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REGULARITY AND LOCALITY OF POINT DEFECTS IN MULTILATTICES

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Abstract. We formulate a model for a point defect embedded in a homogeneous multilattice crystal with an empirical interatomic potential interaction. Under a natural, phonon stability assumption we quantify the decay of the long-range elastic fields with increasing distance from the defect.

These decay estimates are an essential ingredient in quantifying approximation errors in coarse-grained models and in the construction of optimal numerical methods for approximating crystalline defects.

1. Introduction

The mechanical and electrical properties of crystalline materials are heavily influenced by defects in the crystalline lattice [25]. These range from point defects (the subject of the present work) including vacancies, interstitials, impurities; line defects including the preeminent dislocation; planar defects including grain boundaries; and many others including cracks and voids. Modeling each of these defects relies in some form on resolving the long-range elastic fields generated by the defects. Whether this is accomplished via an empirical potential, continuum PDE, or multiscale method, all of these approximations rely on *decay and regularity* of the elastic fields sufficiently far away from the defect. For example, a key use of these decay rates is in establishing rigorous asymptotic results for atomistic-to-continuum methods for multilattices [21]. These decay rates have long been known in the engineering and materials community from elasticity theory [8, 2, 10] and computational techniques [12, 9, 15, 28, 10], and can in fact be thought of as a means of classifying defects [17, 11]. While related mathematical results for the decay of scalar potential fields in a linearized model defined on a lattice were obtained in [18], the first mathematical result for proving these decay rates for an empirical atomistic model of point defects and dislocations in Bravais lattices appeared only recently in [7] .

The present work is an extension of [7] to multilattices, which are crystals with more than one atom per unit cell. Multilattice descriptions allow for a much greater swath of materials to be considered including hcp metals, diamond cubic structures, and the recently discovered two dimensional materials, graphene and hexagonal boron-nitride, among several others [20]. For the sake of simplicity of presentation, we only consider point defects in the present paper; however, there do not seem to be major obstacles in combining the analysis for point defects presented here with that of dislocations for Bravais lattices in [7] to also obtain analogous results for dislocations in multilattices.

The method of obtaining these decay rates for point defects in multilattices is similar to that of Bravais lattices; we show that the point defect solution satisfies a linearized equation and then convert L^1 integrability of the solution in Fourier space into algebraic decay in real

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space. These integrability conditions are determined from the Green's matrix of the linearized problem. Herein lies the main difference between the Bravais lattice and multilattice cases: the Green's matrix for a multilattice accounts for relative shifts between atoms in each unit cell which leads to a different structure than in the Bravais lattice case.

In Theorem 4 we recover the result from the Bravais lattice case [7] that the discrete strain field decays at a rate of r^{-d} where d is space dimension and r is the distance from the defect. The additional new result is that the relative shifts (which are indeed also a form of strain) also decay at a rate of r^{-d}.

In the process of proving this result, we also establish a convenient connection between phonon stability and stability in a natural discrete energy-norm, extending an analogous observation for Bravais lattices [7]. This in particular leads to a simplified proof of the fact [6] that atomistic stability (phonon stability) implies stability of the Cauchy–Born continuum model (see also [13]).

Outline. We begin by introducing the notation for formulating the atomistic defect problem on a multilattice and the assumptions required of the atomistic potential in Section 2. Our main result, Theorem 4, is also presented there. We divide the proof of Theorem 4 into two sections. In Section 3, we review the required facts of the Fourier transform and state them in the specificity and version required for the application at hand. Section 3 also reviews the multilattice Cauchy–Born model and proves that atomistic stability implies Cauchy–Born stability, closely mirroring the approach of [13]. Section 4 subsequently provides the linearized equation that the point defect satisfies, gives an expression for the Green's matrix associated to this equation, and then proves our main result.

2. Model and Main Results

A multilattice is a union of shifted Bravais lattices: we fix $\mathsf{F} \in \mathbb{R}^{d\times d}$ with $\det(\mathsf{F}) = 1$, $d \in \{2,3\}$ and $p_0, \dots, p_{S-1} \in \mathbb{R}^d$ with $p_0 = 0$ and define a multilattice $\mathcal{M}$ by

$$\mathcal{M} := \bigcup_{\alpha=0}^{S-1} \left(\mathsf{F}\mathbb{Z}^d + p_\alpha\right).$$

The set $\mathsf{F}\mathbb{Z}^d$ is a Bravais lattice and comprises the set of *sites* in the lattice; we denote it by $\mathcal{L} := \mathsf{F}\mathbb{Z}^d$. (The conditions $\det(\mathsf{F}) = 1$ and $p_0 = 0$ are merely for convenience of notation and do not restrict the generality of the analysis.) Deformations and displacements of atoms of species α at site $\xi \in \mathcal{L}$ are, respectively, denoted by $y_\alpha(\xi) : \mathbb{R}^d \to \mathbb{R}^n$ and $u_\alpha(\xi) : \mathbb{R}^d \to \mathbb{R}^n$, where we permit $n = d$ or $n = d+1$ when $d = 2$. The set of all S deformations and displacements are denoted by $\boldsymbol{y}(\xi) : \mathcal{L}^S \to \mathbb{R}^n$ and $\boldsymbol{u}(\xi) : \mathcal{L}^S \to \mathbb{R}^n$ where $\mathcal{L}^S = \mathcal{L} \times \cdots \times \mathcal{L}$.

To describe interactions between atoms, we define a finite difference notation (on either deformations or displacements) indexed by

$$D_{(\rho\alpha\beta)}\boldsymbol{u}(\xi) := u_\beta(\xi+\rho) - u_\alpha(\xi), \qquad \text{where} \\ (\rho\alpha\beta) \in \mathcal{L} \times \{0,\dots,S-1\} \times \{0,\dots,S-1\}.$$

The collection of finite differences describing the interaction of a site ξ is denoted by

$$D\boldsymbol{u}(\xi) := \left(D_{(\rho\alpha\beta)}\boldsymbol{u}(\xi)\right)_{(\rho\alpha\beta)\in\mathcal{R}},$$

where $\mathcal{R} \subset \mathcal{L} \times \{0, \dots, S-1\} \times \{0, \dots, S-1\} \setminus \bigcup_{\alpha=0}^{S-1} \{(0\alpha\alpha)\}$ is a finite interaction range satisfying the conditions

$$\mathrm{span}\{\rho \,|\, (\rho\alpha\alpha) \in \mathcal{R}\} = \mathbb{R}^d \text{ for all } \alpha \in \mathcal{S}, \tag{2.1}$$

$$(0\alpha\beta) \in \mathcal{R} \quad \text{for all } \alpha \neq \beta \in \mathcal{S}\ . \tag{2.2}$$

These two conditions, as well as a further condition (3.1) are made for convenience of notation but do not restrict generality since we can always enlarge the interaction range $\mathcal{R}$ to satisfy them. For future reference, we denote the projection of $\mathcal{R}$ onto the lattice component by

$$\mathcal{R}_1 := \big\{\rho \in \mathcal{L} \,|\, \exists (\rho\alpha\beta) \in \mathcal{R}\big\}$$

and finite differences on individual displacements, u_α, by

$$D_\rho u_\alpha(\xi) := u_\alpha(\xi + \rho) - u_\alpha(\xi), \quad Du_\alpha(\xi) := \big(D_\rho u_\alpha(\xi)\big)_{\rho \in \mathcal{R}_1}.$$

We assume that the atomistic energy may be written (formally) as a sum of site potentials,

$$\hat{\mathcal{E}}^{\mathrm{a}}(\boldsymbol{y}) := \sum_{\xi \in \mathcal{L}} \hat{V}_\xi(D\boldsymbol{y}(\xi)),$$

where the site potential, $\hat{V}_\xi$, is assumed to satisfy:

V.1 There exists $R_{\mathrm{def}} > 0$ such that for all $|\xi| \geq R_{\mathrm{def}}$, $\hat{V}_\xi \equiv \hat{V}$ does not depend on ξ. This assumption is valid for point defects located near the origin.

For the atomistic energy functional to be well-defined (i.e. finite), we will consider an energy difference functional defined on displacements, $\boldsymbol{u}$, from a reference state, $\boldsymbol{y}(\xi)$, which is defined differently depending on whether $d = n$ or not. When $d = n$, which models bulk crystals, we set

$$y_\alpha(\xi) = \xi + p_\alpha,$$

where each $p_\alpha \in \mathbb{R}^d$. If $d = 2$ and $n = 3$, which is the case when modeling monolayer materials such as graphene, then we set

$$y_\alpha(\xi) = \begin{pmatrix} \xi \\ 0 \end{pmatrix} + \begin{pmatrix} p_\alpha \\ 0 \end{pmatrix}.$$

In the latter case, we will drop the third component being equal to zero under the understanding that $\xi, p_\alpha \in \mathbb{R}^d$ are considered as elements in $\mathbb{R}^n$ in this fashion. Thus, ξ, p_α may either denote vectors in $\mathbb{R}^d$ or $\mathbb{R}^n$, but it will always be clear from the context what we mean.

