THEORETICAL STUDY OF ELASTIC FAR-FIELD DECAY FROM DISLOCATIONS IN MULTILATTICES

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Abstract. We extend recent results of [6] characterising the decay of elastic fields generated by defects in crystalline materials to dislocations in multilattices. Specifically, we establish that the elastic field generated by a dislocation in a multilattice can be decomposed into a continuum field predicted by linearised elasticity, and a discrete and nonlinear core corrector representing the defect core. We discuss the consequences of this result for cell size effects in numerical simulations.

1. Introduction

A key approximation in all numerical simulations of crystalline defects is the boundary condition emulating the crystalline far-field. The “quality” of this boundary condition has a significant consequence for the severity of cell-size effects in such simulations. The study of these cell-size effects, such as [6], and the development of new boundary conditions, including [2], begins with a characterisation of the elastic field surrounding the defect core, which was initiated in [6]. Such a characterisation is also interesting in other contexts, e.g., in the study of defect interactions [8]. In the present work, we extend results concerning the decay of elastic far-fields generated by defects in crystalline materials to dislocations in multilattices (also referred to as complex crystals).

While results of this kind have been known in the materials science community from computational experiments and justified by associated continuum results dating back to Volterra [15], we fill a gap in the existing literature by producing the a rigorous proof of such decay estimates for dislocations in multilattices modeled via classical empirical potentials, i.e., in a discrete and fully nonlinear setting.

Our results are vital in establishing convergence of numerical methods for simulating crystal defects including direct atomistic simulations (c.f. [6]) as well as multiscale atomistic-to-continuum methods (c.f. [12]). Indeed, such direct atomistic computational methods date back decades to [4] which investigated computational methods for dislocations in iron (a simple crystal) and later works including [11, 10] which investigated dislocations in silicon and other diamond cubic lattices (a multilattice). Thus, the extension of these decay results from simple lattices to multilattices is vital for physical applications as it enlarges the pool of admissible materials to include all physical crystals including graphene, silicon, and germanium (to name but a few).

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A particularly important application that we have in mind are dislocations in ionic crystals, which provides two significant challenges compared to the setting in \([6]\): multi-lattice structure and long-range (Coulomb) interaction. In the present work, we take the first step, establishing the necessary techniques for multi-lattices, but restrict ourselves to short-range interactions only. In future work, we plan to extend our theory to ionic interactions, which represent a significant additional technical challenge.

Not surprisingly, the decay estimates for the strain and strain gradients generated by a dislocation in the multilattice setting match those of the simple lattice. However, there is a perhaps striking difference in the proof. A fundamental tool that is used to prove decay of the elastic fields in the simple lattice setting is algebraic decay of the residual atomistic forces evaluated at a continuum elasticity predictor displacement. These residual forces are shown to decay at a rate of \(|r|^{-3}\) in \([6]\) where \(r\) is the distance from the dislocation core, but perhaps surprisingly, these same forces do not in general decay at \(|r|^{-3}\) in the multilattice setting. What is true in this setting, however, is that the net force on a multi-lattice site (the sum of the forces on all species of atoms at a single multilattice site) decay at \(|r|^{-3}\). This fact, along with a strong localisation of multilattice shifts then turns out to be sufficient to prove the expected decay of the strain fields for multilattice dislocations.

This paper is organized as follows. First, we describe the multilattice structure and the specific material models admitted in our analysis of dislocations. The main task accomplished in this technical section is defining the potential energy for straight-line dislocations over an appropriate admissible space of multilattice displacements. We show this potential energy is well-defined (finite) under a set of physically motivated assumptions and then state our main result concerning decay of the elastic fields generated by the dislocation. The proof is broken up in a number of separate steps in the following section which closely mimic the results \([6]\) and \([13]\). Finally, we end with a straightforward consequence of the elastic decay rates: convergence of a direct atomistic method for a lattice statics simulation of a dislocation in an infinite crystal, followed by a numerical example of an edge dislocation in silicon confirming our theoretical predictions.

2. Model Problem

We begin by letting \(\mathcal{L}\) denote a Bravais lattice:

\[
\mathcal{L} = B\mathbb{Z}^3, \quad B \in \mathbb{R}^{3\times 3}.
\]

A multilattice, or complex crystal, is obtained by taking a union of shifted lattices,

\[
\mathcal{M} = \bigcup_{\alpha=0}^{s-1} \mathcal{L} + p_{\alpha}^{\text{ref}},
\]

where each \(p_{\alpha}^{\text{ref}} \in \mathbb{R}^3\) represents a shift vector. Without loss of generality, we shall always assume \(p_{0}^{\text{ref}} = 0\). We refer to \(\xi \in \mathcal{L}\) as a lattice site, while \(\xi + p_{\alpha}^{\text{ref}}\) represents an actual atom location. Hence, \(\mathcal{L} + p_{\alpha}^{\text{ref}}\) represents the lattice locations for the \(\alpha\)th species of atom.

We adopt several equivalent descriptions of the kinematics of the multilattice. We denote a deformation field by \(y_\alpha(\xi)\) and a displacement field by \(u_\alpha(\xi)\) for each species \(\alpha\). Note carefully that the argument of both of these fields is a lattice site \(\xi \in \mathcal{L}\). The relationship
between the two is

\[ y_\alpha(\xi) = \xi + p^\text{ref}_\alpha + u_\alpha(\xi). \]

We collect the set of all deformations (and displacements) at a single lattice site into a tuple which we denote by

\[ y(\xi) = (y_0(\xi), \ldots, y_{S-1}), \quad u(\xi) = (u_0(\xi), \ldots, u_{S-1}(\xi)). \]

We now specify our model to a situation to model straight dislocations, mimicking the setup of [6]. For convenience, we shall assume that the lattice is oriented so that the dislocation direction is parallel to the \( x_3 \) direction and the Burger’s vector is of the form

\[ b = (b_1, 0, b_3) \in \mathcal{L}. \]

We further assume, without loss of generality, that the displacement fields are independent of the \( x_3 \)-direction and thus only functions of \( x_1 \) and \( x_2 \). We denote the resulting two-dimensional reference lattice by

\[ \Lambda = \mathbb{A} \mathbb{Z}^2 := \{ (\ell_1, \ell_2) : \ell \in \mathcal{L} \}. \]

Yet another way of describing the multilattice kinematics, motivated by the definition of the multilattice, is by using displacement-shift notation, \((U, p)\). Here, we set

\[ U(\ell_1) = u_0(\ell), \quad p_\alpha(\ell) = u_\alpha(\ell) - u_0(\ell), \quad p(\ell) = (p_0(\ell), \ldots, p_{S-1}(\ell)), \]

though other choices are available and may in fact be preferable depending on symmetries of the underlying multilattice (see, e.g., [9] for one such example).

Having described the multilattice kinematic variables, we now describe the basic assumptions on the potential energy of the multilattice that we require for our analysis. These assumptions will be quite general so as to allow wide-ranging applicability to any classical interatomic potential including (but not limited to) multi-body potentials, pair functionals, bond-order potentials, etc.

The foremost assumption we make is that the atomistic energy may be written as a sum over empirical \textit{site} potentials. Hence the energy of the lattice must be decomposable as a sum:

\[ \mathcal{E}^a(u) = \sum_{\ell \in \Lambda} V_\ell(Du(\ell)), \quad (2.1) \]

where \( V_\ell : (\mathbb{R}^3)^{|\mathcal{R}|} \to \mathbb{R} \) is the site potential at site \( \ell \),

\[ \mathcal{R} = \{ (\rho\alpha\beta) : \rho \in \Lambda, \alpha, \beta = 0, \ldots, S-1 \} \]

is an interaction range allowing us to index pairs of interacting atoms of species \( \alpha \) and \( \beta \) whose sites are connected by a vector \( \rho \), and

\[ Du(\ell) := (D_{(\rho\alpha\beta)}u(\ell))_{\rho \in \mathcal{R}}, \quad D_{(\rho\alpha\beta)}u(\ell) := u_\beta(\ell + \rho) - u_\alpha(\ell) \]

is the interaction stencil of finite differences needed to compute the energy at site \( \ell \in \Lambda \). We assume \( \mathcal{R} \) is finite (this assumption will be justified shortly) and satisfies the conditions

\[ \text{span}\{\rho \mid (\rho\alpha\alpha) \in \mathcal{R}\} = \mathbb{R}^2 \text{ for all } \alpha \in \mathcal{S}, \quad (2.2) \]

\[ (0\alpha\beta) \in \mathcal{R} \quad \text{for all } \alpha \neq \beta \in \mathcal{S}. \quad (2.3) \]
These two conditions, as well as a further condition encoding slip invariance (see condition (2.8)) of the site potential may always be met by enlarging the interaction range if necessary. We set
\[ \mathcal{R}_1 = \{ \rho \in \Lambda : (\rho \alpha \beta) \in \mathcal{R} \} \]
and use \( r_{\text{cut}} \) to denote the cut-off distance for the potential so that if \(|\rho| > r_{\text{cut}}\), then \((\rho \alpha \beta) \notin \mathcal{R}\).

The site potential, \( V_\ell(\cdot) \), is defined by
\[ V_\ell(Du(\ell)) = V(Du^0(\ell) + Du(\ell)) - V(Du^0(\ell)), \tag{2.4} \]
where in this equation, \( V \) represents a site potential for a defect-free lattice, and \( u^0 \) represents a predictor displacement derived from solving a linear elastic model of a dislocation. (This predictor shall be defined in (2.8)).

Having introduced the site potential for the defect and defect-free lattice, we briefly pause to introduce notation for the derivatives of the site potential. As arguments of \( V \) and \( V_\ell \) are finite differences, \( Du(\rho \alpha \beta) \), for \((\rho \alpha \beta) \in \mathcal{R}\), we will write derivatives of the site potentials with respect to each of these arguments as follows. Let \( g = (g(\rho \alpha \beta))_{(\rho \alpha \beta) \in \mathcal{R}} \). Then
\[
[V_\ell,(\rho \alpha \beta)(g)]_i := \frac{\partial V_\ell(g)}{\partial g_{(\rho \alpha \beta)}}, \quad i = 1, \ldots, 3,
\]
\[
V_\ell,(\rho \alpha \beta)(g) := \frac{\partial V_\ell(g)}{\partial g_{(\rho \alpha \beta)}},
\]
\[
[V_\ell,(\rho \alpha \beta)(\tau \gamma \delta)(g)]_{ij} := \frac{\partial^2 V_\ell(g)}{\partial g_{(\tau \gamma \delta)} \partial g_{(\rho \alpha \beta)}}, \quad i, j = 1, \ldots, 3,
\]
and so on with analogous definitions for \( V(\cdot) \) except that we will drop the usage of the comma as a subscript when writing derivatives of \( V(\cdot) \).

We now further define the potential energy for the defect-free (or homogeneous lattice) as
\[ E_{\text{hom}}^a(u) = \sum_{\ell \in \Lambda} V(Du). \tag{2.5} \]
The relevant function space we introduce, over which \( E_{\text{hom}}^a \) and \( E^a \) will be defined, is a quotient space of multilattice displacements whose (semi-)norm,
\[ \|u\|_{a_1}^2 := \sum_{\ell \in \Lambda} |Du(\ell)|_R^2, \quad \text{where } |Du|_R^2 := \sum_{(\rho \alpha \beta) \in \mathcal{R}} |D(\rho \alpha \beta)u(\ell)|^2, \]
is finite. Because this is only a semi-norm, we form the quotient with the kernel of the semi-norm, which is the set of constant multilattice displacements, to obtain the spaces
\[ \mathcal{U} := \mathcal{U}/\mathbb{R}^3, \quad \text{where } \mathcal{U} := \{ u : \mathcal{L}^s \to \mathbb{R}^3, \|u\|_{a_1} < \infty \}. \]
It is then proven in [13] that \( \mathcal{U}_0 \), defined by
\[ \mathcal{U}_0 := \{ u \in \mathcal{U} : Du_0, u_\alpha - u_0 \text{ have compact support for each } \alpha \}, \]
\[ \mathcal{U}_0 := \mathcal{U}_0/\mathbb{R}^3, \]
is dense in $\mathcal{U}$ and subsequently that

**Theorem 1 (Olson and Ortner 2017 [13]).** If the homogeneous multilattice reference configuration, $u = 0$, is an equilibrium of the defect free energy, that is,

$$
\sum_{\ell \in \Lambda} \sum_{(\alpha \beta) \in \mathcal{R}} V_{(\alpha \beta)}(0) \cdot Dv(\ell) = 0, \quad \forall \ v \in \mathcal{U}_0,
$$

(2.6)

and if the homogeneous site potential is $C^4$ with uniformly bounded derivatives, then the energy functional, $\mathcal{E}^a_{\mathrm{hom}}(u)$, is well-defined and $C^3$ on $\mathcal{U}$.

A further assumption on the site potential and multilattice is that the defect-free multilattice be a stable equilibrium of the defect free energy. In essence, this amounts to saying that our model is physically reasonable and is equivalent to the usual assumption of phonon-stability made in the solid-state physics community. For a discussion of this, see [13, 5]. Mathematically, this amounts to a discrete ellipticity condition and allows us to make use of a wide variety of estimates for elliptic systems (in particular for Green’s functions for elliptic equations) of equations after proper translation.

**Assumption 1.** The perfect multilattice reference configuration, $u = 0$, is a stable equilibrium of $\mathcal{E}^a_{\mathrm{hom}}$ in the sense that there exists $\gamma_a > 0$ such that

$$
\langle \delta^2 \mathcal{E}^a_{\mathrm{hom}}(0) v, v \rangle \geq \gamma_a \|v\|_{a_1}^2, \quad \forall \ v \in \mathcal{U}.
$$

(2.7)

Having rigorously defined the defect-free energy and function space over which it is defined, we are now in a position to rigorously define the dislocation energy (2.1) and the admissible space of displacements over which it is defined. To that end, we must (1) encode slip invariance of the atomistic energy into the site potential $V$, (2) define the admissible function space as a proper subset of $\mathcal{U}$ allowing us to employ a finite interaction range in the reference configuration, and (3) define the predictor displacement $u^0$ utilized in (2.4).

