilde{H} \tilde{u}, v \rangle = \sum_{\ell \in \Lambda^h} \left( \langle \delta^2 V(0) - \delta^2 V(e(\ell)) \rangle \tilde{D} \tilde{u}(\ell), \tilde{D} v(\ell) \right) + \langle \delta V(e(\ell)) + \delta^2 V(e(\ell)) \tilde{D} \tilde{u}(\ell) - \delta V(e(\ell) + \tilde{D} \tilde{u}(\ell)), \tilde{D} v(\ell) \rangle \right) \right) - \langle \delta \delta(0), v \rangle
$$

$$
=: \langle g^{(1)} + g^{(2)}, \tilde{D}v \rangle - \langle f, v \rangle, \tag{F.41}
$$

where we employed the force-displacement form (F.25) in the last step.
To estimate \( \tilde{g}^{(1)} \), we have from (F.23) that there exist \( w_j \in L_{j+2}^{\log} \) \((j = 1, 2, 3)\) such that

\[
|\langle g^{(1)}, \tilde{D}v \rangle| = \left| \sum_{\ell \in \Lambda^h} \int_0^1 \left\langle \delta^3 V(te(\ell)), \left( e(\ell), \tilde{D}_z u(\ell), \tilde{D}_z v(\ell) \right) \right\rangle \, dt \right|
\]

\[
\leq \sum_{\ell \in \Lambda^h} \sum_{\rho, \xi \in \Lambda^h} \int_0^1 \left| V_{\rho, \xi}(te(\ell)) D_\rho e(\ell) \tilde{D}_z u(\ell) \tilde{D}_z v(\ell) \right| \, dt \tag{F.42}
\]

\[
\leq C \sum_{\ell \in \Lambda^h} (1 + |\ell|)^{-1} \left( \left( \sum_{k=1}^2 |\tilde{D}u(\ell)|_{w_k, k} \right)^2 \left( \sum_{k' = 1}^2 |\tilde{D}v(\ell)|_{w_{k'}, k'} \right) + |\tilde{D}u(\ell)|_{w_{3, 3}}^2 |\tilde{D}v(\ell)|_{w_{3, 3}} \right) \tag{F.43}
\]

where similar calculations as (E.25)–(E.27) and the decay assumptions (S.L) for dislocations are used for the last estimate.

Again using the same calculations as (E.25)–(E.27), we have the estimate for \( g^{(2)} \)

\[
|\langle g^{(2)}, \tilde{D}v \rangle| \leq C \sum_{\ell \in \Lambda} \left( \left( \sum_{k=1}^2 |\tilde{D}u(\ell)|_{w_k, k} \right)^2 \left( \sum_{k' = 1}^2 |\tilde{D}v(\ell)|_{w_{k'}, k'} \right) + |\tilde{D}u(\ell)|_{w_{3, 3}}^2 |\tilde{D}v(\ell)|_{w_{3, 3}} \right). \tag{F.44}
\]

Combing (F.42) and (F.44), we obtain that

\[
|\langle g^{(1)} + g^{(2)}, \tilde{D}v \rangle| \leq C \sum_{\ell \in \Lambda^h} \left( (1 + |\ell|)^{-2} + \left( \sum_{k=1}^2 |\tilde{D}u(\ell)|_{w_k, k} \right)^2 \right) \left( \sum_{k' = 1}^2 |\tilde{D}v(\ell)|_{w_{k'}, k'} \right)
+ C \sum_{\ell \in \Lambda^h} \left( (1 + |\ell|)^{-2} + |\tilde{D}u(\ell)|_{w_{3, 3}}^2 \right) |\tilde{D}v(\ell)|_{w_{3, 3}}. \tag{F.45}
\]

For the \( \{f, v\} \) group, we have from Lemma F.6 that \(|f(\ell)| \leq C|\ell|^{-3}\), which also implies \(|S f(\ell)| \leq C|\ell|^{-3}\). Then using a similar argument as Lemma F.7, we can derive existence of \( g^{(3)} \), such that

\[
|\langle f, v \rangle| = |\langle g^{(3)}, \tilde{D}v \rangle| \leq \sum_{\ell \in \Lambda^h} (1 + |\ell|)^{-2} |\tilde{D}v(\ell)|_{w_{1, 1}}. \tag{F.46}
\]

Setting \( g := g^{(1)} + g^{(2)} - g^{(3)} \), we obtain from (F.45) and (F.46) the stated result. \( \square \)

Unlike the point defect case, we can not use Lemma D.3 directly, due to the “incompatible finite-difference stencils” \( \tilde{D}u(\ell) \) in (F.40). We will follow a boot-strapping argument in [13] to bypass this obstacle, starting from the following sub-optimal estimate.