This energy difference functional is defined by

$$\mathcal{E}^{\mathrm{a}}(\boldsymbol{u}) := \sum_{\xi \in \mathcal{L}} V_\xi(D\boldsymbol{u}(\xi)), \quad V_\xi(D\boldsymbol{u}) := \hat{V}_\xi(D\boldsymbol{y} + D\boldsymbol{u}) - \hat{V}(D\boldsymbol{y}). \tag{2.3}$$

An auxiliary energy functional needed in the subsequent analysis is the energy of the homogeneous (defect-free) lattice

$$\mathcal{E}^{\mathrm{a}}_{\mathrm{hom}}(\boldsymbol{u}) := \sum_{\xi \in \mathcal{L}} V(D\boldsymbol{u}(\xi)), \qquad V(D\boldsymbol{u}) := \hat{V}(D\boldsymbol{y} + D\boldsymbol{u}) - \hat{V}(D\boldsymbol{y}).$$

Arguments of the site potentials are indexed by $(\rho\alpha\beta) \in \mathcal{R}$. Given $(\rho\alpha\beta), (\tau\gamma\delta) \in \mathcal{R}$ and $\boldsymbol{g} = (\boldsymbol{g}_{(\rho\alpha\beta)})_{(\rho\alpha\beta)\in\mathcal{R}} \in (\mathbb{R}^n)^{\mathcal{R}}$, we will denote derivatives of V_ξ (or $\hat{V}_\xi$) by

$$\begin{aligned}
[V_{\xi,(\rho\alpha\beta)}(\boldsymbol{g})]_i &:= \frac{\partial V_\xi(\boldsymbol{g})}{\partial \boldsymbol{g}^i_{(\rho\alpha\beta)}}, \quad i = 1, \dots, n, \\
V_{\xi,(\rho\alpha\beta)}(\boldsymbol{g}) &:= \frac{\partial V_\xi(\boldsymbol{g})}{\partial \boldsymbol{g}_{(\rho\alpha\beta)}}, \\
[V_{\xi,(\rho\alpha\beta)(\tau\gamma\delta)}(\boldsymbol{g})]_{ij} &:= \frac{\partial^2 V_\xi(\boldsymbol{g})}{\partial \boldsymbol{g}^j_{(\tau\gamma\delta)} \partial \boldsymbol{g}^i_{(\rho\alpha\beta)}}, \quad i, j = 1, \dots, n, \\
V_{\xi,(\rho\alpha\beta)(\tau\gamma\delta)}(\boldsymbol{g}) &:= \frac{\partial^2 V_\xi(\boldsymbol{g})}{\partial \boldsymbol{g}_{(\tau\gamma\delta)} \partial \boldsymbol{g}_{(\rho\alpha\beta)}},
\end{aligned}$$

with higher order derivatives defined analogously. Moreover, it will later be notationally convenient to consider derivatives with $(\rho\alpha\beta) \notin \mathcal{R}$, in which case

$$V_{\xi,(\rho\alpha\beta)}(\boldsymbol{g}) = 0,$$

and so on for higher order derivatives. With this notation, the site potential is additionally assumed to satisfy the following differentiability assumption:

V.2 Each $\hat{V}_\xi : (\mathbb{R}^n)^{\mathcal{R}} \to \mathbb{R}$ is four times continuously differentiable with uniformly bounded derivatives.

The function space on which $\mathcal{E}^{\mathrm{a}}$ will be defined is a quotient space of a set of discrete displacements having a finite "energy" norm,

$$\|\boldsymbol{u}\|^2_{\mathrm{a}_1} := \sum_{\xi\in\mathcal{L}} |D\boldsymbol{u}(\xi)|^2_{\mathcal{R}}, \qquad \text{where } |D\boldsymbol{u}|^2_{\mathcal{R}} := \sum_{(\rho\alpha\beta)\in\mathcal{R}} |D_{(\rho\alpha\beta)}\boldsymbol{u}(\xi)|^2.$$

In view of (2.1) and (2.2), $\|\boldsymbol{u}\|_{\mathrm{a}_1} = 0$ if and only if there exists $v \in \mathbb{R}^n$ such that $u_\alpha = v$ for all $\alpha = 0, \dots, S-1$.

Because of the translation invariance of $\mathcal{E}^{\mathrm{a}}(\boldsymbol{u})$ we will define it on the quotient space

$$\boldsymbol{\mathcal{U}} := \mathcal{U}/\mathbb{R}^n, \qquad \text{where} \quad \mathcal{U} := \left\{\boldsymbol{u} : \mathcal{L}^S \to \mathbb{R}^n, \|\boldsymbol{u}\|_{\mathrm{a}_1} < \infty\right\}.$$

Proving that $\mathcal{E}^{\mathrm{a}}$ is well defined on this space will rely on density of the space of compactly supported test functions, $\boldsymbol{\mathcal{U}}_0$, defined by

$$\begin{aligned}
\mathcal{U}_0 &:= \{\boldsymbol{u} \in \mathcal{U} : Du_0, u_\alpha - u_0 \text{ have compact support for each } \alpha\}, \\
\boldsymbol{\mathcal{U}}_0 &:= \mathcal{U}_0/\mathbb{R}^n.
\end{aligned}$$

It is straightforward to establish that $\boldsymbol{\mathcal{U}}_0$ is dense in $\boldsymbol{\mathcal{U}}$; see Lemma 18 for a proof.

It is clear that $\mathcal{E}^{\mathrm{a}}$ and $\mathcal{E}^{\mathrm{a}}_{\mathrm{hom}}$ are well-defined on $\boldsymbol{\mathcal{U}}_0$ since only finitely many summands will be nonzero in this case. Our choice of function space, $\boldsymbol{\mathcal{U}}$, is justified in the following theorem, and we will prove below in Lemma 9 that the hypothesis of the theorem is in fact equivalent to the lattice energy per unit volume being minimized over the internal shifts. This implies, in particular that (2.4) is straightforward to enforce in practical computations.

Theorem 1. *If the reference configuration $\boldsymbol{y}$ with $y_\alpha(\xi) = \xi + p_\alpha$ is an equilibrium of the defect free energy, that is,*

$$\sum_{\xi\in\mathcal{L}} \sum_{(\rho\alpha\beta)\in\mathcal{R}} \hat{V}_{,(\rho\alpha\beta)}(D\boldsymbol{y}(\xi)) \cdot D\boldsymbol{v}(\xi) = 0, \quad \forall \boldsymbol{v} \in \boldsymbol{\mathcal{U}}_0, \tag{2.4}$$

then the energy functionals, $\mathcal{E}^{\rm a}_{\rm hom}(\boldsymbol{u})$ and $\mathcal{E}^{\rm a}(\boldsymbol{u})$, can be uniquely extended to continuous functions on $\boldsymbol{\mathcal{U}}$ which are well-defined and C^3 on $\boldsymbol{\mathcal{U}}$.

Remark 2. The proof of Theorem 1 is based on the idea that, for $\boldsymbol{u} \in \boldsymbol{\mathcal{U}}_0$, $\mathcal{E}^{\rm a}_{\rm hom}(\boldsymbol{u}) = \bar{\mathcal{E}}^{\rm a}_{\rm hom}(\boldsymbol{u}))$, where

$$\bar{\mathcal{E}}^{\rm a}_{\rm hom}(\boldsymbol{u}) := \sum_{\xi\in\mathcal{L}} \big[V(D\boldsymbol{u}(\xi)) - \sum_{(\rho\alpha\beta)\in\mathcal{R}} V_{,(\rho\alpha\beta)}(D\boldsymbol{y}(\xi)) \cdot D_{(\rho\alpha\beta)}\boldsymbol{u}(\xi)\big].$$

While $\mathcal{E}^{\rm a}_{\rm hom}$ is well-defined only if $D\boldsymbol{u} \in \ell^1$, $\bar{\mathcal{E}}^{a}_{\rm hom}$ is also well-defined for $D\boldsymbol{u} \in \ell^2$. However, since $\bar{\mathcal{E}}^{\rm a}_{\rm hom}$ is the unique continuous extension of $\mathcal{E}^{\rm a}_{\rm hom}$ from $\boldsymbol{\mathcal{U}}_0$ to $\boldsymbol{\mathcal{U}}$ we will continually use $\mathcal{E}^{\rm a}(\boldsymbol{u})_{\rm hom}$ (and $\mathcal{E}^{\rm a}(\boldsymbol{u})$) in lieu of $\bar{\mathcal{E}}^{\rm a}(\boldsymbol{u})$ (and an analogously defined $\bar{\mathcal{E}}^{\rm a}$).

□

Having established that $\mathcal{E}^{\rm a}(\boldsymbol{u})$ is well-defined on the natural energy space $\boldsymbol{\mathcal{U}}$, we are interested in the force equilibrium problem

$$\langle \delta\mathcal{E}^{\rm a}(\boldsymbol{u}^\infty), \boldsymbol{v}\rangle = 0, \qquad \forall\, \boldsymbol{v} \in \boldsymbol{\mathcal{U}}_0. \tag{2.5}$$

Two important special cases are local minima (stable equilibria) and index-1 saddles (transition states between stable equilibria). In the present work we will not go into details about these specific problems but focus on the regularity of equilibria, i.e., solutions to (2.5).