**2.1. Slip Invariance and Admissible Function Space.** To accomplish these three tasks, we assume a dislocation core position $\hat{x} = (\hat{x}_1, \hat{x}_2) \notin \Lambda$ and assume the dislocation branch cut is given by

$$
\Gamma = \left\{ (x_1, x_2) \in \mathbb{R}^2 : x_1 \geq \hat{x}_1 \right\},
$$

which is consistent with our assumption that the Burgers vector is parallel to the $x_1$-direction.

Our final assumption on the homogeneous site potential, $V$, is that it is slip invariant: if we define the operator, $S_0$, acting on multilattice displacements by ($b_{12}$ represents the projection of the Burger’s vector to the $(x_1, x_2)$ plane)

$$
(S_0 w)_\alpha(x) = \begin{cases} 
  w_\alpha(x), & x_2 > \hat{x}_2 \\
  w_\alpha(x - b_{12}) - b, & x_2 < \hat{x}_2,
\end{cases}
$$

then

$$
V(DS_0 w(\ell)) = V(Dw(\ell)), \quad \forall \ell_2 > \hat{x}_2
$$

$$
V(DS_0 w(\ell + b_{12})) = V(Dw(\ell)), \quad \forall \ell_2 < \hat{x}_2.
$$

(2.8)
This condition ensures that the energy of the lattice remains invariant under crystallographic slip by a lattice vector. However, as noted in [6], in order for this condition to not invalidate our assumption of a finite atomistic interaction range, we must define the admissible displacement space for the dislocation energy (2.1) as a proper subset of \( \mathbf{U} \).

For this, we define a continuous, piecewise linear, nodal interpolant of a lattice function \( u \) by \( Iu \). This can be done by creating a partition of the domain whose vertices are exactly the lattice sites \( \ell \in \Lambda \) and taking \( I \) to be the standard \( P_1 \) interpolant. We can then choose a global bound, \( m_A \), for \( \|\nabla Iu_\alpha\|_{L^\infty}, \| Ip_\alpha\|_{L^\infty} \) and a radius \( r_A \) large enough so that

\[
\mathcal{A} := \{ u \in \mathbf{U} : \|\nabla Iu_\alpha\|_{L^\infty}, \| Ip_\alpha\|_{L^\infty} < m_A, \text{ and } |\nabla Iu_\alpha(x)|, | Ip_\alpha(x)| < 1/2, x > r_A, \forall \alpha \},
\]

contains the possible minimizers of the dislocation energy. Arguing as in [6, Appendix B], the principle idea here is that the finite energy criterion on \( x \) \( \| \cdot \|_{L^1} \) in the definition of \( \mathbf{U} \) implies \( \nabla Iu_\alpha \to 0 \) as \( |x| \to \infty \) and similarly for \( Ip_\alpha \to 0 \). Thus, \( m_A \) and \( r_A \) may always be chosen large enough so that a particular local minimum of the dislocation energy is in \( \mathcal{A} \). But then we may always increase these parameters so that all elements of \( \mathbf{U} \) within some ball of arbitrary radius about this minimum are also contained in \( \mathcal{A} \), which permits us to perform our local calculus arguments. Full details may be found in [6, Appendix B].

We may then formulate the slip invariance condition by defining a mapping, \( S \), of both lattice and multilattice functions by

\[
(Su)(\ell) = \begin{cases} 
  u(\ell), & \ell_2 > \hat{x}_2, \\
  u(\ell - b_{12}), & \ell_2 < \hat{x}_2,
\end{cases} \quad (Su)_\alpha(\ell) = \begin{cases} 
  u_\alpha(\ell), & \ell_2 > \hat{x}_2, \\
  u_\alpha(\ell - b_{12}), & \ell_2 < \hat{x}_2,
\end{cases}
\]

and a mapping, \( R = S^* \), of lattice displacements by

\[
Ru(\ell) = \begin{cases} 
  u(\ell), & \ell_2 > \hat{x}_2, \\
  u(\ell + b_{12}), & \ell_2 < \hat{x}_2.
\end{cases}
\]

The slip invariance condition can now be expressed (using the same notation as [6]) as

\[
V(D(u^0 + u)(\ell)) = V(RDS_0(u^0 + u)(\ell)), \quad \forall \ell \in \Lambda, u \in \mathcal{A} \quad (2.10)
\]

We next fix a dislocation core radius \( \hat{r} \) (which is defined in Lemma 2) and upon defining

\[
\Omega_\Gamma = \{ (x_1, x_2) \in \mathbb{R}^2 : x_1 \geq \hat{x}_1 \} \setminus B_{\hat{r}+b_{12}}(\hat{x}),
\]

we (likewise to [6]) define the “elastic strains”

\[
e(\ell) := \left( e_{(\rho\alpha\beta)}(\ell) \right)_{(\rho\alpha\beta) \in \mathcal{R}}, \quad e_{(\rho\alpha\beta)}(\ell) = \begin{cases} 
  RD_{(\rho\alpha\beta)}S_0u^0(\ell), & \ell \in \Omega_\Gamma \\
  D_{(\rho\alpha\beta)}u^0(\ell), & \ell \notin \Omega_\Gamma,
\end{cases}
\]

and

\[
\tilde{D}u(\ell) := \left( \tilde{D}_{(\rho\alpha\beta)}u(\ell) \right)_{(\rho\alpha\beta) \in \mathcal{R}}, \quad \tilde{D}_{(\rho\alpha\beta)}u(\ell) = \begin{cases} 
  RD_{(\rho\alpha\beta)}S u(\ell), & \ell \in \Omega_\Gamma \\
  D_{(\rho\alpha\beta)}u(\ell), & \ell \notin \Omega_\Gamma,
\end{cases}
\]

Using this notation, the slip invariance condition (2.10) may be written as

\[
V(D(u^0 + u)(\ell)) = V(e(\ell) + \tilde{D}u(\ell)), \quad (2.13)
\]
Moreover, we have the identity
\[
\tilde{D}_{(\rho \alpha \beta)} u(\ell) = \tilde{D}_\rho u_0 + \tilde{D}_\rho p_\beta(\ell) + p_\beta(\ell) - p_\alpha(\ell),
\]
which is intuitive, but can be proven via tedious algebraic manipulations and considering the cases (1) \( \ell \notin \Omega_F \) and (2) \( \ell \in \Omega_F \). We have included these manipulations in Appendix [B].

2.1.1. Continuum-Elasticity Dislocation Predictor. Having recalled the well-posedness of the defect-free energy, \( E_{\text{hom}}^a \), in Theorem [1] and having described the fundamental assumptions on the energy (smoothness of the site potential and the coercivity condition of Assumption [1]) and the slip invariance condition on the site potential (condition (2.13)), we are now in a position to complete the definition of the dislocation defect energy first alluded to in (2.1). Specifically, it remains to define the predictor \( u^0 = (U^0, p^0) \) utilized in (2.4).

As is done in the simple lattice case [6], this will be accomplished by a slight modification of the solution of a linearized, elastic problem, where the elasticity tensor is taken from the linearized Cauchy–Born [3, 1] model. Thus, we shall define \( (U^\text{lin}) \) by
\[
\nabla \cdot (C \nabla U^\text{lin}) = 0,
\]
\[
U^\text{lin}(x^+) - U^\text{lin}(x^-) = b, \quad \text{on } \Gamma,
\]
\[
\nabla e_2 U^\text{lin}(x^+) - \nabla e_2 U^\text{lin}(x^-) = 0, \quad \text{on } \Gamma,
\]
where \( C \) is the linearized Cauchy-Born (see [3, 1]) tensor for a multilattice defined by
\[
W(F, p) = V((F \rho + p_\beta - p_\alpha)_{(\rho \alpha \beta) \in \mathbb{R}})
\]
\[
C_{ijkl} = \frac{\partial^2}{\partial F_{ij} \partial F_{kl}} \min_p W(F, p).
\]

It was shown in [13, Equation 3.11] that Assumption [1] implies that linearized Cauchy–Born tensor satisfies a Legendre-Hadamard condition, and therefore the first set of three equations in (2.15) is solvable by the classical techniques of Hirth and Lothe [7]. As we are working with a multilattice, we then must obtain a corresponding set of shift fields, \( p^\text{lin} \). In the Cauchy–Born theory for multilattices, the shift fields are obtained by minimization of the energy density [11]:
\[
p = \arg\min_p V\left((\nabla_\rho U^\text{lin} + p_\beta - p_\alpha)_{(\rho \alpha \beta) \in \mathbb{R}}\right),
\]
but we define \( p^\text{lin} \) by
\[
\frac{\partial^2}{\partial p \partial p} [V(0)] p^\text{lin} = -\partial p_F [V(0)] \nabla U^\text{lin}.
\]
which is equivalent to performing one step of Newton’s method to the minimization problem (2.17) where the initial shift fields are taken to be the reference shifts in the perfect multilattice.

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\frac{\partial^2}{\partial p \partial p} [V(0)] p^\text{lin} = -\partial p_F [V(0)] \nabla U^\text{lin}.
\]
which is equivalent to performing one step of Newton’s method to the minimization problem (2.17) where the initial shift fields are taken to be the reference shifts in the perfect multilattice.

We have carefully not yet defined the predictor, \( u^0 = (U^0, p^0) \), to be exactly \( (U^\text{lin}, p^\text{lin}) \) as the precise definition requires the introduction of a smooth transition function, \( \eta : \mathbb{R} \to \mathbb{R} \), which satisfies \( \eta(x) = 1 \) for \( x \geq 1 \), \( \eta(x) = 0 \) for \( x \leq 0 \), and \( \eta'(x) > 0 \) for \( 0 < x < 1 \); and an
Lemma 3. The function $\tilde{D}$ is bijective on $\mathbb{R}^2 \setminus \Gamma$. Furthermore $U^0$ is then defined and a solution, $\mathbf{p}^0$, to (2.20) exists. These functions satisfy $\nabla^j S_0 u^0(x+) = \nabla^j S_0 u^0(x-)$ and $\nabla^j p^0(x+) = \nabla^j p^0(x-)$ for all $\alpha$, nonnegative integers $j$, and $x \in \Gamma$, and

$$|\nabla^j u^0(x) - \nabla^j u^0(\zeta^{-1}(x))| \lesssim |x|^{-j-1}, \quad |\nabla^j p^0(x) - \nabla^j p^0(\zeta^{-1}(x))| \lesssim |x|^{-j-2}.$$

Proof. As all results concerning displacements are proven in [6], we shall only concern ourselves with the results for the shifts. Once we establish existence of $\mathbf{p}$, the corresponding estimates are immediate from the definition of $\mathbf{p}$ and $\mathbf{p}^\text{lin}$ in (2.18) and (2.20) and the corresponding results for $U^0$ and $U^\text{lin}$.

For existence of a solution to (2.20), we need only note that it was shown in [13, Theorem 3.7] that the atomistic stability assumption, Assumption 1, implies a corresponding estimate on stability of the Cauchy-Born model. In particular, $\frac{\partial^2}{\partial \mathbf{p} \partial \mathbf{p}} [V(0)]$ was shown to be invertible.

It now follows that $(S_0 U^0, \mathbf{p}^0)$ are smooth, which allows us to perform Taylor expansions of finite differences using the $\tilde{D}$ operator:

Lemma 3. With $\mathbf{u}^0 = (U^0, \mathbf{p}^0)$ and $\tilde{D}$ as defined above and $|\ell|$ large enough,

$$\left| \tilde{D}_{(\alpha \beta)} \mathbf{u}^0(\ell) - (\nabla_\rho U^0(\ell) + \mathbf{p}^0(\ell), p^0(\ell)) \right| \lesssim |\ell|^{-2}, \quad \ell \notin \Omega_\Gamma \quad (2.21)$$

$$\left| \tilde{D}_{(\alpha \beta)} \mathbf{u}^0(\ell) - (R \nabla_\rho S_0 U^0(\ell) + \mathbf{p}^0(\ell), p^0(\ell)) \right| \lesssim |\ell|^{-2}, \quad \ell \in \Omega_\Gamma, \quad (2.22)$$