**Lemma F.9.** Under the conditions of Theorem 3.7, there exists \( C > 0 \) such that

\[
|\tilde{D}_\rho u(\ell)| \leq C|\rho|(1 + |\ell|)^{-1}. \tag{F.47}
\]

*Proof.* Let us first consider the case when \( \ell \) lies in the left half-plane \( \ell_1 < \tilde{\ell}_1 \). It is only necessary for us to consider when \(|\ell|\) is sufficiently large, when \( B_{3|\ell|/4}(\ell) \) does not intersect the branch cut \( \Gamma \).

Let \( \eta \) be a cut-off function with \( \eta(x) = 1 \) in \( B_{|\ell|/4}(\ell) \), \( \eta(x) = 0 \) in \( \mathbb{R}^2 \setminus B_{|\ell|/2}(\ell) \) and \( |\nabla \eta| \leq C|\ell|^{-1} \). Further, let \( v(k) := D_\rho \mathcal{G}(k - \ell) \), where \( \mathcal{G} \) is the lattice Green’s function.
associated with the homogeneous finite-difference operator $H$ in (D.2), see Lemma D.2 for the definition of $G$. Then,

$$D \tilde{u}(\ell) = \langle H \tilde{u}, v \rangle = \left( \langle H \tilde{u}, \eta v \rangle - \langle \tilde{H} \tilde{u}, \eta v \rangle \right) + \langle \tilde{H} \tilde{u}, \eta v \rangle + \langle H \tilde{u}, (1 - \eta)v \rangle$$

$$= h^{(1)} + h^{(2)} + h^{(3)},$$

(F.48)

where $\eta v, (1 - \eta)v$ are understood as pointwise function multiplications.

We first compare $H$ and $\tilde{H}$ to estimate $h^{(1)}$. Using Lemma D.2 (ii), we can derive from the definitions of $\tilde{D}$ and $\eta$ that $|\tilde{D}_\sigma[\eta v](k)| \leq C|\sigma| \cdot |\rho|(1 + |\ell - k|)^{-2}$. Moreover, we have from the definition of $\eta$ that if $|k - \ell| > 3|\ell|/4$, then $D_\sigma[\eta v](k) \neq 0$ only when $|\sigma| > |\ell|/4$. Using the definition of $\tilde{D}$ and the fact $B_{\frac{3|\ell|}{4}}(\ell) \cap \Gamma = \emptyset$, we have that if $|k - \ell| \leq 3|\ell|/4$, then $\tilde{D}_\sigma u(k) \neq D_\sigma u(k)$ only when $|\xi| \geq |\ell|/4$. Then we can obtain from the decay assumptions (S.L) for dislocations that

$$h^{(1)} = \langle H \tilde{u}, \eta v \rangle - \langle \tilde{H} \tilde{u}, \eta v \rangle$$

$$= \sum_{k \in \Lambda^b \cap \Omega_r} \sum_{\sigma, \xi \in \Lambda^b_{\sigma}} V_{\sigma, \xi}(0) \left( D_\sigma[\eta v](k) \left( D_\xi \tilde{u}(k) - \tilde{D}_\xi \tilde{u}(k) \right) + \tilde{D}_\xi u(k) \left( D_\sigma[\eta v](k) - \tilde{D}_\sigma[\eta v](k) \right) \right)$$

$$\leq C|\rho| \left( |\ell|^{-2} \sum_{k \in \Lambda^b \cap \Omega_r} (1 + |k - \ell|)^{-2} + |\ell|^{-2} \sum_{k \in \Lambda^b \cap \Omega_r} (1 + |k - \ell|)^{-2} \right)$$

$$\leq C|\rho| |\ell|^{-1}.$$  

(F.49)