Our analysis requires only the following standing assumption:

Assumption A. *(1) The reference configuration, $\boldsymbol{y}$, with $y_\alpha(\xi) = \xi + p_\alpha$ is a stable equilibrium of $\mathcal{E}^{\rm a}_{\rm hom}$, that is, in addition to* (2.4) *we require that there exists $\gamma_{\rm a} > 0$ such that*

$$\langle \delta^2\mathcal{E}^{\rm a}_{\rm hom}(0)\boldsymbol{v}, \boldsymbol{v}\rangle \geq \gamma_{\rm a}\|\boldsymbol{v}\|^2_{\rm a_1}, \quad \forall\, \boldsymbol{v} \in \boldsymbol{\mathcal{U}}_0. \tag{2.6}$$

(2) There exists a solution $\boldsymbol{u}^\infty \in \boldsymbol{\mathcal{U}}$ to (2.5).

Remark 3. Note that Assumption A imposes no additional structure on solutions $\boldsymbol{u}^\infty$ but only on the reference state. Physically, the requirement (2.6) is a minimal assumption on the stability of lattice waves, called *phonon stability*, made throughout the solid state physics literature [3], and is almost universally reasonable.

Moreover, one can readily show (see Lemma 19 in the appendix or [7, Section 2.2] for a related result for Bravais lattices) that, if there exists *any* stable equilibrium of $\mathcal{E}^{\rm a}$, then (2.6) holds as well. □

The decay rates we prove in Theorem 4 below are formulated in terms of the finite difference notation

$$D_\rho u_\alpha(\xi) := u_\alpha(\xi+\rho) - u_\alpha(\xi) \qquad \text{for } \rho \in \mathcal{L}, \quad \alpha \in \mathcal{S}, \qquad \text{and}$$
$$D_{\boldsymbol{\rho}} u_\alpha(\xi) := D_{\rho_1}D_{\rho_2}\cdots D_{\rho_k}u_\alpha(\xi) \qquad \text{for } \boldsymbol{\rho} = (\rho_1,\ldots,\rho_k) \in \mathcal{L}^k.$$

We interpret the finite differences $D_\rho u$ as an "atomistic strain" and the higher order differences as discrete strain gradients.

Theorem 4 (Decay of Displacements and Shifts). *Suppose that Assumption A holds and set $U^\infty = u_0^\infty, p_\alpha^\infty = u_\alpha^\infty - u_0^\infty$. Then*

$$\begin{aligned} \big|D_{\boldsymbol{\rho}}U^\infty(\xi)\big| &\lesssim (1+|\xi|)^{1-d-j}, \quad \forall \boldsymbol{\rho} \in (\mathcal{R}_1)^j, 1 \leq j \leq 3, \quad \textit{and} \\ \big|D_{\boldsymbol{\rho}}p_\alpha^\infty(\xi)\big| &\lesssim (1+|\xi|)^{-d-j}, \quad \forall \boldsymbol{\rho} \in (\mathcal{R}_1)^j, 0 \leq j \leq 2. \end{aligned} \tag{2.7}$$

In the statement of the theorem, we have used the modified Vinogradov notation $A \lesssim B$ to mean there exists a constant $c > 0$ such that $A \leq cB$. The implied constant here (and throughout the remainder of the paper) is allowed to depend upon the interatomic potential, interaction range, and stability constant $\gamma_{\rm a}$.

The rest of the paper is devoted to proving Theorem 4. We will first exhibit a linearized equation which $\boldsymbol{u}^\infty$ satisfies and prove decay rates for the Green's function associated with this linearized problem. The key point in proving the decay rates for the Green's function will be connecting L^1 integrability of a function's Fourier transform with L^∞ decay of the original function. Meanwhile, the L^1 estimates in Fourier space are obtained by comparing the atomistic Green's function with the *Cauchy–Born* continuum Green's function.

Remark 5 (Other point defects). Although superficially we have only included an impurity defect in defining our model energy, Theorem 4 actually applies to arbitrary point defects, including for example vacancies and interstitials.

To see this, consider a defective lattice, $\mathcal{L}^{\rm def}$, with a "defect core radius," $R_{\rm def}$, such that $\mathcal{L} \setminus B_{R_{\rm def}} = \mathcal{L}^{\rm def} \setminus B_{R_{\rm def}}$, and let $u^{\rm def} : \mathcal{L}^{\rm def} \to \mathbb{R}^n$ be an equilibrium of an energy functional analogous to $\mathcal{E}^{\rm a}$, in particular employing the same homogeneous potential V in $\mathcal{L} \setminus B_{R_{\rm def}}$. Then, projecting $u^{\rm def}$ to a displacement $u : \mathcal{L} \to \mathbb{R}^n$ with $u(\xi) = u^{\rm def}(\xi)$ in $\mathcal{L} \setminus B_{R_{\rm def}}$, we obtain a new displacement satisfying

$$\frac{\partial \mathcal{E}^{\rm a}_{\rm hom}(u)}{\partial u_\alpha(\xi)} = 0, \qquad \forall\, |\xi| \geq R'_{\rm def},$$

for some $R'_{\rm def} \geq 0$ but potentially non-zero forces in $B_{R'_{\rm def}}$. By defining $V_\xi(Du) = V(Du) + \boldsymbol{g}_\xi \cdot Du$ with suitable $\boldsymbol{g} \in (\mathbb{R}^n)^{\mathcal{R}}$ for $\xi \in B_{R_{\rm def}}$, we are put precisely in the context of Theorem 4, and thus the decay estimates again apply. $\square$

3. Preliminaries

In this section we collect a range of auxiliary results that are required in the proof of Theorem 4.

3.1. Continuous interpolants of lattice functions.

It is often useful to identify lattice functions with continuous interpolants. To define these, we divide the unit cell $\mathsf{F}[0,1]^d$ into simplices (triangles in $2D$ and tetrahedra in $3D$) so that each vertex of a simplex is one of the vertices of $\mathsf{F}[0,1]^d$. A simplicial decomposition, $\mathcal{T}_{\rm a}$, of $\mathcal{L}$ is completed by performing the same decomposition on the translated cells $\xi + \mathsf{F}[0,1]^d$ for $\xi \in \mathcal{L}$. Note that this can be done in such a way that $\mathcal{T}_{\rm a}$ is *regular*.

For $u : \mathcal{L} \to \mathbb{R}^n$, we then denote the continuous interpolant of u with respect to $\mathcal{T}_{\rm a}$ by Iu. We will also write $I\boldsymbol{u} = (Iu_\alpha)_{\alpha=0}^{S-1}$. By possibly enlarging $\mathcal{R}$ we may assume without loss of generality that

$$\text{if } \operatorname{conv}\{\xi, \xi + \rho\} \text{ is an edge of } \mathcal{T}_{\rm a}, \text{ then } \rho \in \mathcal{R}_1. \tag{3.1}$$

This construction gives rise to a natural alternative norm for multilattice displacements,

$$\|\boldsymbol{u}\|_{{\rm a}_2} := \|\nabla I u_0\|_{L^2(\mathbb{R}^d)} + \sum_{\alpha=0}^{S-1} \|Iu_\alpha - Iu_0\|_{L^2(\mathbb{R}^d)},$$

which turns out to be equivalent to $\|\cdot\|_{\mathrm{a}_1}$.

Lemma 6. *The norms, $\|\cdot\|_{\mathrm{a}_1}$ and $\|\cdot\|_{\mathrm{a}_2}$, are equivalent on the set of multilattice displacements $\boldsymbol{u} : \mathcal{L}^S \to \mathbb{R}^n$.*

Proof. From (3.1) it is clear that $\|\cdot\|_{\mathrm{a}_2} \lesssim \|\cdot\|_{\mathrm{a}_1}$. To prove the opposite, let $\omega := \bigcup\{T \in \mathcal{T}_{\mathrm{a}} | T \cap \mathcal{R}_1 \neq \emptyset\}$ (the minimal patch of elements T covering the interaction neighbourhood), then

$$|D\boldsymbol{u}(\xi)|^2 \le C\Big(\|\nabla I u_0\|^2_{L^2(\xi+\omega)} + \textstyle\sum_\alpha \|I u_\alpha - I u_0\|^2_{L^2(\xi+\omega)}\Big). \tag{3.2}$$

This follows from the fact that both sides of the inequality involve only finitely many degrees of freedom and, if the right-hand side vanishes, then so does the left-hand side.

The stated result now follows by summing (3.2) over $\mathcal{L}$. □

3.2. **Semi-discrete Fourier transform for multilattices.** The first Brillouin zone, $\mathcal{B}$, is defined as the Voronoi cell associated with the origin in the dual lattice, $\mathsf{B}\mathbb{Z}^d$, with $\mathsf{B} = \mathsf{F}^{-\top}$. For a lattice function $u : \mathcal{L} \to \mathbb{R}^n$, the semidiscrete Fourier transform, and its inverse are, respectively, defined by

$$\hat{u}(k) = \sum_{\xi\in\mathcal{L}} e^{-2\pi i \xi\cdot k} u(\xi), \quad \text{for } k \in \mathcal{B}, \qquad \check{v}(\xi) = \int_{\mathcal{B}} e^{2\pi i \xi\cdot k} v(k)\, dk, \quad \text{for } \xi \in \mathcal{L}.$$

As usual, the discrete Fourier transform is well-defined for $\ell^1(\mathcal{L})$ functions and otherwise defined through continuity.