$$|e(\ell)| \lesssim |\ell|^{-1}, \quad (2.23)$$

$$|\tilde{D}_{-\rho} e(\ell)| \lesssim |\ell|^{-2}. \quad (2.24)$$
Proof. We first prove (2.21) and consider the two cases as to whether \( \ell \in \Omega_{\Gamma} \). If \( \ell \notin \Omega_{\Gamma} \), then \( \bar{D} = D \), \((U^0, p^0)\) is smooth, and we have a straightforward Taylor expansion
\[
\bar{D}_{(\rho, \beta)} u^0(\ell) = D_{(\rho, \beta)} u^0(\ell) = D_{\rho, p^0}(\ell) + D_{\rho, p^0}(\ell) - p^0(\ell)
\]
\[
= \nabla_{\rho, p^0}(\ell) + p^0(\ell) - p^0(\ell) + O(\|\nabla^2 U^0\|_{L^\infty(B_{\text{cut}}(\ell))}) + O(\|p^0\|_{L^\infty(B_{\text{cut}}(\ell))}),
\]
and now from \([7]\), we know that \(|\nabla^2 U^0| \lesssim |\ell|^{-2} \) and thus \(|\nabla^2 U^0| \lesssim |\ell|^{-2} \) from Theorem \(2\) which further implies \(|\nabla p^0(\ell)| \lesssim |\ell|^{-2} \) from (2.18). Hence
\[
|\bar{D}_{(\rho, \beta)} u^0(\ell) - (\nabla_{\rho, p^0}(\ell) + p^0(\ell) - p^0(\ell))| \lesssim |\ell|^{-2}.
\]
If \( \ell \in \Omega_{\Gamma} \), then \( \bar{D} = RD_{\rho, S_0} \),
\[
\bar{D}_{(\rho, \beta)} u^0(\ell) = (\bar{D}_{\rho, S_0} U^0)(\ell) + (\bar{D}_{\rho, S_0} p^0)(\ell) + p^0(\ell) - p^0(\ell)
\]
\[
= (RD_{\rho, S_0} U^0)(\ell) + p^0(\ell) - p^0(\ell) + O(\|\nabla^2 S_0 U^0\|_{L^\infty(B_{\text{cut}}(\ell))}) + O(\|p^0\|_{L^\infty(B_{\text{cut}}(\ell))}),
\]
which, because \( S_0 \) simply represents a shift by one Burger’s vector, implies
\[
|\bar{D}_{(\rho, \beta)} u^0(\ell) - (\nabla_{\rho, S_0} U^0(\ell) + p^0(\ell) - p^0(\ell))| \lesssim O(\|\nabla^2 U^0\|_{L^\infty(B_{\text{cut}}(\ell))}) + O(\|\nabla p^0\|_{L^\infty(B_{\text{cut}}(\ell))})
\]
\[
\lesssim O(\|\nabla^2 U^0\|_{L^\infty(B_{\text{cut}}+b_1(\ell))}) + O(\|\nabla p^0\|_{L^\infty(B_{\text{cut}}+b_1(\ell))})
\]
\[
\lesssim |\ell|^{-2}.
\]
In order to prove (2.23), we consider only the case \( \ell \notin \Omega_{\Gamma} \) as the other case is analogous:
\[
|e(\ell)| \leq |\bar{D}_{(\rho, \beta)} u^0(\ell) - (\nabla_{\rho, S_0} U^0(\ell) + p^0(\ell) - p^0(\ell)) + |\nabla_{\rho, S_0} U^0(\ell) + p^0(\ell) - p^0(\ell)|
\]
\[
\lesssim |\ell|^{-2} + |\nabla_{\rho, S_0} U^0(\ell) + p^0(\ell) - p^0(\ell)|
\]
\[
\leq |\ell|^{-2} + |\nabla_{\rho, S_0} U^0(\ell) + p^0(\ell) - p^0(\ell)|.
\]
From \([7]\), we know that \(|\nabla U^0| \lesssim |\ell|^{-1} \) and thus \(|\nabla U^0| \lesssim |\ell|^{-1} \) from Theorem \(2\) which further implies \(|p^0(\ell)| \lesssim |\ell|^{-1} \) from (2.18). Thus
\[
|e(\ell)| \lesssim |\ell|^{-1}.
\]
For (2.24), we apply Taylor remainder estimates analogous to those proven in (2.21) and (2.22), and for brevity, we consider only the case \( \ell \in \Omega_{\Gamma} \):
\[
|\bar{D}_{(\rho, \beta)} e(\ell)| = |\bar{D}_{(\rho, \beta)}(RD_{\rho, S_0} U^0 + \bar{D}_{(\rho, \beta)} + p^0(\ell) - p^0(\ell))|
\]
\[
= |RD_{(\rho, \beta)}(\bar{D}_{(\rho, \beta)} + p^0(\ell) - p^0(\ell)) + RD_{(\rho, \beta)} p^0(\ell) - RD_{(\rho, \beta)} p^0(\ell)|
\]
\[
= |\bar{D}_{(\rho, \beta)}(\bar{D}_{(\rho, \beta)} + p^0(\ell) - p^0(\ell)) + RD_{(\rho, \beta)} p^0(\ell) - RD_{(\rho, \beta)} p^0(\ell)|
\]
\[
+ O(\|\nabla^2 S_0 U^0\|_{L^\infty(B_{\text{cut}}(\ell))}) + O(\|\nabla^2 p^0\|_{L^\infty(B_{\text{cut}}(\ell))})
\]
We may again utilize [7], to see that $|\nabla^2 U^\text{lin}| \lesssim |\ell|^{-2}$ and $|\nabla^3 U^\text{lin}| \lesssim |\ell|^{-3}$ and thus $|\nabla^2 S_0 U^0| \lesssim |\ell|^{-2}$ and $|\nabla^3 S_0 U^0| \lesssim |\ell|^{-3}$ from Theorem 2. Obtaining corresponding estimates on the shifts from (2.18) gives (2.24).

□

Next, we estimate the decay of the residual forces from the homogeneous energy when evaluated at the continuum dislocation predictor; these decay estimates will turn out to be vital in proving the decay estimates for the dislocation strain fields themselves. For ease of notation and visual clarity, throughout the proof, we will use the notation to $\|\cdot\|_{L^\infty}$ to represent $\|\cdot\|_{L^\infty(B_{cut}+b_1(\ell))}$, and $\sum_{\gamma}$ will represent a summation over which $\gamma$ is held fixed.

**Lemma 4.** Suppose that $(U, p)$ are smooth. The force on an atomistic degree of freedom $(\eta, \gamma)$ for $\eta \in \Lambda$ and $\gamma \in \{0, \ldots, S - 1\}$ and $\ell$ large enough is given by

$$\frac{\partial \mathcal{E}^{a}_{\text{hom}}}{\partial u_\gamma}(\eta)|_{(U, p)} = \sum_{(\tau_\chi)(\rho_\alpha\gamma)} \gamma \sum_{\gamma} V_{(\rho_\alpha\gamma)(\tau_\chi)}(0) \left[ \nabla_{\tau_\chi}^2 U(\eta) - \nabla_{\tau_\chi} p_\gamma(\eta) + \nabla_{\tau_\chi} p_\gamma(\eta) \right]$$

$$+ \sum_{(\tau_\chi)(\rho_\alpha\gamma)} \left\{ \sum_{\gamma} V_{(\rho_\alpha\gamma)(\tau_\chi)}(0) - \sum_{(\rho_\gamma\alpha)} V_{(\rho_\gamma\alpha)(\tau_\chi)}(0) \right\} \left[ (\nabla_{\tau_\chi} U + p_\chi(\eta) - p_\chi(\eta)) \right]$$

$$+ \sum_{(\tau_\chi)(\rho_\alpha\gamma)} \left\{ \sum_{\gamma} V_{(\rho_\alpha\gamma)(\tau_\chi)}(0) - \sum_{(\rho_\gamma\alpha)} V_{(\rho_\gamma\alpha)(\tau_\chi)}(0) \right\} \left[ \frac{1}{2} \nabla_{\tau_\chi}^2 U + \nabla_{\tau_\chi} p_\gamma(\eta) \right]$$

$$+ O\left( \|\nabla^2 U\|_{L^\infty} \|\nabla u\|_{L^\infty} + \|\nabla p\|_{L^\infty} \|p\|_{L^\infty} + \|\nabla^3 U\|_{L^\infty} + \|\nabla^2 p\|_{L^\infty} \right).$$

(2.25)

In particular, if $(U, p) = (U^0, p^0)$, and if $\ell$ is large enough and $\ell \notin \Omega_\Gamma$, then

$$\sum_{\gamma} \frac{\partial \mathcal{E}^{a}_{\text{hom}}}{\partial u_\gamma}(\eta)|_{(U, p)} = O(|\ell|^{-3}),$$

(2.26)

and if $\ell \in \Omega_\Gamma$ and if $(U, p) = (SU^0, Sp^0)$, then

$$\sum_{\gamma} \frac{\partial \mathcal{E}^{a}_{\text{hom}}}{\partial u_\gamma}(\eta)|_{(U, p)} = O(|\ell|^{-3}),$$

(2.27)

**Proof.** First, we establish the expression in (2.25). Observe that

$$\frac{\partial \mathcal{E}^{a}}{\partial u_\gamma}(\eta)|_{(U, p)} = \sum_{(\rho_\alpha\gamma)} V_{(\rho_\alpha\gamma)}(Du(\eta) - \rho) - \sum_{(\rho_\gamma\alpha)} V_{(\rho_\gamma\alpha)}(Du(\eta)).$$
which we now Taylor expand about 0 to obtain

\[
\frac{\partial \mathcal{E}^a}{\partial u_\gamma(\eta)}|_{(\mathbf{u},p)}
\]

\[
= \sum_\gamma V_{(\rho\gamma\gamma)}(0) - \sum_\gamma V_{(\rho\gamma\alpha)}(0)
\]

\[
+ \sum_\gamma \sum_\gamma V_{(\rho\alpha\gamma)(\tau\chi\chi)}(0)(D_{(\tau\chi\chi)}\mathbf{u}(\eta - \rho)) - \sum_\gamma \sum_\gamma V_{(\rho\gamma\alpha)(\tau\chi\chi)}(0)(D_{(\tau\chi\chi)}\mathbf{u}(\eta))
\]

\[
+ \frac{1}{2} \int_0^1 (1 - t)^2 \sum_\gamma \sum_\gamma \sum_\gamma V_{(\rho\gamma\alpha)(\tau\chi\chi)(\sigma\mu\nu)}(tD\mathbf{u})(D_{(\tau\chi\chi)}\mathbf{u}(\eta - \rho))(D_{(\sigma\mu\nu)}\mathbf{u}(\eta - \rho)) dt
\]

\[
- \frac{1}{2} \int_0^1 (1 - t)^2 \sum_\gamma \sum_\gamma \sum_\gamma V_{(\rho\gamma\alpha)(\tau\chi\chi)(\sigma\mu\nu)}(tD\mathbf{u})(D_{(\tau\chi\chi)}\mathbf{u}(\eta))(D_{(\sigma\mu\nu)}\mathbf{u}(\eta)) dt
\]

\[
= \sum_\gamma \sum_\gamma V_{(\rho\alpha\gamma)(\tau\chi\chi)}(0)(D_{(\tau\chi\chi)}\mathbf{u}(\eta - \rho)) - \sum_\gamma \sum_\gamma V_{(\rho\gamma\alpha)(\tau\chi\chi)}(0)(D_{(\tau\chi\chi)}\mathbf{u}(\eta))
\]

\[
+ \mathcal{O}(\|\nabla^2\mathbf{U}\|_L^\infty\|\nabla\mathbf{u}\|_L^\infty + \|\nabla\mathbf{p}\|_L^\infty\|\mathbf{p}\|_L^\infty),
\]

(2.28)

where in obtaining the last line we have used that \(\partial p_\gamma W(0) = 0\) in the equilibrated reference configuration, which implies \(0 = \sum_\gamma V_{(\rho\alpha\gamma)}(0) - \sum_\gamma V_{(\rho\gamma\alpha)}(0)\) [13, A.4], and we Taylor expanded the finite differences in the remainder term. Next, we rewrite this as

\[
\frac{\partial \mathcal{E}^a}{\partial u_\gamma(\eta)}|_{(\mathbf{u},p)}
\]

\[
= \sum_\gamma \left\{ \sum_\gamma V_{(\rho\alpha\gamma)(\tau\chi\chi)}(0)(D_{(\tau\chi\chi)}\mathbf{u}(\eta - \rho) - D_{(\tau\chi\chi)}\mathbf{u}(\eta)) + \sum_\gamma V_{(\rho\gamma\alpha)(\tau\chi\chi)}(0)(D_{(\tau\chi\chi)}\mathbf{u}(\eta)) \right\}
\]

\[
- \sum_\gamma V_{(\rho\gamma\alpha)(\tau\chi\chi)}(0)(D_{(\tau\chi\chi)}\mathbf{u}(\eta)) + \mathcal{O}(\|\nabla^2\mathbf{U}\|_L^\infty\|\nabla\mathbf{u}\|_L^\infty + \|\nabla\mathbf{p}\|_L^\infty\|\mathbf{p}\|_L^\infty)
\]

\[
= \sum_\gamma \left\{ \sum_\gamma V_{(\rho\alpha\gamma)(\tau\chi\chi)}(0) \right\} (D_{(\tau\chi\chi)}\mathbf{u}(\eta))
\]

\[
+ \sum_\gamma \left\{ \sum_\gamma V_{(\rho\gamma\alpha)(\tau\chi\chi)}(0) - \sum_\gamma V_{(\rho\gamma\alpha)(\tau\chi\chi)}(0) \right\} (D_{(\tau\chi\chi)}\mathbf{u}(\eta))
\]

\[
+ \mathcal{O}(\|\nabla^2\mathbf{U}\|_L^\infty\|\nabla\mathbf{u}\|_L^\infty + \|\nabla\mathbf{p}\|_L^\infty\|\mathbf{p}\|_L^\infty).
\]

(2.29)
We then rewrite term $A_1$ and then Taylor expand (keeping only the lowest order error terms) to produce

\[
A_1 = \sum_{(\gamma)} \sum_{(\rho)} V_{(\rho\gamma)(\tau)}(0) \left[ D_{-\rho}(U(\eta + \tau) - U(\eta) + p_\chi(\eta + \tau) - p_\eta(\eta)) \right] \\
= \sum_{(\gamma)} \sum_{(\rho)} V_{(\rho\gamma)(\tau)}(0) \left[ D_{-\rho}(\nabla U(\eta) + p_\chi(\eta + \tau) - p_\eta(\eta) + p_\chi(\eta)) \right] \\
+ \mathcal{O}(\|\nabla^3 U\|_{L^\infty}) \\
= \sum_{(\gamma)} \sum_{(\rho)} V_{(\rho\gamma)(\tau)}(0) \left[ D_{-\rho}(\nabla U(\eta) + \nabla p_\chi(\eta) + p_\chi(\eta)) \right] \\
+ \mathcal{O}(\|\nabla^3 U\|_{L^\infty} + \|\nabla^2 p\|_{L^\infty}) \\
= \sum_{(\gamma)} \sum_{(\rho)} V_{(\rho\gamma)(\tau)}(0) \left[ D_{-\rho}(\nabla U(\eta) + p_\chi(\eta) - p_\eta(\eta)) \right] \\
+ \mathcal{O}(\|\nabla^3 U\|_{L^\infty} + \|\nabla^2 p\|_{L^\infty}) \\
= \sum_{(\gamma)} \sum_{(\rho)} V_{(\rho\gamma)(\tau)}(0) \left[ \nabla^2_{-\rho} U(\eta) - \nabla p_\chi(\eta) + \nabla p_\eta(\eta) \right] + \mathcal{O}(\|\nabla^3 U\|_{L^\infty} + \|\nabla^2 p\|_{L^\infty}).
\]
Focusing now on term $A_2$, we note that

$$A_2 = \sum_{(\tau \chi)} \left\{ \sum_{(\rho \alpha \gamma)} V_{\gamma}(\rho \alpha \gamma)(\tau \chi)(0) - \sum_{(\rho \gamma \alpha)} V_{\gamma}(\rho \gamma \alpha)(\tau \chi)(0) \right\} (D_{(\tau \chi)}u(\eta))$$