Using Lemma D.2, F.8 and same calculations as (D.10)–(D.12), we have that there exist $w_j \in \mathcal{L}_{j+\frac{1}{2}} \log (j = 1, 2, 3)$ such that

$$h^{(2)} = \langle \tilde{H} u, \eta v \rangle = \langle g, \tilde{D} \eta v \rangle$$

$$\leq C|\rho| \sum_{k \in \Lambda^b} \left( (1 + |k|)^{-2} + \sum_{j=1}^{3} |\tilde{D} u(k)|_{w_j, j}^2 \right) (1 + |\ell - k|)^{-2}$$

$$\leq C|\rho| \left( |\ell|^{-2} \log |\ell| + \sum_{k \in \Lambda^b} (1 + |\ell - k|)^{-2} \left( \sum_{j=1}^{3} |\tilde{D} u(k)|_{w_j, j}^2 \right) \right).$$  

(F.50)

To estimate the last group in (F.48), we note that the definition of $\eta$ and Lemma D.2 implies $|D_\sigma[(1 - \eta)v](k)| \leq C|\sigma| \cdot |\rho|(1 + |\ell - k|)^{-2}$. Moreover, if $|k - \ell| \leq |\ell|/8$, then $D_\sigma[(1 - \eta)v](k) \neq 0$ only when $|\sigma| > |\ell|/8$. Hence, we have from the decay assumptions (S.L) for dislocations that there exist $w_j \in \mathcal{L}_{j+\frac{1}{2}} \log (j = 1, 2)$ such that

$$h^{(3)} = \langle H \tilde{u}, (1 - \eta)v \rangle$$

$$= \sum_{k \in \Lambda^b} \sum_{\rho, \xi \in \Lambda^b} V_{\rho, \xi}(0) D_\rho \tilde{u}(k) D_\xi (1 - \eta)v(k) + \sum_{k \in \Lambda^b} \sum_{\rho, \xi \in \Lambda^b} V_{\rho, \xi}(0) D_\rho \tilde{u}(k) D_\xi (1 - \eta)v(k)$$

$$\leq C|\rho| \left( |\ell|^{-2} \sum_{|k - \ell| \leq \frac{|\ell|}{4}} (1 + |\ell - k|)^{-2} + \sum_{|k - \ell| > \frac{|\ell|}{4}} |\ell - k|^{-2} \left( \sum_{j=1}^{2} |\tilde{D} u(k)|_{w_j, j}^2 \right) \right)$$

$$\leq C|\rho| |\ell|^{-1}.$$  

(F.51)
Combining (F.48)–(F.51) and the definition (A.1), we have that if \( \ell \) lies in the left half-plane and \( |\ell| \) sufficiently large, then there exist \( w_j \in L_{j+2}^{\log} \) \( (j = 1, 2, 3) \) such that

\[
\sum_{k=1}^{3} |Du(\ell)|_{w_{j,k}} \leq C \left( |\ell|^{-1} + \sum_{k \in \Lambda^h} (1 + |\ell - k|)^{-2} \left( \sum_{j=1}^{3} |\tilde{D}u(k)|_{w_{j,j}}^2 \right) \right).
\]

We can extend this estimate to the case when \( \ell \) lies in the right half-plane by a reflection argument as used in the proof of Lemma F.6. We replace the branch-cut \( \Gamma \) by \( \Gamma \) used in the proof of Lemma F.6. We replace the branch-cut \( \Gamma \) by \( \Gamma \) and repeating the argument used to show (D.15)–(D.19) verbatim, we deduce that (F.52) holds, but with \( u \) replaced by \( Su \) and for all \( \ell_1 > \hat{x}_1 \).

We can now consider arbitrary \( \ell \) and follow the proof of Lemma D.3. By taking

\[
w(r) := \sup_{\ell \in \Lambda^h, |\ell| \geq r} \left( \sum_{k=1}^{3} |Du(\ell)|_{w_{j,k}} \right)
\]

and repeating the argument used to show (D.15)–(D.19) verbatim, we deduce that \( \omega(r) \leq C r^{-1} \). Inserting this estimate into (F.49)–(F.51) gives us \( |D_{\rho}u(\ell)| \leq C |\rho| \cdot |\ell|^{-1} \), which together with the definition of \( \tilde{D} \) leads to \( |\tilde{D}_{\rho}u(\ell)| \leq C |\rho| \cdot |\ell|^{-1} \).

Having established a preliminary pointwise decay estimate on \( \tilde{D}u \), we now apply a boot-strapping technique to obtain an optimal bound.