The semidiscrete Fourier transform (and its inverse) possesses the usual transform properties; for the task at hand, the most important of these is the connection between L^1 integrability of a function's (semidiscrete) Fourier transform and its derivatives and the L^∞ decay of the original function and its derivatives.

As the first Brillouin zone is a finite domain, and many of the fields involved will be either smooth or only singular at the origin, we will be most concerned with the behavior of the Fourier transform near the origin. For this reason, we introduce a "big O notation"

$$f(k) = \mathcal{O}(g(k)) \quad \text{if and only if} \quad \exists\, C > 0 \text{ s.t. } |f(k)| \le C|g(k)| \text{ for all } k \in \mathcal{B},$$

which is modified from the standard notation in that we require the upper bound in the entire domain of definition $\mathcal{B}$.

Theorem 7. *Suppose that $f : \mathcal{L} \to \mathbb{R}^n$ is a function such that $\hat{f}, \nabla\hat{f}, \cdots, \nabla^m \hat{f} \in L^1(\mathcal{B})$, then*

$$|f(\xi)| \lesssim (1 + |\xi|)^{-m}, \quad \forall\, \xi \in \mathcal{L}.$$

Proof. The proof uses standard techniques and while related results exist throughout the literature [29, 26], we were unable to find a statement of the specificity that we require here, hence we include a proof for convenience and completeness.

Let γ be any multiindex with $|\gamma| \le m$. Then using the fact that

$$(\partial_\gamma \hat{f})^\vee(\xi) = \int_{\mathcal{B}} e^{2\pi i \xi\cdot k} \partial_\gamma \hat{f}(k)\, dk = (2\pi i)^{|\gamma|} \xi^\gamma \int_{\mathcal{B}} e^{2\pi i \xi\cdot k} \hat{f}(k) = (2\pi i)^{|\gamma|} \xi^\gamma f(\xi)$$

and

$$\|f\|_{\ell^\infty} \le \|\hat{f}\|_{L^1},$$

we see that
$$(2\pi)^{|\gamma|}\|\xi^\gamma f(\xi)\|_{\ell^\infty} = \|(2\pi i)^{|\gamma|}\xi^\gamma f(\xi)\|_{\ell^\infty} \leq \ \|\partial_\gamma \hat{f}\|_{L^1}.$$
This in turn implies $|\xi|^m f(\xi)$ is bounded. □

Since we will later employ Taylor expansions in Fourier space along with operating with finite differences, a useful (and almost immediate) corollary of this result is the following.

Corollary 8. *Let $f : \mathcal{L} \to \mathbb{R}^n$, and assume there is an integer $s \geq -1$ such that $\nabla^j \hat{f}(k) = \mathcal{O}(k^{s-j})$ for all nonnegative integers j. Then*
$$|D_{\boldsymbol{\rho}} f(\xi)| \lesssim (1+|\xi|)^{-s-d+1-t} \qquad \textit{for} \quad \xi \in \mathcal{L}, \quad \boldsymbol{\rho} \in (\mathcal{R}_1)^t, \quad t \geq 0.$$

Proof. Let $\boldsymbol{\rho} = \rho_1 \cdots \rho_t \in (\mathcal{R}_1)^t$. By Theorem 7, to prove the stated decay, it is sufficient to show that
$$\nabla^j \widehat{D_{\boldsymbol{\rho}} f}(k) \in L^1(\mathcal{B}) \qquad \text{for} \quad j = 0, \dots, t+s+d-1.$$
To that end we first note that
$$\widehat{D_{\boldsymbol{\rho}} f}(k) = (e^{2\pi i k\cdot\rho_1} - 1)(e^{2\pi i k\cdot\rho_2} - 1)\cdots(e^{2\pi i k\cdot\rho_t} - 1)\hat{f}.$$
Next, we observe that
$$\nabla^j\big((e^{2\pi i k\cdot\rho_1} - 1)(e^{2\pi i k\cdot\rho_2} - 1)\cdots(e^{2\pi i k\cdot\rho_t} - 1)\big) = \mathcal{O}(k^{t-j}) \quad \text{for } j \geq 0,$$
while $\nabla^j \hat{f}(k) = \mathcal{O}(k^{s-j})$ for $j \geq 0$ by assumption. Therefore,
$$\int_{\mathcal{B}} \Big|\nabla^j\big((e^{2\pi i k\cdot\rho_1} - 1)(e^{2\pi i k\cdot\rho_2} - 1)\cdots(e^{2\pi i k\cdot\rho_t} - 1)\big)\hat{f}\Big|\, dk \lesssim \int_{B_R(0)} |k|^{t+s-j}\, dk.$$
Hence, $\widehat{D_{\boldsymbol{\rho}} f}(k) \in L^1(\mathcal{B})$ provided $t+s-j+d-1 > -1$. This last statement is true for $0 \leq j \leq t+s+d-1$, and we obtain the desired result. □

3.3. **The multilattice Cauchy–Born model.** The next ingredient for our analysis is the Cauchy–Born energy functional. We will later compare the Hessian of a linearized atomistic model with that of the Cauchy–Born Hessian in order to glean information about the atomistic Green's matrix from the Cauchy–Born Green's matrix. The Cauchy–Born energy functional was originally proposed by Cauchy for Bravais lattices [4] and was later extended to multilattices [3]. The fundamental idea behind the original Cauchy rule for Bravais lattices was that the atomistic and continuum kinematics could be related by assuming that a continuum strain affected the atomistic model by straining the lattice basis vectors as if they were part of the continuous medium [4]. The adaptation of this to multilattices proceeded by further assuming that the relative shifts between atoms inside each unit cell were equilibrated [3].

For our purposes, we will introduce both the classical Cauchy–Born energy for multilattices, and a variant used in [16, 21], which maintains the relative shifts in each unit cell as degrees of freedom in the energy functional. Throughout this section, we will employ the displacement-shift kinematic description of the multilattice. That is, we define a base displacement at each Bravais lattice site by $U(\xi) = u_0(\xi)$ and then define the relative shifts within each unit cell by $p_\alpha(\xi) = u_\alpha(\xi) - u_0(\xi)$ and $\boldsymbol{p} = (p_0, \dots, p_{S-1})$. In this notation, the "non-classical" variant of the Cauchy–Born strain energy density functional is defined for $\mathsf{G} \in \mathbb{R}^{n\times d}$ and $\boldsymbol{p} \in \mathbb{R}^n$ by
$$\hat{W}(\mathsf{G}, \boldsymbol{p}) := \hat{V}\big((\mathsf{G}\rho + p_\beta - p_\alpha)_{(\rho\alpha\beta)\in\mathcal{R}}\big),$$

and for $U \in \mathrm{C}^1(\mathbb{R}^d, \mathbb{R}^n)$ and $p_\alpha \in \mathrm{C}^0(\mathbb{R}^d, \mathbb{R}^n)$ by

$$W((U, \boldsymbol{p})) := V\big((\nabla_\rho U + p_\beta - p\alpha)_{(\rho\alpha\beta)\in\mathcal{R}}\big).$$

The Cauchy–Born continuum energy is then, formally, defined by

$$\mathcal{E}^{\mathrm{c}}(U, \boldsymbol{p}) = \int_{\mathbb{R}^d} W((U, \boldsymbol{p}))\, dx.$$

The classical variant of the Cauchy–Born rule [3] additionally enforces that the shifts in each unit cell are equilibrated in the sense that the energy in each unit cell is minimized. Thus, it defines a strain energy density functional on $\mathbb{R}^{n\times d}$ by

$$\bar{W}(\mathsf{G}) := \min_{\boldsymbol{p}\in(\mathbb{R}^d)^S} \hat{V}\big((\mathsf{G}\rho + p_\beta - p\alpha)_{(\rho\alpha\beta)\in\mathcal{R}}\big). \tag{3.3}$$

A useful relation between the classical Cauchy–Born rule and the atomistic model is that minimizing $\hat{V}$ with respect to the shifts in each unit cell is equivalent to the equilibrium condition that we used in Theorem 1 to show that $\mathcal{E}^{\mathrm{a}}$ is well-defined.