$$= \sum_{(\tau \chi)} \left\{ \sum_{(\rho \alpha \gamma)} V_{\gamma}(\rho \alpha \gamma)(\tau \chi)(0) - \sum_{(\rho \gamma \alpha)} V_{\gamma}(\rho \gamma \alpha)(\tau \chi)(0) \right\} (U(\tau + \eta) - U(\eta) + p_\chi(\eta + \tau) - p_\chi(\eta))$$

$$= \sum_{(\tau \chi)} \left\{ \sum_{(\rho \alpha \gamma)} \sum_{(\rho \gamma \alpha)} V_{\gamma}(\rho \alpha \gamma)(\tau \chi)(0) - V_{\gamma}(\rho \gamma \alpha)(\tau \chi)(0) \right\} (\nabla_\tau U + \frac{1}{2} \nabla^2 U + p_\chi(\eta + \tau) - p_\chi(\eta) + 0(\|\nabla^3 U\|_{L^\infty})$$

$$= \sum_{(\tau \chi)} \left\{ \sum_{(\rho \alpha \gamma)} \sum_{(\rho \gamma \alpha)} V_{\gamma}(\rho \alpha \gamma)(\tau \chi)(0) - V_{\gamma}(\rho \gamma \alpha)(\tau \chi)(0) \right\} (\nabla_\tau U + \frac{1}{2} \nabla^2 U + \nabla_\tau p_\chi(\eta) + p_\chi(\eta) - p_\chi(\eta)) + 0(\|\nabla^3 U\|_{L^\infty} + \|\nabla^2 p\|_{L^\infty})$$

$$= \sum_{(\tau \chi)} \left\{ \sum_{(\rho \alpha \gamma)} \sum_{(\rho \gamma \alpha)} V_{\gamma}(\rho \alpha \gamma)(\tau \chi)(0) - V_{\gamma}(\rho \gamma \alpha)(\tau \chi)(0) \right\} (\nabla_\tau U + p_\chi(\eta) - p_\chi(\eta))$$

$$+ \sum_{(\tau \chi)} \left\{ \sum_{(\rho \alpha \gamma)} \sum_{(\rho \gamma \alpha)} V_{\gamma}(\rho \alpha \gamma)(\tau \chi)(0) - V_{\gamma}(\rho \gamma \alpha)(\tau \chi)(0) \right\} \left( \frac{1}{2} \nabla^2 U + \nabla_\tau p_\chi(\eta) + 0(\|\nabla^3 U\|_{L^\infty} + \|\nabla^2 p\|_{L^\infty}) \right)$$

$$= \sum_{(\tau \chi)} \left\{ \sum_{(\rho \alpha \gamma)} \sum_{(\rho \gamma \alpha)} V_{\gamma}(\rho \alpha \gamma)(\tau \chi)(0) - V_{\gamma}(\rho \gamma \alpha)(\tau \chi)(0) \right\} (\nabla_\tau U + p_\chi(\eta) - p_\chi(\eta))$$

$$+ 0(\|\nabla^3 U\|_{L^\infty} + \|\nabla^2 p\|_{L^\infty}). \quad (2.31)$$

Inserting the expressions (2.30) and (2.31) into (2.29) yields the desired expression for $\frac{\partial \sigma_{\text{hom}}}{\partial u_\chi(\eta)}$ in (2.25).

To establish (2.26), we observe that from Appendix A, $(U, p)$ is a solution to the linear elastic Cauchy-Born model provided

$$\langle \partial_{GG} W(0) \nabla U, \nabla V \rangle + \sum_\nu \langle \partial_{Gp_\nu} W(0) \nabla U, q_\nu \rangle + \sum_\mu \langle \partial_{p_\mu G} W(0) p_\mu, \nabla V \rangle$$

$$+ \sum_{\mu, \nu} \langle \partial_{p_\mu p_\nu} W(0) p_\mu, q_\nu \rangle = 0, \quad \forall (W, q) \in C^\infty_\theta.$$ \quad (2.32)

In strong form, this reads

$$\nabla \cdot (\partial_{GG} W(0) \nabla U) + \sum_\mu \nabla \cdot (\partial_{p_\mu G} W(0) p_\mu) = 0,$$

$$\partial_{Gp_\nu} W(0) \nabla U + \sum_\mu \partial_{p_\mu p_\nu} W(0) p_\mu = 0, \quad \text{for each species } \nu. \quad (2.33)$$
It is then a simple calculus exercise to compute (see also [13] for the same expressions)

\[
\partial^2_{G_{\alpha n}} W(0) = \sum_{(\rho \alpha \mu) \in R} \sum_{(\tau \chi) \in R} V_{i,(\rho \alpha \mu)(\tau \chi)}^{\nu}(0) \tau_n - \sum_{(\rho \mu \alpha) \in R} \sum_{(\tau \chi) \in R} V_{i,(\rho \mu \alpha)(\tau \chi)}^{\nu}(0) \tau_n
\]

\[
\partial^2_{G_{\alpha n} G_{rs}} = \sum_{(\rho \alpha \mu) \in R} \sum_{(\tau \chi) \in R} V_{i,(\rho \alpha \mu)(\tau \chi)}^{mr}(0) \rho_n \tau_s
\]

\[
\partial^2_{p^\mu p^\gamma} W(0) = \sum_{(\tau \mu) \in R} \sum_{(\rho \gamma \alpha) \in R} \sum_{(\tau \mu) \in R} \sum_{(\rho \gamma \alpha) \in R} V_{i,(\rho \gamma \alpha)(\tau \mu)}^{kl}(0) \rho_n \tau_s
\]

and therefore

\[
- [\nabla \cdot (\partial_{GG} W(0) \nabla U)]_m = - \sum_{(\rho \alpha \mu) \in R} V_{i,(\rho \alpha \mu)(\tau \chi)}^{mr}(0) \rho_n \tau_s u_{r,sn} = \sum_{(\rho \alpha \mu) \in R} V_{i,(\rho \alpha \mu)(\tau \chi)}^{mr} \nabla^2_{-\rho,\tau} u_{r,s},
\]

and

\[
[\nabla \cdot (\partial_{Gp^\mu} W(0)p^\mu)]_m = \sum_{(\rho \alpha \mu) \in R} \sum_{(\tau \chi) \in R} V_{i,(\rho \alpha \mu)(\tau \chi)}^{il}(0) \tau_n p^l_{\mu,n} - \sum_{(\rho \mu \alpha) \in R} \sum_{(\tau \chi) \in R} V_{i,(\rho \mu \alpha)(\tau \chi)}^{il}(0) \tau_n p^l_{\mu,n}
\]

\[
= \sum_{(\rho \alpha \mu) \in R} \sum_{(\tau \chi) \in R} V_{i,(\rho \alpha \mu)(\tau \chi)}^{il}(0) (\nabla \tau p^l_\mu)^l - \sum_{(\rho \mu \alpha) \in R} \sum_{(\tau \chi) \in R} V_{i,(\rho \mu \alpha)(\tau \chi)}^{il}(0) (\nabla \tau p^l_\mu)^l = \sum_{(\tau \chi) \in R} \sum_{(\rho \alpha \mu) \in R} V_{i,(\tau \chi)(\rho \alpha \mu)}^{il}(0) (\nabla \rho p^l_\chi)^l - \sum_{(\tau \chi) \in R} \sum_{(\rho \mu \alpha) \in R} V_{i,(\tau \chi)(\rho \mu \alpha)}^{il}(0) (\nabla \rho p^l_\chi)^l
\]

where in obtaining the last line we have merely relabeled \( \tau \) to \( \rho, \iota \) to \( \alpha \) and \( \chi \) to \( \mu \). We use (2.35) and (2.36) to compute the summation over \( \gamma \) of (1) in (2.25), which is valid since \( U^\text{lin} \) is smooth in this region:

\[
\sum_{(\tau \chi) \in R} \sum_{(\rho \alpha \mu) \in R} V_{i,(\rho \alpha \mu)(\tau \chi)}^{il}(0) \left[ \nabla_{\tau,\rho}^2 U(\eta) - \nabla_{\rho} p_\chi(\eta) + \nabla_{\rho} p_\chi(\eta) \right]
\]

\[
= - \nabla \cdot (\partial_{GG} W(0) \nabla U) + \sum_{(\tau \chi) \in R} \sum_{(\rho \alpha \mu) \in R} V_{i,(\tau \chi)(\rho \alpha \mu)}^{il}(0) \left[ - \nabla_{\rho} p_\chi(\eta) + \nabla_{\rho} p_\chi(\eta) \right] \text{ by Clairaut’s Thm.}
\]

\[
= - \nabla \cdot (\partial_{GG} W(0) \nabla U) - \sum_{\mu} \nabla \cdot (\partial_{Gp^\mu} W(0)p^\mu) = 0 \text{ by (2.33)}.
\]

(2.37)

When summing over \( \gamma \) in terms (2a) and (2b) of (2.25), the terms in braces disappear, which when combined with (2.37) yields the second component of (2.26). Moreover, even
if $\gamma$ is not summed over, then term (2a) vanishes at the linear elastic solution due to the second constraint of (2.33) and due to the expressions (2.34): indeed, we may observe that

$$[\partial_{\rho \mu} W(0) \nabla U],$$

while

$$(2a) = \sum_{(\rho \alpha \gamma)} \{ \sum_{(\rho \alpha)} \gamma V_{\gamma}(\rho \alpha \gamma)(0) \} (p_\gamma(\eta) - p_\eta(\eta))$$

$$= \sum_{(\rho \alpha \gamma)} \sum_{(\rho \alpha)} \gamma V_{\gamma}(\rho \alpha \gamma)(0) p_\alpha(\eta) - \sum_{(\rho \alpha)} \sum_{(\rho \alpha \gamma)} \gamma V_{\gamma}(\rho \alpha \gamma)(0) p_\alpha(\eta)$$

$$- \sum_{(\rho \alpha \gamma)} \sum_{(\rho \alpha)} V_{\rho}(\rho \alpha \gamma)(0) p_\gamma(\eta) + \sum_{(\rho \alpha \gamma)} \sum_{(\rho \alpha)} V_{\rho}(\rho \alpha \gamma)(0) p_\gamma(\eta)$$

$$= \sum_{(\rho \alpha \gamma)} \sum_{(\rho \alpha)} V_{\rho}(\rho \alpha \gamma)(0) p_\alpha(\eta) - \sum_{(\rho \alpha)} \sum_{(\rho \alpha \gamma)} V_{\rho}(\rho \alpha \gamma)(0) p_\alpha(\eta)$$

$$- \sum_{(\rho \alpha \gamma)} \sum_{(\rho \alpha)} V_{\rho}(\rho \alpha \gamma)(0) p_\gamma(\eta) + \sum_{(\rho \alpha \gamma)} \sum_{(\rho \alpha)} V_{\rho}(\rho \alpha \gamma)(0) p_\gamma(\eta)$$

$$= \sum_{\chi} \partial_{\rho \gamma} W(0) p_\chi.$$

We may now replace the linear elastic solution with $(U^0, P^0)$ and make an at most $|\ell|^{-3}$ error according to Lemma 3 in (1) and 2b which yields (2.26) when combined with decay estimates for the remainder terms used previously in Lemma 3. Moreover, even though $SP^0$ is not smooth, we are still able to use Taylor expansions of $D_\rho p^0$ just as we did in Lemma 3 so that we may replace $(U^0, P^0)$ with $(SU^0, SP^0)$ to obtain (2.27).

We have now fully defined all ingredients in the dislocation energy (2.1),

$$\mathcal{E}^a(u) = \sum_{\ell \in \Lambda} V_\ell(Du(\ell)),$$

and we can further show this energy is well-defined and continuously Frechet differentiable over the admissible displacements, $\mathcal{A}$, defined in (2.9).

**Theorem 5 (Dislocation Energy is well-defined).** Under the hypotheses on the site potential and coercivity of the defect-free energy, the atomistic energy function, $\mathcal{E}^a$, is well defined and belongs to $C^3(\mathcal{A})$, provided the site potential is $C^4$. More generally, a $C^{k+1}$ site potential yields a $C^k$ energy.

It should come as no surprise that the proof makes heavy use of techniques previously used in [6, 13].
Proof of Theorem 5. We proceed as in the proof of [6, Lemma 3.2]. Namely, we recall the definition of the atomistic energy as

$$\mathcal{E}^a(u) = \sum_{\ell \in \Lambda} V_\ell(Du(\ell)),$$

and note that if $u$ belongs to the space $U_0$, then

$$\langle \delta \mathcal{E}^a(0), u \rangle = \frac{d}{dt} \left[ \mathcal{E}^a(0 + tu) \right]_{t=0} = \sum_{\ell \in \Lambda} \langle \delta V_\ell(0), Du(\ell) \rangle,$$

as this becomes a finite sum (and hence we can differentiate term-by-term), and thus

$$\mathcal{E}^a(u) = \sum_{\ell \in \Lambda} \left[ V_\ell(Du(\ell)) - \langle \delta V_\ell(0), Du(\ell) \rangle \right] + \langle \delta \mathcal{E}^a(0), u \rangle$$

for these displacements $u$. If we can show that (1)

$$\sum_{\ell \in \Lambda} \left[ V_\ell(Du(\ell)) - \langle \delta V_\ell(0), Du(\ell) \rangle \right]$$

is well-defined for displacements having finite energy and is differentiable and (2) that

$$\langle \delta \mathcal{E}^a(0), u \rangle$$

is a bounded linear functional, then we will have that $\mathcal{E}^a$ agrees with a $C^k$ functional on the dense subset, $U_0$, of $\mathcal{U}$, and hence may be uniquely extended to a $C^k$ functional on $\mathcal{A}$.

Showing that the function

$$\sum_{\ell \in \Lambda} \left[ V_\ell(Du(\ell)) - \langle \delta V_\ell(0), Du(\ell) \rangle \right]$$

is well defined and continuously differentiable can be done verbatim to [13, Theorem 2.1] by simply replacing the homogeneous site potential, $V$, in that work with $V_\ell$ in the present work so we omit the details.