**Proof of Theorem 3.7.** Without loss of generality, we may assume \( \ell \) belongs to the left half-plane, i.e. \( \ell_1 < \hat{x}_1 \). The right half-plane case can be obtained by the reflection arguments used in the proof of Lemma F.6 and F.9. We again define \( v \) as in the proof of Lemma F.9, and write

\[
D_{\rho}u(\ell) = \langle H\bar{u}, v \rangle
= \langle \tilde{H}\bar{u}, v \rangle + \sum_{k \in \Lambda^h \cap \Omega_T} \left( \langle \delta^2 V(0)\tilde{D}u(k), Dv(k) \rangle - \langle \delta^2 V(0)\tilde{D}u(k), \tilde{D}v(k) \rangle \right)
=: T_1 + T_2.
\]

To estimate the first group we note that \( T_1 = \langle g, \tilde{D}v \rangle \), hence we can employ the residual estimates from Lemma F.8. Combining the estimates in Lemma D.2, F.8 and F.9 yields

\[
|T_1| \leq \sum_{k \in \Lambda} (1 + |k|)^{-2} (1 + |\ell - k|)^{-2} \leq C |\ell|^{-2} \log |\ell|.
\]

To estimate \( T_2 \), we will combine the result in Lemma F.9 and a similar calculation as (F.49):

\[
T_2 = \langle H\bar{u}, v \rangle - \langle \tilde{H}\bar{u}, v \rangle
= \sum_{k \in \Lambda^h \cap \Omega_T} \sum_{\sigma, \xi \in \Lambda^h} V_{\sigma,\xi}(0) \left( D_{\sigma}v(k) \left( D_{\xi}u(k) - \tilde{D}_{\xi}u(k) \right) + \tilde{D}_{\xi}u(k) \left( D_{\sigma}v(k) - \tilde{D}_{\sigma}v(k) \right) \right)
\leq C |\rho| \left( \sum_{k \in \Lambda^h \cap \Omega_T} (1 + |k|)^{-2} (1 + |\ell - k|)^{-2} + \sum_{k \in \Lambda^h \cap \Omega_T} (1 + |k|)^{-1} (|k| + |\ell|)^{-2} \right)
\leq C |\rho| |\ell|^{-2} \log |\ell|.
\]
where we have used the facts that if $\Gamma \cap B_{|k|/2}(k) = \emptyset$, then $D_{\sigma}u(k) \neq \tilde{D}_{\sigma}u(k)$ only when $|\sigma| > |k|/2$, and if $\Gamma \cap B_{|k|/2}(k) \neq \emptyset$, then $|\ell - k| \geq \frac{1}{2}(|\ell| + |k|)$. Collecting (F.53) and (F.54) completes the proof of our desired result.

\[ \Box \]

References

[1] Balluffi, R. Introduction to Elasticity Theory for Crystal Defects. Cambridge University Press, 2012.

[2] Cai, W., Bulatov, V., Chang, J., Li, J., and Yip, S. Periodic image effects in dislocation modelling. Philosophical Magazine 83 (2003), 539–567.

[3] Cances, E., and Bris, C. L. Mathematical modelling of point defects in materials science. Math. Models Methods Appl. Sci. 23 (2013), 1795.

[4] Cances, E., Deleurence, A., and Lewin, M. A new approach to the modelling of local defects in crystals: The reduced hartree-fock case. Comm. Math. Phys. 281 (2008), 129–177.

[5] Catto, I., Bris, C. L., and Lions, P. The Mathematical Theory of Thermodynamic Limits: Thomas-Fermi Type Models. Oxford University Press, 1998.

[6] Chen, H., Kermode, J., Nazar, F., and Ortner, C. Locality of the reduced Hartree-Fock model with Yukawa poential. In preparation.

[7] Chen, H., Lu, J., and Ortner, C. Thermodynamic limits of crystal defects with finite temperature tight binding. arxiv:1607.06850.

[8] Chen, H., Nazar, F., and Ortner, C. Geometry equilibration of crystalline defects in quantum and atomistic descriptions. arXiv:1709.02770v1.

[9] Chen, H., and Ortner, C. QM/MM methods for crystalline defects. part 1: Locality of the tight binding model. Multiscale Model. Simul. 14 (2016), 232–264.