Lemma 9. *Recall the multilattice is defined by* $\mathcal{M} := \bigcup_{\alpha=0}^{S-1}\big(\mathsf{F}\mathbb{Z}^d + p_\alpha\big)$*, and let* $\boldsymbol{y}$ *be the reference deformation defined by* $y_\alpha(\xi) = \xi + p_\alpha$*. If* $d = n$*, then set* $\mathsf{G} = I_{d\times d} \in \mathbb{R}^{d\times d}$*, and if* $d \neq n$*, set* $\mathsf{G} = \begin{pmatrix} I_{d\times d} \\ \boldsymbol{0} \end{pmatrix}$ *and consider each* $p_\alpha \in \mathbb{R}^d$ *to be in* $\mathbb{R}^n$ *via* $p_\alpha = \begin{pmatrix} p_\alpha \\ 0 \end{pmatrix}$*. Then the following two conditions are equivalent:*

$$\begin{aligned} &\partial_{\boldsymbol{p}} \hat{W}(\mathsf{G}, \boldsymbol{p}) = \partial_{\boldsymbol{p}} \hat{V}\big((\mathsf{G}\rho + p_\beta - p_\alpha)_{(\rho\alpha\beta)\in\mathcal{R}}\big) = 0, \qquad \textit{and} \\ &\sum_{\xi\in\mathcal{L}} \sum_{(\rho\alpha\beta)\in\mathcal{R}} \hat{V}_{,(\rho\alpha\beta)}(D\boldsymbol{y}(\xi)) \cdot D_{(\rho\alpha\beta)}\boldsymbol{v}(\xi) = 0, \qquad \forall\, \boldsymbol{v} \in \boldsymbol{\mathcal{U}}_0. \end{aligned}$$

Proof. We define the test function $\boldsymbol{v}$ by $v_\gamma(\zeta) = 1$, $v_\gamma(\xi) = 0$ for $\xi \neq \zeta$, and $v_\beta(\xi) = 0$ for all $\beta \neq \gamma$. Then a straightforward computation (see Appendix A.4) yields

$$\langle \mathcal{E}^{\mathrm{a}}_{\mathrm{hom}}(\boldsymbol{0}), \boldsymbol{v}\rangle = \partial_{p_\gamma} \hat{W}(\mathsf{G}, \boldsymbol{p}), \tag{3.4}$$

which implies that the result. □

Another relation between the Cauchy–Born rule and the atomistic model is the fact that the stability assumption, Assumption A, implies an analogous stability condition for the Cauchy–Born energy functional.

For the purpose of proving this auxiliary result, we temporarily consider a finite continuum domain $\Omega = (-1/2, 1/2]^d$, a corresponding finite atomistic domain

$$\Omega_\epsilon := \{-1/2 + \epsilon, -1/2 + 2\epsilon, \cdots, 1/2 - \epsilon, 1/2\}^d,$$

associated atomistic and continuum energies, and appropriate norms defined by

$$\mathcal{E}^{\rm a}_\epsilon(\boldsymbol{u}^\epsilon) := \epsilon^d \sum_{\xi\in\Omega_\epsilon} V_\xi(D^\epsilon \boldsymbol{u}^\epsilon) \quad \text{where} \quad D^\epsilon_{(\rho\alpha\beta)}\boldsymbol{u}^\epsilon(\xi) := \frac{u^\epsilon_\beta(\xi+\epsilon\rho) - u^\epsilon_\alpha(\xi)}{\epsilon}$$

$$\|\boldsymbol{u}^\epsilon\|^2_{\mathrm{a},\epsilon} = \|\nabla I_\epsilon u^\epsilon_0\|^2_{L^2(\Omega)} + \sum_{\alpha=0}^{S-1} \epsilon^{-2}\|I_\epsilon u^\epsilon_\alpha - I_\epsilon u^\epsilon_0\|^2_{L^2(\Omega)}, \qquad \text{and}$$

$$\mathcal{E}^{\rm c}_\Omega(U,\boldsymbol{p}) = \int_\Omega V\Big((\nabla_\rho U(x) + p_\beta(x) - p_\alpha(x))_{(\rho\alpha\beta)\in\mathcal{R}}\Big)\,dx,$$

$$\|(U,\boldsymbol{p})\|^2_{\mathrm{c},\Omega} := \|\nabla U\|^2_{L^2(\Omega)} + \sum_{\alpha=0}^{S-1} \|p_\alpha - p_0\|^2_{L^2(\Omega)},$$

$$\|(U,\boldsymbol{p})\|^2_{\mathrm{c},\mathbb{R}^d} := \|\nabla U\|^2_{L^2(\mathbb{R}^d)} + \sum_{\alpha=0}^{S-1} \|p_\alpha - p_0\|^2_{L^2(\mathbb{R}^d)}.$$

We will evaluate $\mathcal{E}^{\rm c}_\Omega$ only for $(U,\boldsymbol{p}) \in C^1_{\rm per}(\Omega) \times (C_{\rm per}(\Omega))^{S-1}$, where per denotes periodic functions. For such fields $(U,\boldsymbol{p})$ we define the corresponding atomistic fields

$$u^\epsilon_\alpha(\xi) = U(\xi) + \epsilon p_\alpha(\xi) \quad \text{and} \quad \boldsymbol{u}^\epsilon = (u^\epsilon_\alpha)_{\alpha=0}^{S-1}. \tag{3.5}$$

The next result is a scaled variant of [16, Proposition 3.1], proven by a straightforward Taylor expansion.

Lemma 10. *Let $U \in C^3(\Omega), p_\alpha \in C^2(\Omega)$, and $\boldsymbol{u}^\epsilon$ given by (3.5). Then there exists a constant C, independent of ϵ, such that*

$$|\mathcal{E}^{\rm a}_\epsilon(\boldsymbol{u}^\epsilon) - \mathcal{E}^{\rm c}_\Omega((U,\boldsymbol{p}))| \le C\epsilon.$$

Arguing as in [14, Lemma 3.2], Lemma 10 implies convergence of hessians. The proof requires only minor adjustments.

Lemma 11. *Let $Z \in \mathrm{C}^3(\Omega), q_\alpha \in \mathrm{C}^2(\Omega)$ and $\boldsymbol{z}^\epsilon$ define analogously to (3.5), then*

$$\langle \delta^2\mathcal{E}^{\rm a}_\epsilon(0)\boldsymbol{z}^\epsilon, \boldsymbol{z}^\epsilon\rangle - \langle \delta^2\mathcal{E}^{\rm c}_\Omega(0)(Z,\boldsymbol{q}),(Z,\boldsymbol{q})\rangle \to 0, \quad \textit{as } \epsilon \to 0.$$

We have now assembled the necessary prerequisites to prove that atomistic stability, Assumption A, implies stability of the Cauchy–Born model.

Theorem 12 (Cauchy–Born Stability). *Suppose $Z \in H^1_{\rm loc}(\mathbb{R}^d,\mathbb{R}^n), q_\alpha \in L^2(\mathbb{R}^d,\mathbb{R}^n)$ with $\nabla Z, q_\alpha$ having compact support. Then there exists $\gamma_{\rm c} > 0$ such that*

$$\big\langle \delta^2\mathcal{E}^{\rm c}(0)(Z,\boldsymbol{q}),(Z,\boldsymbol{q})\big\rangle \ge \gamma_{\rm c}\big\|(Z,\boldsymbol{q})\big\|^2_{\mathrm{c},\mathbb{R}^d}. \tag{3.6}$$

Proof. This proof largely follows the Bravais lattice case [13]; the main additional step is the correct choice of rescaling the shifts.

Suppose $(Z, \boldsymbol{q})$ is supported in $B_{R/2}$. Rescaling $Z_R(x) := R^{-1}Z(Rx)$ and $q_{R,\alpha}(x) := q_\alpha(Rx)$, we obtain that $(Z_R, \boldsymbol{q}_R)$ has support contained in $B_{1/2}(0)$, while

$$\big\langle \delta^2\mathcal{E}^{\rm c}(0)(Z,\boldsymbol{q}),(Z,\boldsymbol{q})\big\rangle = R^d\big\langle \delta^2\mathcal{E}^{\rm c}(0)(Z_R,\boldsymbol{q}_R),(Z_R,\boldsymbol{q}_R)\big\rangle, \quad \text{and}$$
$$\|(Z,\boldsymbol{q})\|^2_{{\rm c},\mathbb{R}^d} = R^d\|(Z_R,\boldsymbol{q}_R)\|^2_{{\rm c},\Omega}.$$

In particular, stability for $(Z, \boldsymbol{q})$ implies stability for $(Z_R, \boldsymbol{q}_R)$ and vice-versa, that is, we drop the subscript R and assume, without loss of generality, that $(Z, \boldsymbol{q})$ has support in $B_{1/2}$. Moreover, by density of smooth functions we may also assume that $(Z, \boldsymbol{q}) \in {\rm C}^3 \times ({\rm C}^2)^{S-1}$.