To show that $\langle \delta \mathcal{E}^a(0), u \rangle = \sum_{\ell \in \Lambda} \langle \delta V_\ell(0), Du(\ell) \rangle$ is a bounded functional, we recall first the identity (2.14)

$$\tilde{D}u(\ell) = \tilde{D}_\rho u_0 + \tilde{D}_\rho p_\beta(\ell) + p_\beta(\ell) - p_\alpha(\ell).$$
Using this identity and the definition of $e(\ell)$ from (2.11), we have

$$
\sum_{\ell \in \Lambda} \langle \delta V(0), Du(\ell) \rangle = \sum_{\ell \in \Lambda} \langle \delta V(e(\ell)), D\bar{u}(\ell) \rangle
$$

$$
= \sum_{\ell \in \Lambda} \sum_{(\rho, \beta)} V(\rho, \beta) e(\ell) \cdot D(\rho, \beta) u(\ell)
$$

$$
= \sum_{\ell \in \Lambda} \sum_{(\rho, \beta)} V(\rho, \beta) e(\ell) \cdot [\tilde{D}_\rho u_0(\ell) + \tilde{D}_\rho p(\ell) + p(\ell) - p(\ell)]
$$

$$
= \sum_{\ell \in \Lambda} \sum_{(\rho, \beta)} V(\rho, \beta) e(\ell) \cdot [\tilde{D}_\rho u_0(\ell) + \tilde{D}_\rho p(\ell) + p(\ell) - p(\ell)]
$$

$$
+ \sum_{\ell \in \Lambda} \sum_{(\rho, \beta)} V(\rho, \beta) e(\ell) \cdot [p(\ell) - p(\ell)].
$$

For term $T_2$, we have

$$
T_2 = \sum_{\ell \in \Lambda} \sum_{(\rho, \beta)} V(\rho, \beta) e(\ell) \cdot [p(\ell) - p(\ell)]
$$

$$
= \sum_{\ell \in \Lambda} \sum_{(\rho, \beta)} [V(\rho, \beta) e(\ell) - V(\rho, \beta) e(0)] \cdot [p(\ell) - p(\ell)]
$$

$$
+ \sum_{\ell \in \Lambda} \sum_{(\rho, \beta)} [V(\rho, \beta) e(0) - V(\rho, \beta) e(0)] \cdot [p(\ell) - p(\ell)]
$$

$$
= \sum_{\ell \in \Lambda} \sum_{(\rho, \beta)} [V(\rho, \beta) e(\ell) - V(\rho, \beta) e(0)] \cdot [p(\ell) - p(\ell)]
$$

$$
+ \sum_{\ell \in \Lambda} \sum_{(\rho, \beta)} [V(\rho, \beta) e(0) - V(\rho, \beta) e(0)] \cdot [p(\ell) - p(\ell)]
$$

$$
= \sum_{\ell \in \Lambda} \sum_{(\rho, \beta)} [V(\rho, \beta) e(\ell) - V(\rho, \beta) e(0)] \cdot [p(\ell) - p(\ell)]
$$

$$
+ \sum_{\ell \in \Lambda} \sum_{(\rho, \beta)} [V(\rho, \beta) e(0) - V(\rho, \beta) e(0)] \cdot [p(\ell) - p(\ell)]
$$

$$
= \sum_{\ell \in \Lambda} \sum_{(\rho, \beta)} [V(\rho, \beta) e(\ell) - V(\rho, \beta) e(0)] \cdot [p(\ell) - p(\ell)]
$$

$$
+ \sum_{\ell \in \Lambda} \sum_{(\rho, \beta)} [V(\rho, \beta) e(0) - V(\rho, \beta) e(0)] \cdot [p(\ell) - p(\ell)]
$$

$$
= \sum_{\ell \in \Lambda} \sum_{(\rho, \beta)} [V(\rho, \beta) e(\ell) - V(\rho, \beta) e(0)] \cdot [p(\ell) - p(\ell)]
$$

$$
+ \sum_{\ell \in \Lambda} \sum_{(\rho, \beta)} [V(\rho, \beta) e(0) - V(\rho, \beta) e(0)] \cdot [p(\ell) - p(\ell)]
$$

$$
= \sum_{\ell \in \Lambda} \sum_{(\rho, \beta)} [V(\rho, \beta) e(\ell) - V(\rho, \beta) e(0)] \cdot [p(\ell) - p(\ell)]
$$

$$
+ \sum_{\ell \in \Lambda} \sum_{(\rho, \beta)} [V(\rho, \beta) e(0) - V(\rho, \beta) e(0)] \cdot [p(\ell) - p(\ell)]
$$

$$
= \sum_{\ell \in \Lambda} \sum_{(\rho, \beta)} [V(\rho, \beta) e(\ell) - V(\rho, \beta) e(0)] \cdot [p(\ell) - p(\ell)]
$$

$$
+ \sum_{\ell \in \Lambda} \sum_{(\rho, \beta)} [V(\rho, \beta) e(0) - V(\rho, \beta) e(0)] \cdot [p(\ell) - p(\ell)]
$$

where we have used Lemma 3 in the obtaining the final line. Now by Lemma 4, term (2a) vanishes, which is exactly the term immediately above up to an $O(\ell^{-2})$ error. But this is
then summable so that

$$|T_2| \lesssim \|p\|_{L^2} \lesssim \|u\|_{a_1}.$$ 

For term $T_1$, we utilize [6, Lemma 5.7] which allows to write “integrate $\tilde{D}$ by parts:”

$$T_1 = \sum_{\ell \in \Lambda} \sum_{(\rho \alpha \beta)} V_{(\rho \alpha \beta)}(e(\ell)) \cdot [\tilde{D}_\rho u_0(\ell) + \tilde{D}_\rho p_\beta(\ell)]$$

$$= \sum_{\ell \in \Lambda} \sum_{(\rho \alpha \beta)} \tilde{D}_\rho (V_{(\rho \alpha \beta)}(e(\ell))) \cdot [u_0(\ell) + p_\beta(\ell)]$$

$$= \sum_{\ell \in \Lambda} \sum_{(\rho \alpha \beta)} \tilde{D}_\rho (V_{(\rho \alpha \beta)}(e(\ell))) \cdot u_0(\ell) + \sum_{\ell \in \Lambda} \sum_{(\rho \alpha \beta)} \tilde{D}_\rho (V_{(\rho \alpha \beta)}(e(\ell))) \cdot p_\beta(\ell).$$

(2.40)

Next, observe that by Lemma [4] if $\ell \not\in \Omega_\Gamma$,

$$\left| \sum_{(\rho \alpha \beta)} \tilde{D}_\rho (V_{(\rho \alpha \beta)}(e(\ell))) \right| = \left| \sum_{(\rho \alpha \beta)} D_\rho (V_{(\rho \alpha \beta)}(Du_0^0)) \right| = \left| \sum_{\gamma} \frac{\partial \mathcal{E}^a}{\partial u_\gamma(\ell)}|_{(Du_0^0, p_0^0)} \right| \lesssim |\ell|^{-3},$$

(2.41)

and if $\ell \in \Omega_\Gamma$,

$$\left| \sum_{(\rho \alpha \beta)} \tilde{D}_\rho (V_{(\rho \alpha \beta)}(e(\ell))) \right| = \left| \sum_{(\rho \alpha \beta)} RD_\rho S(V_{(\rho \alpha \beta)}(RDS_0 u_0^0)) \right|$$

$$= \left| \sum_{(\rho \alpha \beta)} RD_\rho S(V_{(\rho \alpha \beta)}(DS_0 u_0^0)) \right|$$

$$= \left| \sum_{(\rho \alpha \beta)} RD_\rho (V_{(\rho \alpha \beta)}(DS_0 u_0^0)) \right|$$

$$= \left| \sum_{\gamma} \frac{\partial \mathcal{E}^a}{\partial u_\gamma(\ell)}|_{(S_0 Du_0^0, S p_0^0)} \right| \lesssim |\ell|^{-3}.$$ 

(2.42)

Moreover,

$$\left| \tilde{D}_\rho (V_{(\rho \alpha \beta)}(e(\ell))) \right| \lesssim |\ell|^{-2},$$

(2.43)

since

$$\left| \tilde{D}_\rho (V_{(\rho \alpha \beta)}(e(\ell))) \right| = \left| \tilde{D}_\rho (V_{(\rho \alpha \beta)}(0) + \sum_{(\tau \gamma \delta)} V_{(\rho \alpha \beta)(\tau \gamma \delta)} e_{(\tau \gamma \delta)}(\ell)) \right| + \mathcal{O}(|\epsilon_{(\tau \gamma \delta)}(\ell)|^2)$$

$$\lesssim |\ell|^{-2}$$

by (2.23) and (2.24).

Inserting estimates (2.41), (2.42), and (2.43) into (2.40), we obtain

$$|T_1| \lesssim \left| \sum_{\ell \in \Lambda} f(\ell) \cdot u_0(\ell) \right| + \sum_{\ell \in \Lambda} \sum_{(\rho \alpha \beta)} |1 + |\ell||^{-2}|p_\beta(\ell)||$$

(2.44)

where $|f(\ell)| \lesssim |\ell|^{-3}$ for sufficiently large $|\ell|$. We may then apply [6, Corollary 5.2] to deduce the existence of $g : \Lambda \to (\mathbb{R}^2)^R$, such that

$$\sum_{\ell \in \Lambda} f(\ell) \cdot u_0(\ell) = \sum_{\ell \in \Lambda} g_\rho(\ell) D_\rho u_0(\ell)$$

where $|g_\rho(\ell)| \lesssim |\ell|^{-3}$ for sufficiently large $|\ell|$.
where $|g_\rho(\ell)| \lesssim |\ell|^{-2}$ for sufficiently large $|\ell|$. This can then be inserted into (2.44) to yield

$$|T_1| \lesssim \sum_{\ell \in \Lambda} \sum_{\beta \in S} |1 + |\ell||^{-2} |D_\rho u_0(\ell) + p_\beta(\ell)| \lesssim \|u\|_{a_1},$$

where we have applied the Cauchy-Schwarz inequality and summability of $|\ell|^{-2}$ in the final inequality. Combining our estimates for $T_1$ and $T_2$ shows $\langle \delta E^a(0), \cdot \rangle$ is a bounded linear functional and thus completes the proof. □

This concludes our introductory section defining all of the perquisites necessary to state our main result concerning decay of the elastic far-fields in a multilattice generated by a straight dislocation. These decay rates are phrased in terms of finite differences (alternatively, they could be written as derivatives of smooth interpolants of lattice functions) using the notation

$$D_\rho u_\alpha(\xi) := u_\alpha(\xi + \rho) - u_\alpha(\xi) \quad \text{for} \quad \rho \in \Lambda, \quad \alpha \in S,$$

and

$$D_\rho u_\alpha(\xi) := D_\rho_1 D_\rho_2 \cdots D_\rho_k u_\alpha(\xi) \quad \text{for} \quad \rho = (\rho_1, \ldots, \rho_k) \in \Lambda^k.$$

**Theorem 6 (Decay of Dislocation far-fields).** Let $u^\infty = (U^\infty, P^\infty) \in A$ be a local minimizer of $E^a(u)$, and suppose the site potential is $C^k$ with $k \geq 4$, satisfies the slip invariance condition, and Assumption [1] is satisfied. Then for all $|\ell|$ large enough,

$$|D_\rho U_\infty(\ell)| \lesssim |\ell|^{-2} \log |\ell|, \quad \forall \rho \in \mathcal{R}_1, \quad \text{and}$$

$$|p^\infty_\alpha(\ell)| \lesssim |\ell|^{-2} \log |\ell|, \quad \forall \rho \in \mathcal{R}_1.$$  \hspace{1cm} (2.45)

**Remark 1.** Though we have only stated the decay of the elastic strains, brute-force computations may also be used to show that corresponding decay estimates also hold for strain gradients (and the corresponding shift gradients) in the sense that

$$|\tilde{D}_\rho U_\infty(\ell)| \lesssim |\ell|^{-1-j} \log |\ell|, \quad \forall \rho \in (\mathcal{R}_1)^j, 1 \leq j \leq k-2, \quad \text{and}$$

$$|D_\rho p^\infty_\alpha(\ell)| \lesssim |\ell|^{-2-j} \log |\ell|, \quad \forall \rho \in (\mathcal{R}_1)^j, 0 \leq j \leq k-3.$$  \hspace{1cm} (2.46)

We remark on how to prove such a result at the end of the proof of Theorem 6 but choose not to state this as part of the theorem as we ourselves do not go through a rigorous proof. These decay rates may also be validated by numerical computations. □

### 3. Proof of Theorem 6

The main idea of proving Theorem 6 is to show that $u^\infty$ solves a linearized problem whose Green’s function may be estimated in terms of existing Green’s function estimates developed in [13] for point defects in multilattices. The residual terms found in this linearization process are estimated in close analogy to [6], and then the two estimates are combined to yield the theorem. It is with this breakdown in mind that we split this section into separate subsections. In Section 3.1 we derive the linearized problem and corresponding estimates on the residual; in Section 3.2 we recall the needed properties of the Green’s function (matrix). Finally, in Section 3.3 we combine these results in a “pure” analysis problem to derive the estimates (2.45).
3.1. Linearized Problem and Residual Estimates. Our goal here is to establish

**Lemma 7.** There exists \( \bar{f} : \Lambda \to (\mathbb{R}^3)^{\mathcal{R}} \) such that

\[
\sum_{\ell \in \Lambda} \langle \delta^2 V(0) \tilde{D} u^\infty, \tilde{D} v \rangle = \sum_{\ell \in \Lambda} \sum_{(\rho, \beta) \in \mathcal{R}} \bar{f}_{(\rho, \beta)}(\ell) \cdot \tilde{D}_{(\rho, \beta)} v(\ell) - \langle \delta \mathcal{E}^a(0), v \rangle
\]

where \( \bar{f}_{(\rho, \beta)} \) satisfies

\[
|\bar{f}_{(\rho, \beta)}(\ell)| \lesssim |\ell|^{-2} + |\tilde{D} u^\infty(\ell)|^2.
\]