[10] Chen, H., and Ortner, C. QM/MM methods for crystalline defects. part 2: Consistent energy and force-mixing. Multiscale Model. Simul. 15 (2017), 184–214.

[11] Csányi, G., Albaret, T., Moras, G., Payne, M., and Vita, A. D. Multiscale hybrid simulation methods for material systems. J. Phys.: Condens. Matter 17 (2005), R691–R703.

[12] Daw, M., and Baskes, M. Embedded-Atom Method: Derivation and Application to Impurities, Surfaces, and other Defects in Metals. Physical Review B 20 (1984).

[13] Ehrlacher, V., Ortner, C., and Shapeev, A. Analysis of boundary conditions for crystal defect atomistic simulations. Archive for Rational Mechanics and Analysis 222, 3 (2016), 1217–1268.

[14] E.T., B. Exponential polynomials. Annals of Mathematics 35 (1934), 258–277.

[15] Finnis, M. A simple empirical $n$-body potential for transition metals. Phil. Mag. A. 50 (1984), 45–55.

[16] Finnis, M. Interatomic Forces in Condensed Matter. Oxford University Press, Oxford, 2003.

[17] Goringe, C., Bowler, D., and Hernández, E. Tight-binding modelling of materials. Rep. Prog. Phys. 60 (1997), 1447–1512.

[18] Gupta, R. Lattice relaxation at a metal surface. Phys. Rev. B 23 (1981), 6265.

[19] Hine, N., Freusch, K., Foulkes, W., and Finnis, M. Supercell size scaling of density functional theory formation energies of charged defects. Phys. Rev. B Auguest 2008 (2009), 1–13.

[20] Hudson, T., and Ortner, C. On the stability of Bravais lattices and their Cauchy–Born approximations. ESAIM:M2AN 46 (2012), 81–110.

[21] Hudson, T., and Ortner, C. Existence and stability of a screw dislocation under anti-plane deformation. ArXiv e-prints 1304.2500 (2013).

[22] Jones, J. On the Determination of Molecular Fields. III. From Crystal Measurements and Kinetic Theory Data. Proc. Roy. Soc. London A. 106 (1924), 709–718.

[23] Li, X., Luskin, M., Ortner, C., and Shapeev, A. Theory-based benchmarking of the blended force-based quasicontinuum method. Comput. Methods Appl. Mech. Engrg. 268 (2014), 763–781.

[24] Li, X., Ortner, C., Shapeev, A., and Van Koten, B. Analysis of blended atomistic/continuum hybrid methods. ArXiv 1404.4878.

[25] Makov, G., and Payne, M. Periodic boundary conditions in ab initio calculations. Phys. Rev. B 51 (Feb 1995), 4014–4022.

[26] Morse, P. Diatomic Molecules According to the Wave Mechanics. II. Vibrational Levels. Phys.Rev. 34f (1929), 57–64.

[27] Nazar, F. Electronic structure of defects in the Thomas-Fermi-von Weizsäcker model of crystals. PhD thesis, University of Warwick, 2016.
[28] Nazar, F., and Ortner, C. Locality of the Thomas-Fermi-von Weizsäcker equations. Arch. Ration. Mech. Anal. 224, 3 (2017), 817–870.

[29] Olson, D., and Ortner, C. Regularity and locality of point defects in multilattices. Appl. Math. Res. Express 1-41 (2017).

[30] Ortner, C., and Shapeev, A. Interpolants of lattice functions for the analysis of atomistic/continuum multiscale methods. arXiv:1204.3705.

[31] Ortner, C., and Theil, F. Justification of the Cauchy–Born approximation of elastodynamics. Arch. Ration. Mech. Anal. 207 (2013).

[32] Ortner, C., and Zhang, L. Atomistic/continuum blending with ghost force correction. ArXiv 1407.0053.

[33] Sinclair, J. Improved atomistic model of a bcc dislocation core. J. Appl. Phys. 42 (1971), 5231.

[34] Solovej, J. Proof of the ionization conjecture in a reduced Hartree-Fock model. Invent. Math. 104 (1991), 291–311.

[35] Yip, S., Ed. Handbook of Materials Modelling. Springer, 2005.

[36] Yukawa, H. On the interaction of elementary particles. Proc. Phys. Math. Soc. Japan. 17 (1935), 48–57.

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