We can now interpret $(Z, \boldsymbol{q})$ as periodic with respect to the domain Ω and, for $N \in \mathbb{N}$, $\epsilon := 1/N$, let $\boldsymbol{z}^\epsilon$ be the corresponding periodic atomistic test function defined via (3.5). Then, Lemma 11 implies

$$\big|\langle \delta^2\mathcal{E}^{\rm a}_\epsilon(0)\boldsymbol{z}^\epsilon,\boldsymbol{z}^\epsilon\rangle - \langle \delta^2\mathcal{E}^{\rm c}_\Omega(0)(Z,\boldsymbol{q}),(Z,\boldsymbol{q})\rangle\big| \to 0 \quad \text{as } N\to\infty. \tag{3.7}$$

From standard finite element interpolation error estimates we can deduce that

$$\|\boldsymbol{z}^\epsilon\|_{{\rm a},\epsilon} \to \|(Z,\boldsymbol{q})\|_{{\rm c},\Omega} \quad \text{as } N\to\infty \quad (\epsilon\to 0). \tag{3.8}$$

We now rescale $\boldsymbol{z}_N(\xi) := N\boldsymbol{z}^\epsilon(\xi/N)$ if $\xi/N \in \Omega$ and $\boldsymbol{z}_N(\xi) = 0$ otherwise. Assumption A and norm equivalence, Lemma A.6, then imply

$$\begin{aligned} 0 < \gamma_{\rm a}' \le \frac{\langle \delta^2\mathcal{E}^{\rm a}(0)\boldsymbol{z}_N,\boldsymbol{z}_N\rangle}{\|\boldsymbol{z}_N\|^2_{{\rm a}_2}} &= \frac{\langle \delta^2\mathcal{E}^{\rm a}_\epsilon(0)\boldsymbol{z}^\epsilon,\boldsymbol{z}^\epsilon\rangle}{\|\boldsymbol{z}^\epsilon\|^2_{{\rm a},\epsilon}} \\ &\to \frac{\langle \delta^2\mathcal{E}^{\rm c}_\Omega(0)(Z,\boldsymbol{q}),(Z,\boldsymbol{q})\rangle}{\|(Z,\boldsymbol{q})\|^2_{{\rm c},\Omega}} \qquad \text{as } N\to\infty, \end{aligned}$$

where we have used (3.7) and (3.8) in the final line. Finally, for $(Z, \boldsymbol{q})$ supported in Ω we have

$$\frac{\langle \delta^2\mathcal{E}^{\rm c}_\Omega(0)(Z,\boldsymbol{q}),(Z,\boldsymbol{q})\rangle}{\|(Z,\boldsymbol{q})\|^2_{{\rm c},\Omega}} = \frac{\langle \delta^2\mathcal{E}^{\rm c}(0)(Z,\boldsymbol{q}),(Z,\boldsymbol{q})\rangle}{\|(Z,\boldsymbol{q})\|^2_{{\rm c},\mathbb{R}^d}},$$

which completes the proof. □

3.4. **Lattice Green's function.** Having established the basic facts of the Fourier transform and Cauchy–Born model that we require, we now turn towards deriving the lattice Green's function to which we will apply these facts. Applying the standard *continuous* Fourier transform on $\mathbb{R}^d$ to both sides of (3.6) and applying the Plancherel theorem, we obtain

$$\begin{aligned} \gamma_{\rm c}\Big(\int_{\mathbb{R}^d} 4\pi^2|k|^2|\hat{Z}(k)|^2 + \sum_{\alpha=0}^{S-1}|\hat{q}_\alpha(k)|^2\,dk\Big) &\le \big\langle \delta^2\mathcal{E}^{\rm c}(0)(Z,\boldsymbol{q}),(Z,\boldsymbol{q})\big\rangle \\ &= \int_{\mathbb{R}^d}\begin{pmatrix}\hat{Z}^*\\ \hat{\boldsymbol{q}}^*\end{pmatrix}\begin{pmatrix}J_{00}(k) & J_{0\boldsymbol{p}}(k)\\ J^*_{0\boldsymbol{p}}(k) & J_{\boldsymbol{pp}}(k)\end{pmatrix}\begin{pmatrix}\hat{Z}\\ \hat{\boldsymbol{q}}\end{pmatrix}dk, \end{aligned}$$

where

$$
\begin{aligned}
J_{00}(k) &:= \sum_{(\rho\alpha\beta)\in\mathcal{R}} \sum_{(\tau\gamma\delta)\in\mathcal{R}} 4\pi^2(\tau\cdot k)V_{,(\rho\alpha\beta)(\tau\gamma\delta)}(0)(\rho\cdot k)\\
[J_{0\boldsymbol{p}}(k)]_\beta &:= \sum_{\rho\in\mathcal{R}_1}\sum_{\alpha=0}^{S-1}\sum_{(\tau\gamma\delta)\in\mathcal{R}} -2\pi i(k\cdot\tau)\big[V_{,(\rho\alpha\beta)(\tau\gamma\delta)}(0) - V_{,(\rho\beta\alpha)(\tau\gamma\delta)}(0)\big],\\
J_{\boldsymbol{p}0} &= J_{0\boldsymbol{p}}^*\\
[J_{\boldsymbol{pp}}(k)]_{\beta\delta} &:= \sum_{\rho,\tau\in\mathcal{R}_1}\sum_{\alpha,\gamma=0}^{S-1}\big[V_{,(\rho\alpha\beta)(\tau\gamma\delta)}(0) + V_{,(\rho\beta\alpha)(\tau\delta\gamma)}(0) - V_{,(\rho\beta\alpha)(\tau\gamma\delta)}(0) \qquad (3.9)\\
&\qquad\qquad - V_{,(\rho\alpha\beta)(\tau\delta\gamma)}(0)\big],\\
J^{-1}(k) &:= \begin{pmatrix} M^{-1} & -M^{-1}J_{0\boldsymbol{p}}J_{\boldsymbol{pp}}^{-1}\\ -J_{\boldsymbol{pp}}^{-1}J_{\boldsymbol{p}0}M^{-1} & J_{\boldsymbol{pp}}^{-1}J_{\boldsymbol{p}0}M^{-1}J_{0\boldsymbol{p}}J_{\boldsymbol{pp}}^{-1} + J_{\boldsymbol{pp}}^{-1}\end{pmatrix}, \text{ where}\\
M &:= J_{00} - J_{0\boldsymbol{p}}J_{\boldsymbol{pp}}^{-1}J_{\boldsymbol{p}0}. \qquad (3.10)
\end{aligned}
$$

By taking the test pair with $\boldsymbol{q} = \boldsymbol{0}$, we see that this implies

$$\gamma_{\rm c}\Big(\int_{\mathbb{R}^d} 4\pi^2|k|^2|\hat{Z}(k)|^2\,dk\Big) \le \int_{\mathbb{R}^d}\hat{Z}^*J_{00}(k)\hat{Z}\,dk,$$

and in particular we obtain

$$J_{00}(k) \ge \gamma_{\rm c}4\pi^2|k|^2 I_{n\times n} \qquad \text{for } k\in\mathbb{R}^d\setminus\{0\}.$$

In a similar fashion, by testing with pairs having $Z = 0$, we see that

$$\gamma_{\rm c}\Big(\int_{\mathbb{R}^d}\sum_{\alpha=0}^{S-1}|\hat{q}_\alpha(k)|^2\,dk\Big) \le \int_{\mathbb{R}^d}\hat{\boldsymbol{q}}^*J_{\boldsymbol{pp}}\hat{\boldsymbol{q}}\,dk,$$

where $J_{\boldsymbol{pp}}$ is symmetric and independent of k, hence

$$J_{\boldsymbol{pp}} \ge \gamma_{\rm c}I_{(S-1)n\times(S-1)n}.$$

Next, we note that $M = J_{00} - J_{0\boldsymbol{p}}J_{\boldsymbol{pp}}^{-1}J_{\boldsymbol{p}0}$ is the Schur complement of $J_{\boldsymbol{pp}}$ in J. [27, Theorem 5] or [31, Corollary 2.3] imply that the eigenvalues of M interlace those of J, so in particular we obtain that $M(k) \ge c|k|^2$ for some $c > 0$. Letting $\mathrm{A}_{ijkl} := \frac{\partial\bar{W}(\mathsf{G})}{\partial\mathsf{G}_{ij}\partial\mathsf{G}_{kl}}$ with G defined as in Lemma 9, we obtain

$$\int_{\mathbb{R}^d}\mathrm{A}_{ijkl}Z_{i,j}Z_{k,l}\,dx =: \int_{\mathbb{R}^d}\mathrm{A} : \nabla Z : \nabla Z\,dx = \int_{\mathbb{R}^d}\hat{Z}^*M\hat{Z}\,dk \gtrsim \|\nabla Z\|^2_{\mathbb{R}^d}. \qquad (3.11)$$

The proof of (3.11), presented in § A.5, is a tedious algebraic manipulation, the key observation being that $\partial_{\boldsymbol{p}}\hat{W}((\mathsf{F},\boldsymbol{p})) = 0$, which we have proven holds in Lemma 9 since we assume the reference configuration is in equilibrium.

It follows from (3.11) that A satisfies the Legendre–Hadamard ellipticity condition. We can therefore apply [19, Equation 6.2.15] to obtain bounds on the Green's matrix for the linearized continuum elasticity operator.

Lemma 13. *Let M be defined by* (3.10)*. Then the Green's function, $\check{M}(x)$, for the differential operator* $\operatorname{div}\big(\mathrm{A}\nabla\cdot\big)$ *satisfies the decay rates*

$$|\nabla^j\check{M}(x)| \lesssim (1+|x|)^{2-d-j}. \qquad (3.12)$$

4. Proof of Theorem 4

To prove our main result, Theorem 4, we first linearize the equilibrium equation (2.5) about the ground state. We then use the decay estimate (3.12) for the Cauchy–Born Green's function to obtain a corresponding estimate for the atomistic Green's function. This will then allow us to prove the decay rates for the displacements and shifts stated in Theorem 4.