**Proof.** As \( u^\infty \) solves the atomistic Euler-Lagrange equations,

\[
0 = \langle \delta \mathcal{E}^a(u^\infty), v \rangle, \quad \forall v \in \mathcal{U}_0,
\]

we may simply Taylor expand (using (2.13))

\[
0 = \sum_{\ell \in \Lambda} \langle \delta V(e(\ell) + \tilde{D} u^\infty(\ell)), \tilde{D} v \rangle
\]

\[
= \sum_{\ell \in \Lambda} \left[ \langle \delta V(e(\ell) + \tilde{D} u^\infty(\ell)) - \delta V(e(\ell)) - \delta^2 V(e(\ell)) \tilde{D} u^\infty, \tilde{D} v \rangle \right]
\]

\[
+ \sum_{\ell \in \Lambda} \langle \delta^2 V(e(\ell)) - \delta^2 V(0) \tilde{D} u^\infty(\ell), \tilde{D} v \rangle
\]

\[
+ \sum_{\ell \in \Lambda} \langle \delta^2 V(0) \tilde{D} u^\infty(\ell), \tilde{D} v \rangle + \sum_{\ell \in \Lambda} \langle \delta V(e(\ell)), \tilde{D} v \rangle.
\]

We then rearrange terms to arrive at

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

\[
- \sum_{\ell \in \Lambda} \langle \delta^2 V(e(\ell)) - \delta^2 V(0) \tilde{D} u^\infty(\ell), \tilde{D} v \rangle
\]

\[
- \sum_{\ell \in \Lambda} \langle \delta V(e(\ell)), \tilde{D} v \rangle.
\]

Upon defining

\[
\bar{f}_{(\rho, \beta)} = -V_{(\rho, \beta)}(e(\ell) + \tilde{D} u^\infty(\ell)) + V_{(\rho, \beta)}(e(\ell)) + \sum_{(\tau, \gamma, \delta)} V_{(\rho, \beta)(\tau, \gamma, \delta)}(e(\ell)) \tilde{D}_{(\tau, \gamma, \delta)} u^\infty(\ell)
\]

\[
- \sum_{(\tau, \gamma, \delta)} (V_{(\rho, \beta)(\tau, \gamma, \delta)}(e(\ell)) \tilde{D}_{(\tau, \gamma, \delta)} u^\infty(\ell) - V_{(\rho, \beta)(\tau, \gamma, \delta)}(0) \tilde{D}_{(\tau, \gamma, \delta)} u^\infty(\ell)),
\]

it only remains to establish the given estimate on \( \bar{f}_{(\rho, \beta)} \). However, this is a straightforward consequence of Taylor's Theorem and the aforementioned decay estimates on \( e_{(\tau, \gamma, \delta)}(\ell) \) stated in Lemma 3.

\( \square \)
Next, we must estimate the term \( \langle \delta \mathcal{E}^\alpha(0), \mathbf{v} \rangle = \sum_{\ell \in \Lambda} \langle \delta V(\ell), \mathbf{Dv} \rangle \).

**Theorem 8.** There exists \( \bar{f} : \Lambda \to (\mathbb{R}^3)^R, \ g : \Lambda \to (\mathbb{R}^3)^R, \) and \( k : \Lambda \to (\mathbb{R}^3)^S \) such that for \( \mathbf{v} = (v_0, q) \in \mathcal{U}_0, \)

\[
\langle \bar{H} \mathbf{u}^\infty, \mathbf{v} \rangle := \sum_{\ell \in \Lambda} \langle \delta^2 V(0) \mathbf{D} \mathbf{u}^\infty, \mathbf{Dv} \rangle = \sum_{\ell \in \Lambda} \left( \sum_{(\rho, \beta) \in \mathcal{R}} \mathbf{f}_{(\rho, \beta)}(\ell) \cdot \mathbf{D}_{(\rho, \beta)} \mathbf{v}(\ell) + \langle g(\ell), Dv_0(\ell) \rangle + \langle k(\ell), q(\ell) \rangle \right),
\]

where for sufficiently large \(|\ell|\), \( f_{(\rho, \beta)}, g_\rho, k_\gamma \) satisfy

\[
|f_{(\rho, \beta)}(\ell)| \lesssim |\ell|^{-2} + |\mathbf{D} \mathbf{u}^\infty(\ell)|^2 \\
|g_\rho(\ell)| \lesssim |\ell|^{-2} \\
|k_\gamma(\ell)| \lesssim |\ell|^{-2}.
\]

**Proof.** From Lemma \[7\]

\[
\sum_{\ell \in \Lambda} \langle \delta^2 V(0) \mathbf{D} \mathbf{u}^\infty, \mathbf{Dv} \rangle = \sum_{\ell \in \Lambda} \sum_{(\rho, \beta) \in \mathcal{R}} f_{(\rho, \beta)}(\ell) \cdot \mathbf{D}_{(\rho, \beta)} \mathbf{v}(\ell) - \sum_{\ell \in \Lambda} \langle \delta V(\mathbf{D} \mathbf{u}^0), \mathbf{Dv} \rangle,
\]

and

\[
\sum_{\ell \in \Lambda} \langle \delta V(\mathbf{D} \mathbf{u}^0), \mathbf{Dv} \rangle = \sum_{\ell \in \Lambda} \sum_{(\rho, \beta)} V_{(\rho, \beta)}(\mathbf{D} \mathbf{u}^0) \cdot \mathbf{D}_{(\rho, \beta)} \mathbf{v}
\]

\[
= \sum_{\ell \in \Lambda} \sum_{(\rho, \beta)} V_{(\rho, \beta)}(\mathbf{D} \mathbf{u}^0) \cdot (\mathbf{D}_\rho v_0 + \mathbf{D}_\rho q_\beta + q_\beta - q_\alpha)
\]

\[
= \sum_{\ell \in \Lambda} \sum_{(\rho, \beta)} V_{(\rho, \beta)}(\mathbf{D} \mathbf{u}^0) \cdot \mathbf{D}_\rho v_0 + \sum_{\ell \in \Lambda} \sum_{(\rho, \beta)} V_{(\rho, \beta)}(\mathbf{D} \mathbf{u}^0) \cdot \mathbf{D}_\rho q_\beta
\]

\[
+ \sum_{\ell \in \Lambda} \sum_{(\rho, \beta)} V_{(\rho, \beta)}(\mathbf{D} \mathbf{u}^0) \cdot (q_\beta - q_\alpha)
\]

\[
=: B_1 + B_2 + B_3.
\]

We observe that \( B_3 \) was exactly the term, \( T_2 \), estimated in Theorem \[5\] where we saw that

\[
B_3 = \langle k_1, q \rangle, \quad |k_1(\ell)| \lesssim |\ell|^{-2}.
\]

Meanwhile, \( B_2 \) is the second term of \( T_1 \) in \([2.40]\), which we saw could be estimated by

\[
B_2 = \sum_{\ell \in \Lambda} \sum_{(\rho, \beta)} V_{(\rho, \beta)}(\mathbf{D} \mathbf{u}^0) \cdot \mathbf{D}_\rho q_\beta
\]

\[
= \sum_{\ell \in \Lambda} \mathbf{D}_{-\rho} \sum_{(\rho, \beta)} V_{(\rho, \beta)}(\ell) \cdot q_\beta = \langle k_2, q \rangle, \quad |k_2(\ell)| \lesssim |\ell|^{-2}.
\]

Thus,

\[
B_2 + B_3 = \langle k, q \rangle, \quad |k(\ell)| \lesssim |\ell|^{-2}.
\] (3.3)
Next, we observe $B_1$ is precisely the first term estimated in $T_1$ in (2.40) so, as in Theorem 5, there exists $g : \Lambda \rightarrow (\mathbb{R}^d)^{\mathbb{R}_1}$ with $|g(\ell)| \lesssim |\ell|^{-2}$ and

$$B_1 = \sum_{\ell \in \Lambda} \sum_{\rho \in \mathbb{R}_1} g_{\rho}(\ell) \cdot D_\rho v_0(\ell).$$

\[ \square \]

### 3.2. Green’s Function.

Having defined our linearized problem and estimated the residual in Theorem 8, we will proceed to estimate the decay of $u^\infty$ in the current section. Doing that will require comparing the atomistic Green’s matrix for the homogeneous energy derived in [13] for point defects to the Green’s matrix for the dislocation solution. Thus, we will introduce the homogeneous Green’s function and the corresponding estimates for its decay here.

From [13], we let $\xi \in \mathcal{B}$, where $\mathcal{B}$ is the first Brillouin zone associated to the atomic lattice, denote the Fourier variable and set

\[
\hat{H}_{00}(\xi) := \sum_{(\rho_{\alpha}\beta) \in \mathcal{R}} \sum_{(\tau_{\gamma}\delta) \in \mathcal{R}} (e^{-2\pi i \xi \cdot \tau} - 1)V_{(\rho_{\alpha}\beta)(\tau_{\gamma}\delta)}(0)(e^{2\pi i \xi \cdot \rho} - 1),
\]

\[
[\hat{H}_{0\beta}(\xi)]_{\beta} := \sum_{\rho \in \mathbb{R}_1} \sum_{\alpha = 0}^{S-1} \sum_{(\tau_{\gamma}\delta) \in \mathcal{R}} [(e^{-2\pi i \xi \cdot \tau} - 1)V_{(\rho_{\alpha}\beta)(\tau_{\gamma}\delta)}(0)(e^{2\pi i \xi \cdot \rho} - 1) - (e^{-2\pi i \xi \cdot \tau} - 1)V_{(\rho_{\alpha}\beta)(\tau_{\gamma}\delta)}(0)],
\]

\[
[\hat{H}_{\beta 0}(\xi)]_{\delta} := \sum_{\tau \in \mathbb{R}_1} \sum_{\gamma = 0}^{S-1} \sum_{(\rho_{\alpha}\beta) \in \mathcal{R}} [(e^{-2\pi i \xi \cdot \tau} - 1)V_{(\rho_{\alpha}\beta)(\tau_{\gamma}\delta)}(0)(e^{2\pi i \xi \cdot \rho} - 1) - V_{(\rho_{\alpha}\beta)(\tau_{\delta}\gamma)}(0)(e^{2\pi i \xi \cdot \rho} - 1)],
\]

\[
[\hat{H}_{\beta \delta}(\xi)]_{\beta\delta} := \sum_{\rho, \tau \in \mathbb{R}_1} \sum_{\alpha, \gamma = 0}^{S-1} [e^{-2\pi i \xi \cdot \tau}V_{(\rho_{\alpha}\beta)(\tau_{\gamma}\delta)}(0)e^{2\pi i \xi \cdot \rho} + V_{(\rho_{\alpha}\beta)(\tau_{\delta}\gamma)}(0) - e^{-2\pi i \xi \cdot \tau}V_{(\rho_{\alpha}\beta)(\tau_{\gamma}\delta)}(0) - e^{2\pi i \xi \cdot \rho}V_{(\rho_{\alpha}\beta)(\tau_{\delta}\gamma)}(0)],
\]

and define the *dynamical matrix* [16],

\[
\hat{H}(\xi) := \begin{bmatrix} \hat{H}_{00}(\xi) & \hat{H}_{0\beta}(\xi) \\ \hat{H}_{\beta 0}(\xi) & \hat{H}_{\beta \delta}(\xi) \end{bmatrix}. \tag{3.4}
\]

It has the property that

\[
\langle H u^\infty, v \rangle := \langle \delta^2 \mathcal{E}^\infty_{\text{hom}}(0) u^\infty, v \rangle = \int_{\mathcal{B}} \left[ \hat{Z}(\xi) \right]^* \hat{H}(\xi) \left[ \hat{U}^\infty(\xi) \right] d\xi, \quad \forall v = (Z, q) \in \mathcal{U}. \tag{3.5}
\]

The atomistic Green’s matrix for the homogeneous energy is then defined by

\[
\mathcal{G} := (\hat{H}^{-1})^\vee, \tag{3.6}
\]
where $\mathcal{V}$ denotes the inverse Fourier transform. It follows from Assumption [1] that $H$ is an invertible operator (see also [13]). Upon partitioning $\mathcal{G}$ as

$$
\begin{pmatrix}
G_{00} & G_{0p} \\
G_{p0} & G_{pp}
\end{pmatrix},
$$

several important decay estimates for the individual blocks were established in [13] Theorem 4.4: for $\rho \in (\mathcal{R}_1)^t, t \geq 0$ and $|\rho| := t \in \mathbb{Z},$

$$
|D_\rho G_{00}(\ell)| \lesssim (1 + |\ell|)^{-d-|\rho|+2} |\rho| \geq 1,
$$

$$
|D_\rho G_{0p}(\ell)| \lesssim (1 + |\ell|)^{-d-|\rho|+1} |\rho| \geq 0,
$$

$$
|D_\rho G_{pp}| \lesssim (1 + |\ell|)^{-d-|\rho|} |\rho| \geq 0.
$$

### 3.3. Analysis Problem

We fix $\ell \in \Lambda$ and define the lattice function $v = (Z, q)$ by $v = \sum_m G(k - \ell)e_m$ where $e_m$ is the $m$th standard basis vector. Using the relation (3.5), we may write our infinite-domain dislocation solution as

$$
\begin{pmatrix}
U^\infty(\ell) \\
p^\infty(\ell)
\end{pmatrix} = \langle Hu^\infty, v \rangle = \sum_m \int_{\mathcal{B}} e^{2\pi i \xi \ell} \left[ \hat{U}^\infty(\xi) \right]_m \hat{\epsilon}_m d\xi
$$

where $H$ is defined in (3.5) and $\mathcal{G}$ is the associated Green’s matrix defined in (3.6). Thus,

$$
\begin{pmatrix}
D_\tau U^\infty(\ell) \\
p^\infty(\ell)
\end{pmatrix} = \sum_m \left\langle H(k) \begin{pmatrix} U^\infty(k) \\ p^\infty(k) \end{pmatrix}, \begin{pmatrix} D_\tau G_{00}(k - \ell) & G_{0p}(k - \ell) \\ D_\tau G_{p0}(k - \ell) & G_{pp}(k - \ell) \end{pmatrix} \hat{\epsilon}_m \right\rangle
$$

As in [6], we consider two cases depending on the location of $\ell$ in the lattice:

#### 3.3.1. Case 1. $B_{3/4|\ell|}(\ell) \cap \Gamma = \emptyset$

In this case we take a bump function $\eta(x)$ from [6]: define $s_1 := 1/2|\ell| - r_{cut}, s_2 := 1/2|\ell|, \eta = 1$ in $B_{s_1/2}(\ell), \eta = 0$ outside of $B_{s_1}(\ell)$, and $|\nabla \eta(x)| \lesssim |\ell|^{-1}$. We then make the substitution

$$
\begin{pmatrix}
D_\tau U^\infty(\ell) \\
p^\infty(\ell)
\end{pmatrix} = \sum_m \left\langle H(k) \begin{pmatrix} U^\infty(k) \\ p^\infty(k) \end{pmatrix}, \eta(k - \ell) \begin{pmatrix} D_\tau G_{00}(k - \ell) & G_{0p}(k - \ell) \\ D_\tau G_{p0}(k - \ell) & G_{pp}(k - \ell) \end{pmatrix} \hat{\epsilon}_m \right\rangle
$$

$$
+ \left\langle H(k) \begin{pmatrix} U^\infty(k) \\ p^\infty(k) \end{pmatrix}, (1 - \eta(k - \ell)) \begin{pmatrix} D_\tau G_{00}(k - \ell) & D_\tau G_{0p}(k - \ell) \\ G_{p0}(k - \ell) & G_{pp}(k - \ell) \end{pmatrix} \hat{\epsilon}_m \right\rangle.
$$
Using the product rule for finite differences, decay estimates on Equation 6.31, and thus we likewise obtain for sufficiently large $\ell$

$$\max\{|DU^\infty(\ell)|, |P^\infty(\ell)|\} \lesssim |\ell|^{-1} + \|(1 + |\ell - k|)^{-1} D\hat{u}^\infty(k)\|e(\Lambda \cap B_{2}(\ell)).$$

(3.17)
3.3.2. Case 2. \( B_{3/4}(\ell) \cap \Gamma \neq \emptyset \)

We argue as in [6] by using a reflection argument whereby the branch cut \( \Gamma = \{(x_1, x_2) : x_2 = \hat{x}_2, x_1 > \hat{x}_1\} \) is replaced by \( \Gamma_S = \{(x_1, x_2) : x_2 = \hat{x}_2, x_1 < \hat{x}_1\} \) and the energy is replaced by

\[
\mathcal{E}_S(u) = \sum_{\ell \in \Lambda} V(D(S_0u_0 + u)).
\]

For this energy, we have that \( \langle \delta \mathcal{E}_S(Su^\infty), \nu \rangle = 0 \) since

\[
\langle \delta \mathcal{E}_S(Su^\infty), \nu \rangle = \sum_{\ell \in \Lambda} \sum_{\rho, \beta} V_{(\rho, \beta)}(D(S_0u_0 + Su^\infty))D_{(\rho, \beta)}\nu
= \sum_{\ell \in \Lambda} \sum_{\rho, \beta} V_{(\rho, \beta)}(D(S_0u_0 + Su^\infty)) \cdot (D\rho v_0(\ell) + q_\beta(\ell + \rho) - q_\alpha(\ell))
= \sum_{\ell \in \Lambda} \sum_{\rho, \beta} SRV_{(\rho, \beta)}(D(S_0u_0 + Su^\infty)) \cdot (D\rho v_0(\ell) + q_\beta(\ell + \rho) - q_\beta(\ell) + q_\beta(\ell) - q_\alpha(\ell))
= \sum_{\ell \in \Lambda} \sum_{\rho, \beta} V_{(\rho, \beta)}(RD(S_0u_0 + Su^\infty)) \cdot (R(D\rho v_0(\ell) + q_\beta(\ell + \rho) - q_\beta(\ell) + q_\beta(\ell) - q_\alpha(\ell)))
= \sum_{\ell \in \Lambda} \sum_{\rho, \beta} V_{(\rho, \beta)}(e(\ell) + \tilde{D}u^\infty) \cdot (RD\rho v_0(\ell) + RD\rho q_\beta(\ell) + Rq_\beta(\ell) - Rq_\alpha(\ell))
= \sum_{\ell \in \Lambda} \sum_{\rho, \beta} V_{(\rho, \beta)}(e(\ell) + \tilde{D}u^\infty) \cdot (RD\rho Sw_0(\ell) + RD\rho Sr_\beta(\ell) + r_\beta(\ell) - r_\alpha(\ell))
= \sum_{\ell \in \Lambda} \sum_{\rho, \beta} V_{(\rho, \beta)}(e(\ell) + \tilde{D}u^\infty) \cdot \tilde{D}w(\ell)
= \langle \delta \mathcal{E}(u^\infty), w \rangle = 0,
\]

where \( w_0 = Rv_0, r_\gamma = Rq_\gamma, \) and \( w_\gamma = w_0 + r_\gamma. \) As we have only reflected the branch cut, this problem is identical to the previous case in the sense that an estimate for \( Su^\infty \) now exists in the \( x \geq \hat{x}_1 \) plane (where there is no branch cut):

\[
\max\{|DSU^\infty(\ell)|, |Sp^\infty(\ell)|\} \lesssim |\ell|^{-1} + \|(1 + |\ell - k|)^{-1}DSu^\infty(k)|_{\mathcal{E}(\Lambda \cap B_s(\ell))}.
\]

As \( R \) simply represents a translation operation by one Burger’s vector, we then also have

\[
\max\{|RDSU^\infty(\ell)|, |RSp^\infty(\ell)|\} \lesssim |\ell|^{-1} + \|(1 + |\ell - k|)^{-1}RDSu^\infty(k)|_{\mathcal{E}(\Lambda \cap B_s(\ell))},
\]

or

\[
\max\{|\tilde{D}U^\infty(\ell)|, |p^\infty(\ell)|\} \lesssim |\ell|^{-1} + \|(1 + |\ell - k|)^{-1}\tilde{D}u^\infty(k)|_{\mathcal{E}(\Lambda \cap B_s(\ell))}.
\]

It is now immediate from the proof of [6, Lemma 6.7] that

\[
\max\{|\tilde{D}U^\infty(\ell)|, |p^\infty(\ell)|\} \lesssim |\ell|^{-1}.
\] (3.18)
Thus far, we have carefully set everything up so that we may use the techniques and analysis of \cite{ref} to complete the proof of Theorem \ref{thm:main}. The primary idea is to obtain suboptimal estimates as in \eqref{3.18}, which translates into higher regularity of the residual in Theorem \ref{thm:main}, which can then in turn be used to prove higher regularity of $\tilde{D}u^\infty$.

We return to equation \eqref{3.11} and set

$$v = \sum_m \begin{pmatrix} D_r G'_{00}(k - \ell) \\ D_r G'_{p0}(k - \ell) \\ G'_{pp}(k - \ell) \end{pmatrix} \hat{e}_m$$

to write

$$\begin{pmatrix} D_r U^\infty(\ell) \\ p^\infty(\ell) \end{pmatrix}$$

$$= \sum_{k \in \Lambda} \langle \delta^2 V(0) Du^\infty, Dv \rangle + \sum_{k \in \Lambda} \langle \delta^2 V(0) \tilde{D}u^\infty, \tilde{D}v \rangle - \sum_{k \in \Lambda} \langle \delta^2 V(0) \tilde{D}u^\infty, \tilde{D}v \rangle$$

$$= \sum_{k \in \Lambda} \left( \sum_{\rho, \beta, \alpha \in \mathcal{R}} \tilde{f}_{(\rho, \beta)}(k) \cdot \tilde{D}_{(\rho, \beta)} \cdot v(k + (g, Dv_0(k)) + (k, q(k))) \right) \text{ by Theorem } \ref{thm:main}$$

$$+ \sum_{k \in \Lambda} \langle \delta^2 V(0) Du^\infty, Dv \rangle - \sum_{k \in \Lambda} \langle \delta^2 V(0) \tilde{D}u^\infty, \tilde{D}v \rangle. \quad \text{(3.19)}$$

It follows from Equation \eqref{3.18} that $|\tilde{f}_{(\rho, \beta)}(k)| \lesssim (1 + |k|)^{-2}$ and from the decay estimates on $\mathcal{G}$ that

$$\left| \sum_{k \in \Lambda} \left( \sum_{\rho, \beta, \alpha \in \mathcal{R}} \tilde{f}_{(\rho, \beta)}(k) \cdot \tilde{D}_{(\rho, \beta)} \cdot v(k + (g, Dv_0(k)) + (k, q(k))) \right) \right| \lesssim \sum_{k \in \Lambda} (1 + |k|)^{-2}(1 + |\ell - k|)^{-2} \lesssim |\ell|^{-2} \log |\ell|.$$ \quad \text{(3.20)}

Next, we assume $\ell_1 < \hat{x}_1$ so that we have $\tilde{D} = D$ for $\ell$ large enough, which means

$$\sum_{k \in \Lambda} \langle \delta^2 V(0) Du^\infty, Dv \rangle - \sum_{k \in \Lambda} \langle \delta^2 V(0) \tilde{D}u^\infty, \tilde{D}v \rangle$$

is nonzero for only those $k \in \Lambda$ within $r_{cut}$ of the branch cut, $\Gamma$. If we let $\Lambda_T$ (as in \cite{ref}) denote the set of all such $k$, we have

$$\sum_{k \in \Lambda} \langle \delta^2 V(0) Du^\infty, Dv \rangle - \sum_{k \in \Lambda} \langle \delta^2 V(0) \tilde{D}u^\infty, \tilde{D}v \rangle = \sum_{k \in \Lambda} \langle \delta^2 V(0) Du^\infty, Dv \rangle - \sum_{k \in \Lambda} \langle \delta^2 V(0) \tilde{D}u^\infty, \tilde{D}v \rangle. \quad \text{(3.21)}$$

In this case we can simply use the suboptimal bounds directly on $u^\infty$ and the decay estimates for $\mathcal{G}$ to get

$$\sum_{k \in \Lambda} \langle \delta^2 V(0) Du^\infty, Dv \rangle - \sum_{k \in \Lambda} \langle \delta^2 V(0) \tilde{D}u^\infty, \tilde{D}v \rangle \lesssim \sum_{k \in \Lambda} (1 + |k|)^{-1}(1 + |\ell - k|)^{-2}. \quad \text{(3.22)}$$
As $U_\Gamma$ is simply a strip, this summation is now effectively one dimensional and can be bounded by noting $|\ell - k| \gtrsim |\ell| + |k|$ when $\ell_1 < \hat{x}_1$ and $k \in U_\Gamma$ so

$$\sum_{k \in U_\Gamma} (1 + |k|)^{-1}(1 + |\ell - k|)^{-2} \lesssim \int_{|\ell|}^{\infty} \frac{1}{|\ell||k|^1 + |k|^2} dk \lesssim |\ell|^{-2}\log|\ell|. \quad (3.23)$$

In the case $\ell_1 > \hat{x}_1$, then we may simply perform another reflection argument by placing the branch cut in the left-half plane. It therefore follows from (3.23) and (3.20) that in fact

$$\max\{|\tilde{D} U_\infty^{\infty}(\ell)|, |p_\infty^{\infty}(\ell)|\} \lesssim |\ell|^{-2}\log|\ell|, \quad (3.24)$$

for all large enough $|\ell|$. This completes the proof of Theorem 6.

As for the case for higher order derivatives (differences) alluded to in Remark 1:

$$\max\{|\tilde{D}^j U_\infty^{\infty}(\ell)|, |D^{j-1} p_\infty^{\infty}(\ell)|\} \lesssim |\ell|^{-1-j}\log|\ell|,$$

we simply give a high-level view of the argument as it is nearly identical to that given in [6, Proof of Theorem 3.6] but with our usual modifications to extend to the multilattice case. The principal idea is to again write

$$\begin{pmatrix} D_\tau U_\infty^{\infty}(\ell) \\ p_\infty^{\infty}(\ell) \end{pmatrix} = \sum_m \langle H(k) \begin{pmatrix} U_\infty^{\infty}(k) \\ p_\infty^{\infty}(k) \end{pmatrix}, \begin{pmatrix} D_\tau G_{00}(k - \ell) & G_{0p}(k - \ell) \\ D_\tau G_{p0}(k - \ell) & G_{pp}(k - \ell) \end{pmatrix} \tilde{e}_m \rangle \quad (3.25)$$

and take higher finite differences in succession. At each stage, the estimates on the residual can be improved by taking into account the decay proven in the previous order finite differences, and thus improved estimates can be obtained rigorously via an induction argument.

4. Applications and Numerical Examples

Having proven our main result, in this section, we use it to prove a result concerning convergence of a numerical method to the true defect solution, $u_\infty$. We illustrate this with a numerical example of an edge dislocation in silicon.