4.1. **Linearized Equation.** The linearized equation that $\boldsymbol{u}^\infty$ satisfies is formed by linearizing the defect-free energy $\mathcal{E}^{\rm a}_{\rm hom}$ about the reference state $\boldsymbol{u} = \boldsymbol{0}$. The key point in this linearization is that the residual is quadratic in terms of the defect solution.

Theorem 14. *There exists* $f : \mathcal{L} \to (\mathbb{R}^n)^{\mathcal{R}}$ *such that*

$$\langle \delta^2 \mathcal{E}^{\rm a}_{\rm hom}(0)\boldsymbol{u}^\infty, \boldsymbol{v}\rangle = \sum_{\xi\in\mathcal{L}} \sum_{(\rho\alpha\beta)\in\mathcal{R}} f_{(\rho\alpha\beta)}(\xi)\cdot D_{(\rho\alpha\beta)}\boldsymbol{v}(\xi) =: \langle f, D\boldsymbol{v}\rangle, \quad \forall\, \boldsymbol{v}\in\boldsymbol{\mathcal{U}}_0, \tag{4.1}$$

$$\text{where} \quad |f(\xi)|_{\mathcal{R}} \lesssim |D\boldsymbol{u}^\infty(\xi)|^2_{\mathcal{R}} \qquad \text{for } |\xi| \geq R_{\rm def}. \tag{4.2}$$

Proof. By (2.4), $\langle \delta\mathcal{E}^{\rm a}_{\rm hom}(0), \boldsymbol{v}\rangle = 0$ for all $\boldsymbol{v}\in\boldsymbol{\mathcal{U}}_0$. Hence

$$\begin{aligned}
\langle \delta^2 \mathcal{E}^{\rm a}_{\rm hom}(0)\boldsymbol{u}^\infty, \boldsymbol{v}\rangle &= \langle \delta^2 \mathcal{E}^{\rm a}_{\rm hom}(0)\boldsymbol{u}^\infty, \boldsymbol{v}\rangle - \langle \delta\mathcal{E}^{\rm a}_{\rm hom}(\boldsymbol{u}^\infty), \boldsymbol{v}\rangle + \langle \delta\mathcal{E}^{\rm a}_{\rm hom}(\boldsymbol{u}^\infty), \boldsymbol{v}\rangle \\
&= \Big\{\langle \delta^2 \mathcal{E}^{\rm a}_{\rm hom}(0)\boldsymbol{u}^\infty, \boldsymbol{v}\rangle + \langle \delta\mathcal{E}^{\rm a}_{\rm hom}(0), \boldsymbol{v}\rangle - \langle \delta\mathcal{E}^{\rm a}_{\rm hom}(\boldsymbol{u}^\infty), \boldsymbol{v}\rangle\Big\} + \langle \delta\mathcal{E}^{\rm a}_{\rm hom}(\boldsymbol{u}^\infty), \boldsymbol{v}\rangle \\
&= -L_1[\boldsymbol{u}^\infty, \boldsymbol{v}] + \langle \delta\mathcal{E}^{\rm a}_{\rm hom}(\boldsymbol{u}^\infty), \boldsymbol{v}\rangle,
\end{aligned}$$

where L_1 is a linearization residual of the form

$$L_1[\boldsymbol{u}^\infty, \boldsymbol{v}] := \sum_{\xi\in\mathcal{L}} \left\langle \frac{1}{2}\int_0^1 \delta^3 V(tD\boldsymbol{u}^\infty(\xi))[(1-t)D\boldsymbol{u}^\infty(\xi), (1-t)D\boldsymbol{u}^\infty(\xi)], D\boldsymbol{v}(\xi)\right\rangle dt. \tag{4.3}$$

Next, note that $\langle \delta\mathcal{E}^{\rm a}(\boldsymbol{u}^\infty), \boldsymbol{v}\rangle = 0$ for all test functions $\boldsymbol{v}$ since $\boldsymbol{u}^\infty$ is a critical point of $\mathcal{E}^a$, and recall that $V_\xi \equiv V$ for $|\xi| \geq R_{\rm def}$. Thus,

$$\begin{aligned}
\langle \delta\mathcal{E}^{\rm a}_{\rm hom}(\boldsymbol{u}^\infty), \boldsymbol{v}\rangle &= \langle \delta\mathcal{E}^{\rm a}_{\rm hom}(\boldsymbol{u}^\infty), \boldsymbol{v}\rangle - \langle \delta\mathcal{E}^{\rm a}(\boldsymbol{u}^\infty), \boldsymbol{v}\rangle \\
&= \sum_{\xi\in\mathcal{L}\cap B_{R_{\rm def}}(0)} \Big\langle \delta V(D\boldsymbol{u}^\infty(\xi)) - \delta V(D\boldsymbol{u}^\infty(\xi)), D\boldsymbol{v}(\xi)\Big\rangle
\end{aligned} \tag{4.4}$$

Combining (4.3) and (4.4), we define

$$\begin{aligned}
&f_{(\rho\alpha\beta)}(\xi) \\
&= \begin{cases} \tfrac{1}{2}\int_0^1 \delta^3 V(t\boldsymbol{u}^\infty(\xi))[(1-t)\boldsymbol{u}^\infty(\xi), (1-t)\boldsymbol{u}^\infty(\xi)]\,dt \\ \qquad + V_{,(\rho\alpha\beta)}(D\boldsymbol{u}^\infty(\xi)) - V_{\xi,(\rho\alpha\beta)}(D\boldsymbol{u}^\infty(\xi)), \quad \text{if} \quad \xi\in B_{R_{\rm def}}(0), \\ \tfrac{1}{2}\int_0^1 \delta^3 V(t\boldsymbol{u}^\infty(\xi))[(1-t)\boldsymbol{u}^\infty(\xi), (1-t)\boldsymbol{u}^\infty(\xi)]\,dt, \quad \text{if} \quad \xi\notin B_{R_{\rm def}}(0), \end{cases}
\end{aligned}$$

and note that $f_{(\rho\alpha\beta)}(\xi)$ satisfies the desired bounds since $B_{R_{\rm def}}(0)$ is finite and since the third derivative of V is bounded by our assumptions on the site potential. □

4.2. **Dynamical Matrix and Green's Function.** We now construct a Green's function representation for the solution of the linearized equation (4.2) so we convert it to an equation in Fourier space. We rewrite the left-hand side in real space in terms of the displacements $U^\infty := u_0^\infty$ and $Z := v_0$ and the shifts $p_\alpha^\infty := u_\alpha^\infty - u_0^\infty$ and $q_\alpha := v_\alpha - v_0$,

$$\begin{aligned}\langle \delta^2 \mathcal{E}^{\rm a}_{\rm hom}(0)\boldsymbol{u}^\infty, \boldsymbol{v}\rangle &= \sum_{\xi\in\mathcal{L}} \sum_{(\rho\alpha\beta)\in\mathcal{R}} \sum_{(\tau\gamma\delta)\in\mathcal{R}} [D_{(\tau\gamma\delta)}\boldsymbol{v}(\xi)]^T V_{,(\rho\alpha\beta)(\tau\gamma\delta)}(0)[D_{(\rho\alpha\beta)}\boldsymbol{u}^\infty(\xi)] \\ &= \sum_{\xi\in\mathcal{L}} \sum_{(\rho\alpha\beta)\in\mathcal{R}} \sum_{(\tau\gamma\delta)\in\mathcal{R}} [v_\delta(\xi+\tau) - v_\gamma(\xi)]^T V_{,(\rho\alpha\beta)(\tau\gamma\delta)}(0)[u^\infty_\beta(\xi+\rho) - u^\infty_\alpha(\xi)] \\ &= \sum_{\xi\in\mathcal{L}} \sum_{(\rho\alpha\beta)\in\mathcal{R}} \sum_{(\tau\gamma\delta)\in\mathcal{R}} [Z(\xi+\tau) - Z(\xi) + q_\delta(\xi+\tau) - q_\gamma(\xi)]^T V_{,(\rho\alpha\beta)(\tau\gamma\delta)}(0) \\ &\qquad \big[U^\infty(\xi+\rho) - U^\infty(\xi) + p^\infty_\beta(\xi+\rho) - p^\infty_\alpha(\xi)\big],\end{aligned}$$