4.1. Algorithm. A simple, yet effective algorithm for approximating a single, straight-line dislocation in an infinite crystal is to fix some finite computational domain $\Omega \subset \Lambda$ and define the approximation space

$$\mathcal{U}_\Omega := \{u \in \mathcal{A} : u_\alpha = 0, \forall \ell \notin \Omega\}.$$ 

In this situation, all displacements in $\mathcal{U}_\Omega$ are given a boundary condition which is just the continuum-elasticity predictor $u^0 = (U^0, p^0)$. If we parametrize the “size” of $\Omega$ by a radius

$$\Omega(R) = \sup\{r > 0 : B_r(\xi) \subset \Omega, \xi \in \Omega\},$$

it is straightforward to prove

**Theorem 9.** Suppose that $u_\infty \in \mathcal{A}$ is a solution to the atomistic Euler-Lagrange equations $\langle \delta \mathcal{E}^a(u_\infty), v_\cdot \rangle = 0$ for all $v \in \mathcal{U}_0$ and that Assumption 1 holds. Then there exists $R_0$ such that for all domains $\Omega$ with $\Omega(R) \geq R_0$, there exists a solution $u_\Omega$ to

$$u_\Omega = \arg\min_{u_\Omega} \mathcal{E}^a(u)$$
which satisfies
\[ \| \mathbf{u}_\Omega - \mathbf{u}^\infty \|_{a_1} \lesssim R^{-1} \log R. \] (4.1)

Proof. For simplicity we assume that \( \Omega \) is chosen so that
\[ \Omega(R) = \sup \{ r > 0 : B_r(0) \subset \Omega \}. \]
As in any Galerkin method, the key here is in estimating the best approximation error of \( \mathbf{u}^\infty \) in the space \( \mathbf{U}_\Omega \). This was accomplished in the work [13, Lemma A.1] and [12, Lemma 12] where an approximation, \( \Pi \mathbf{u}^\infty \in \mathbf{U}_\Omega \), to \( \mathbf{u}^\infty \) was defined, and it was shown that
\[ \| \mathbf{u}^\infty - \Pi \mathbf{u}^\infty \|_{a_1} \lesssim \| \nabla I U \|_{L^2 \left( \mathbb{R}^2 \setminus B_{R/2}(0) \right)} + \| I p \|_{L^2 \left( \mathbb{R}^2 \setminus B_{R/2}(0) \right)}, \]
where we recall \( I \) was a piecewise linear interpolation operator. Using the decay estimates in Theorem 6, we may then estimate these last two terms and have
\[ \| \mathbf{u}^\infty - \Pi \mathbf{u}^\infty \|_{a_1} \lesssim R^{-1} \log R. \]
By continuity, Assumption 1 implies
\[ \langle \delta^2 \mathcal{E}^a(\Pi \mathbf{u}^\infty), \mathbf{v} \rangle \gtrsim \| \mathbf{v} \|^2_{a_1}, \quad \forall \mathbf{v} \in \mathbf{U}_0, \]
(with a possibly different implied constant). Moreover,
\[ \langle \delta \mathcal{E}^a(\Pi \mathbf{u}^\infty), \mathbf{v} \rangle = \langle \delta \mathcal{E}^a(\Pi \mathbf{u}^\infty), \mathbf{v} \rangle - \langle \delta \mathcal{E}^a(\mathbf{u}^\infty), \mathbf{v} \rangle \lesssim \| \Pi \mathbf{u}^\infty - \mathbf{u}^\infty \|_{a_1} \| \mathbf{v} \|_{a_1} \]
so we may apply the inverse function theorem to deduce the existence of a solution \( \mathbf{u}_\Omega \in \mathbf{U}_\Omega \) to
\[ \langle \delta \mathcal{E}^a(\mathbf{u}), \mathbf{v} \rangle = 0, \quad \forall \mathbf{v} \in \mathbf{U}_\Omega, \]
which satisfies
\[ \| \mathbf{u}_\Omega - \Pi \mathbf{u}^\infty \|_{a_1} \lesssim R^{-1} \log R. \]
But then
\[ \| \mathbf{u}_\Omega - \mathbf{u}^\infty \|_{a_1} \lesssim R^{-1} \log R \]
as well. \( \square \)

4.2. Edge Dislocation in Silicon. The structure of silicon is two interpenetrating FCC lattices, where in the definition of a multilattice, we may take:
\[
\mathbf{B} = \frac{1}{2} \begin{pmatrix}
0 & 1 & 1 \\
1 & 0 & 1 \\
1 & 1 & 0
\end{pmatrix}, \quad \mathbf{p}_0 = \mathbf{0}, \quad \mathbf{p}_1 = \begin{pmatrix} 1/4 \\ 1/4 \\ 1/4 \end{pmatrix}.
\]
We consider an edge dislocation with Burger’s vectors \( \mathbf{b} = \frac{1}{2}(110) \) in the \{\overline{1}11\} slip plane such that the dislocation line has direction \( \langle 112 \rangle \), which is also the system analyzed in [11]. (Here, we have chosen units so that the lattice constant is unity.)
We choose to model silicon with a Stilinger-Weber type potential [14], and the analytical solution to the continuum elasticity predictor problem may then be obtained from [7] after which the shifts may be solved for.
We now perform a self-convergence study in the \( \| \cdot \|_{a_1} \) norm for increasing values of \( R \) and plot the results in the blue curve of Figure 1 which shows very good \( R^{-1} \) decay as
expected from the theory. We additionally plot several other curves in the figure, which are discussed below and are obtained by using various other continuum elasticity predictors for \( u^0 = (U^0, p^0) \).

**Figure 1.** Energy Error for Silicon Edge Dislocation using Stilinger-Weber potential.

The red and green curves are derived by using isotropic and anisotropic continuum elasticity solutions [7] where the elasticity constants in \( C \) are obtained from empirical tables [7] and not Cauchy–Born theory. This is for example the approach taken in [11]. We then solve for the continuum displacement, \( U \), and subsequently, the shifts before carrying out our numerical algorithm described above. We note that a lower order convergence appears, but at the moment, we have no explanation as to why these models still appear to be converging, though one possible explanation would be a pre-asymptotic effect in the highly symmetric diamond cubic lattice. Alternatively, there may very well be some form of convergence occurring that deserves further investigation. The final purple curve uses a slightly modified Cauchy-Born predictor using the modified Cauchy-Born energy of [9]. It is only applicable to those multilattice crystals which are single-species two lattices (which silicon is as it is two carbon FCC lattices). Though the convergence matches the regular Cauchy-Born rate, the symmetrized Cauchy-Born energy has the remarkable result that the individual residual forces decay at a higher rate, and would thus lead to simplified proof of our results. Our main interest in this energy was to see if any benefits could be seen, but this simplified setting did not appear to show a significant difference.
Appendix A. Equivalence of Cauchy–Born Equations

Here we show that “standard” Cauchy–Born model is equivalent to the mixed formulation used in the proof of Lemma 4. Namely, we wish to show that if \((U, p)\) solves
\[
\nabla \cdot (C \nabla U) = 0 \tag{A.1}
\]
\[
\frac{\partial^2}{\partial p \partial p} [V\left(\left(0\right)_{\rho_{\alpha\beta} \in \mathbb{R}}\right)] p^{\text{lin}} = -\partial_{p_f}^F [V\left(\left(0\right)_{\rho_{\alpha\beta} \in \mathbb{R}}\right)] \nabla U^{\text{lin}} \tag{A.2}
\]
then \((U, p)\) also solves the mixed variational equation
\[
\langle \partial_{p_f}^F W(0) \nabla U, \nabla V \rangle + \sum_{\nu} \langle \partial_{p_{f\nu}} W(0) \nabla U, q_{\nu} \rangle + \sum_{\mu} \langle \partial_{p_{f\mu}} W(0) p_{\mu}, \nabla V \rangle
\]
\[
+ \sum_{\mu, \nu} \langle \partial_{p_{f\mu} p_{f\nu}} W(0) p_{\mu}, q_{\nu} \rangle = 0, \quad \forall (W, q) \in C^\infty_0.
\]
and vice versa. The main connection between these two lies in the identity
\[
C = \partial_{p_f}^2 W(0) - \partial_{p_{f}}^2 W(0) \left[ \partial_{p p}^2 \left( W(0) \right) \right]^{-1} \partial_{p_f}^2 W(0).
\]

Thus to go from the mixed form to the standard form, we simple take a test function pair with \(\nabla V = 0\) which allows us to obtain the equation for \(p^{\text{lin}}\). We may then choose a test pair with \(q = 0\), integrate by parts and then use the above identity to obtain \(\nabla \cdot (C \nabla U) = 0\). In the opposite direction, we simply multiply (A.1) by a test function \(V\), integrate by parts and substitute (A.2). We then multiply (A.2) by a test function \(q\) and the results of the preceding to computations to yield the mixed form.

Appendix B. Proof of identity (2.14)

Here we establish the identity (2.14):
\[
\tilde{D}_{(\rho_{\alpha\beta})} u(\ell) = \tilde{D}_\rho u_0 + \tilde{D}_\rho p_{\beta}(\ell) + p_{\beta}(\ell) - p_{\alpha}(\ell),
\]
by considering the cases (1) \(\ell \notin \Omega_\Gamma\) and (2) \(\ell \in \Omega_\Gamma\). For the former, we have
\[
\tilde{D}_{(\rho_{\alpha\beta})} u(\ell) = D_{(\rho_{\alpha\beta})} u(\ell), \quad \ell \notin \Omega_\Gamma,
\]
\[
\quad = D_\rho u_0(\ell) + D_\rho p_{\beta}(\ell) + p_{\beta}(\ell) - p_{\alpha}(\ell)
\]
\[
\quad = \tilde{D}_\rho u_0(\ell) + \tilde{D}_\rho p_{\beta}(\ell) + p_{\beta}(\ell) - p_{\alpha}(\ell), \quad \text{since } \ell \notin \Omega_\Gamma.
\]
For the latter case $\ell \in \Omega_{\Gamma}$, we have

$$
\tilde{D}_{(\rho \alpha \beta)} u(\ell) = R D_{(\rho \alpha \beta)} S u(\ell), \quad \ell \in \Omega_{\Gamma},
$$

$$
= \left\{ \begin{array}{ll}
D_{(\rho \alpha \beta)} S u(\ell), & \ell_2 > \hat{x}_2 \\
D_{(\rho \alpha \beta)} S u(\ell + b_{12}), & \ell_2 < \hat{x}_2
\end{array} \right.
$$

$$
= \left\{ \begin{array}{ll}
(Su)_{\beta}(\ell + \rho) - (Su)_{\alpha}(\ell), & \ell_2 > \hat{x}_2 \\
(Su)_{\beta}(\ell + b_{12} + \rho) - (Su)_{\alpha}(\ell + b_{12}), & \ell_2 < \hat{x}_2
\end{array} \right.
$$

$$
= \left\{ \begin{array}{ll}
(Su)_{\beta}(\ell + \rho) - u_{\alpha}(\ell), & \ell_2 > \hat{x}_2 \\
(Su)_{\beta}(\ell + b_{12} + \rho) - u_{\alpha}(\ell), & \ell_2 < \hat{x}_2
\end{array} \right.
$$

$$
= \left\{ \begin{array}{ll}
u_{\beta}(\ell + \rho) - u_{\alpha}(\ell), & \ell_2 > \hat{x}_2, \ell_2 + \rho_2 > \hat{x}_2 \\
u_{\beta}(\ell + \rho - b_{12}) - u_{\alpha}(\ell), & \ell_2 > \hat{x}_2, \ell_2 + \rho_2 < \hat{x}_2 \\
u_{\beta}(\ell + b_{12} + \rho) - u_{\alpha}(\ell), & \ell_2 < \hat{x}_2, \ell_2 + \rho_2 > \hat{x}_2 \\
u_{\beta}(\ell + \rho) - u_{\alpha}(\ell), & \ell_2 < \hat{x}_2, \ell_2 + \rho_2 < \hat{x}_2
\end{array} \right.
$$

$$
= \left\{ \begin{array}{ll}
u_{0}(\ell + \rho) - u_{0}(\ell) + p_{\beta}(\ell + \rho) - p_{\beta}(l) + p_{\beta}(l) - p_{\alpha}(\ell), & \ell_2 > \hat{x}_2, \ell_2 + \rho_2 > \hat{x}_2 \\
u_{0}(\ell + \rho - b_{12}) - u_{0}(\ell) + p_{\beta}(\ell + \rho - b_{12}) - p_{\beta}(l) + p_{\beta}(l) - p_{\alpha}(\ell), & \ell_2 > \hat{x}_2, \ell_2 + \rho_2 < \hat{x}_2 \\
u_{0}(\ell + b_{12} + \rho) - u_{0}(\ell) + p_{\beta}(\ell + b_{12} + \rho) - p_{\beta}(l) + p_{\beta}(l) - p_{\alpha}(\ell), & \ell_2 < \hat{x}_2, \ell_2 + \rho_2 > \hat{x}_2 \\
u_{0}(\ell + \rho) - u_{0}(\ell) + p_{\beta}(\ell + \rho) - p_{\beta}(l) + p_{\beta}(l) - p_{\alpha}(\ell), & \ell_2 < \hat{x}_2, \ell_2 + \rho_2 < \hat{x}_2
\end{array} \right.
$$

$$
= \left\{ \begin{array}{ll}
(Su)_{0}(\ell + \rho) - (Su)_{0}(\ell) + (Sp)_{\beta}(\ell + \rho) - (Sp)_{\beta}(l) + p_{\beta}(l) - p_{\alpha}(\ell), & \ell_2 > \hat{x}_2, \ell_2 + \rho_2 > \hat{x}_2 \\
(Su)_{0}(\ell + \rho) - (Su)_{0}(\ell) + (Sp)_{\beta}(\ell + \rho) - (Sp)_{\beta}(l) + p_{\beta}(l) - p_{\alpha}(\ell), & \ell_2 > \hat{x}_2, \ell_2 + \rho_2 < \hat{x}_2 \\
(Su)_{0}(\ell + b_{12} + \rho) - (Su)_{0}(\ell + b_{12}) + (Sp)_{\beta}(l + b_{12} + \rho) - (Sp)_{\beta}(l + b_{12}) + p_{\beta}(l) - p_{\alpha}(\ell), & \ell_2 < \hat{x}_2, \ell_2 + \rho_2 > \hat{x}_2 \\
(Su)_{0}(\ell + b_{12} + \rho) - (Su)_{0}(\ell + b_{12}) + (Sp)_{\beta}(l + b_{12} + \rho) - (Sp)_{\beta}(l + b_{12}) + p_{\beta}(l) - p_{\alpha}(\ell), & \ell_2 < \hat{x}_2, \ell_2 + \rho_2 < \hat{x}_2
\end{array} \right.
$$

$$
= \left\{ \begin{array}{ll}
D_{\rho}(Su)_{0}(\ell) + D_{\rho}(Sp)_{\beta}(l) + p_{\beta}(l) - p_{\alpha}(\ell), & \ell_2 > \hat{x}_2 \\
D_{\rho}(Su)_{0}(\ell + b_{12}) + D_{\rho}(Sp)_{\beta}(l + b_{12}) + p_{\beta}(l) - p_{\alpha}(\ell), & \ell_2 < \hat{x}_2
\end{array} \right.
$$

$$
= RD_{\rho}(Su)_{0}(\ell) + RD_{\rho}(Sp)_{\beta}(l) + p_{\beta}(l) - p_{\alpha}(\ell) = \tilde{D}_{\rho} u_{0}(\ell) + \tilde{D}_{\rho} p_{\beta}(l) + p_{\beta}(l) - p_{\alpha}(\ell).
$$
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