and then use the Plancherel Theorem to obtain

$$\begin{aligned}&\langle \delta^2 \mathcal{E}^{\rm a}_{\rm hom}(0)\boldsymbol{u}^\infty, \boldsymbol{v}\rangle \\ &= \int_{\mathcal{B}} \sum_{(\rho\alpha\beta)\in\mathcal{R}} \sum_{(\tau\gamma\delta)\in\mathcal{R}} \big[(e^{2\pi i k\cdot\tau} - 1)\hat{Z}(k) + e^{2\pi i k\cdot\tau}\hat{q}_\delta(k) - \hat{q}_\gamma(k)\big]^* V_{,(\rho\alpha\beta)(\tau\gamma\delta)}(0) \\ &\qquad \big[(e^{2\pi i k\cdot\rho} - 1)\hat{U}^\infty(k) + e^{2\pi i k\cdot\rho}\hat{p}^\infty_\beta(k) - \hat{p}^\infty_\alpha(k)\big] \\ &= \int_{\mathcal{B}} \sum_{(\rho\alpha\beta)\in\mathcal{R}} \sum_{(\tau\gamma\delta)\in\mathcal{R}} [(e^{2\pi i k\cdot\tau} - 1)\hat{Z}(k)]^* V_{,(\rho\alpha\beta)(\tau\gamma\delta)}(0)[(e^{2\pi i k\cdot\rho} - 1)\hat{U}^\infty(k)] \\ &\quad + \int_{\mathcal{B}} \sum_{(\rho\alpha\beta)\in\mathcal{R}} \sum_{(\tau\gamma\delta)\in\mathcal{R}} [(e^{2\pi i k\cdot\tau} - 1)\hat{Z}(k)]^* V_{,(\rho\alpha\beta)(\tau\gamma\delta)}(0)[e^{2\pi i k\cdot\rho}\hat{p}^\infty_\beta(k) - \hat{p}^\infty_\alpha(k)] \\ &\quad + \int_{\mathcal{B}} \sum_{(\rho\alpha\beta)\in\mathcal{R}} \sum_{(\tau\gamma\delta)\in\mathcal{R}} [e^{2\pi i k\cdot\tau}\hat{q}_\delta(k) - \hat{q}_\gamma(k)]^* V_{,(\rho\alpha\beta)(\tau\gamma\delta)}(0)[(e^{2\pi i k\cdot\rho} - 1)\hat{U}^\infty(k)] \\ &\quad + \int_{\mathcal{B}} \sum_{(\rho\alpha\beta)\in\mathcal{R}} \sum_{(\tau\gamma\delta)\in\mathcal{R}} [e^{2\pi i k\cdot\tau}\hat{q}_\delta(k) - \hat{q}_\gamma(k)]^* V_{,(\rho\alpha\beta)(\tau\gamma\delta)}(0)[e^{2\pi i k\cdot\rho}\hat{p}^\infty_\beta(k) - \hat{p}^\infty_\alpha(k)].\end{aligned} \tag{4.5}$$

In analogy to the Cauchy–Born Hessian, we now define

$$\begin{aligned}H_{00}(k) &:= \sum_{(\rho\alpha\beta)\in\mathcal{R}} \sum_{(\tau\gamma\delta)\in\mathcal{R}} (e^{-2\pi i k\cdot\tau} - 1)V_{,(\rho\alpha\beta)(\tau\gamma\delta)}(0)(e^{2\pi i k\cdot\rho} - 1), \\ [H_{0\boldsymbol{p}}(k)]_\beta &:= \sum_{\rho\in\mathcal{R}_1} \sum_{\alpha=0}^{S-1} \sum_{(\tau\gamma\delta)\in\mathcal{R}} [(e^{-2\pi i k\cdot\tau} - 1)V_{,(\rho\alpha\beta)(\tau\gamma\delta)}(0)(e^{2\pi i k\cdot\rho}) - (e^{-2\pi i k\cdot\tau} - 1)V_{,(\rho\beta\alpha)(\tau\gamma\delta)}(0)], \\ [H_{\boldsymbol{p}0}(k)]_\delta &:= \sum_{\tau\in\mathcal{R}_1} \sum_{\gamma=0}^{S-1} \sum_{(\rho\alpha\beta)\in\mathcal{R}} [(e^{-2\pi i k\cdot\tau})V_{,(\rho\alpha\beta)(\tau\gamma\delta)}(0)(e^{2\pi i k\cdot\rho} - 1) - V_{,(\rho\alpha\beta)(\tau\delta\gamma)}(0)(e^{2\pi i k\cdot\rho} - 1)], \\ [H_{\boldsymbol{pp}}(k)]_{\beta\delta} &:= \sum_{\rho,\tau\in\mathcal{R}_1} \sum_{\alpha,\gamma=0}^{S-1} \Big[e^{-2\pi i k\cdot\tau}V_{,(\rho\alpha\beta)(\tau\gamma\delta)}(0)e^{2\pi i k\cdot\rho} + V_{,(\rho\beta\alpha)(\tau\delta\gamma)}(0) - e^{-2\pi i k\cdot\tau}V_{,(\rho\beta\alpha)(\tau\gamma\delta)}(0) \\ &\qquad -e^{2\pi i k\cdot\rho}V_{,(\rho\alpha\beta)(\tau\delta\gamma)}(0)\Big],\end{aligned}$$

and note that the matrix

$$H(k) := \begin{bmatrix} H_{00}(k) & H_{0\boldsymbol{p}}(k) \\ H_{\boldsymbol{p}0}(k) & H_{\boldsymbol{pp}}(k) \end{bmatrix}, \tag{4.6}$$

known as the *dynamical matrix* [30], is Hermitian due to $V^{ij}_{,(\rho\alpha\beta)(\tau\gamma\delta)}(0) = V^{ji}_{,(\tau\gamma\delta)(\rho\alpha\beta)}(0)$.

We may now rewrite (4.5) succinctly as

$$\langle \delta^2 \mathcal{E}^{\mathrm{a}}_{\mathrm{hom}}(0)\boldsymbol{u}^\infty, \boldsymbol{v}\rangle = \int_{\mathcal{B}} \begin{bmatrix} \hat{Z}(k) \\ \hat{\boldsymbol{q}}(k) \end{bmatrix}^* H(k) \begin{bmatrix} \hat{U}^\infty(k) \\ \hat{\boldsymbol{p}}^\infty(k) \end{bmatrix} dk. \tag{4.7}$$

In order to give Assumption A an interpretation in terms of H, we introduce a third norm $\|\cdot\|_{\mathrm{a}_3}$ defined for $\boldsymbol{v} \equiv (Z, \boldsymbol{q})$ by

$$\|\boldsymbol{v}\|^2_{\mathrm{a}_3} = \|(Z,\boldsymbol{q})\|^2_{\mathrm{a}_3} := \|2\pi|k|\hat{Z}\|^2_{L^2(\mathcal{B})} + \sum_{\alpha=1}^{S-1} \|\hat{p}_\alpha\|^2_{L^2(\mathcal{B})}.$$

We show in § A.6 that $\|\cdot\|_{\mathrm{a}_3}$ is equivalent to $\|\cdot\|_{\mathrm{a}_2}$ (and hence $\|\cdot\|_{\mathrm{a}_1}$). We then use Assumption A and (4.7) to produce

$$\|(Z,\boldsymbol{q})\|^2_{\mathrm{a}_3} \lesssim \langle \delta^2 \mathcal{E}^{\mathrm{a}}_{\mathrm{hom}}(0)\boldsymbol{v}, \boldsymbol{v}\rangle = \int_{\mathcal{B}} \begin{bmatrix} \hat{Z}(k) \\ \hat{\boldsymbol{q}}(k) \end{bmatrix}^* H(k) \begin{bmatrix} \hat{Z}(k) \\ \hat{\boldsymbol{q}}(k) \end{bmatrix} dk. \tag{4.8}$$

If $\boldsymbol{q} = \boldsymbol{0}$, then (4.8) translates to

$$4\pi^2 \int_{\mathcal{B}} |k|^2 |\hat{Z}(k)|^2\, dk \lesssim \int_{\mathcal{B}} \hat{Z}(k)^* H_{00}(k)\hat{Z}(k)\, dk, \tag{4.9}$$

while if $Z = 0$, (4.8) implies

$$\int_{\mathcal{B}} |\hat{q}(k)|^2\, dk \lesssim \int_{\mathcal{B}} \hat{\boldsymbol{q}}(k)^* H_{\boldsymbol{pp}}(k)\hat{\boldsymbol{q}}(k)\, dk. \tag{4.10}$$

As the inequalities (4.9) and (4.10) are valid for all test functions, it follows that the spectra $\omega_0(k)$ of $H_{00}(k)$ and $\omega_{\boldsymbol{p}}(k)$ of $H_{\boldsymbol{pp}}(k)$ satisfy the bounds

$$\begin{aligned} |k|^2 &\lesssim \omega_0(k) \\ 1 &\lesssim \omega_{\boldsymbol{p}}(k), \end{aligned} \tag{4.11}$$

and in particular that $H_{00}(k)$ and $H_{\boldsymbol{pp}}(k)$ are positive definite for $k \neq 0$.

Remark 15. Since H_{00} and $H_{\boldsymbol{pp}}$ are principal submatrices of H, the Cauchy Interlacing Theorem, the spectral estimates (4.11), and Assumption A imply that there exist three positive eigenvalues, $\lambda^1_{\mathrm{a}}(k), \lambda^2_{\mathrm{a}}(k), \lambda^3_{\mathrm{a}}(k)$, of H which satisfy

$$k^2 \lesssim \lambda^i_{\mathrm{a}}(k) \lesssim k^2 \tag{4.12}$$

and $S \cdot n - 3$ positive eigenvalues, λ^i_{o}, of H which satisfy

$$\lambda^i_{\mathrm{o}} \gtrsim 1. \tag{4.13}$$

These are precisely the (squares of) frequencies associated with the *acoustic* (λ^i_{a}) and *optical* (λ^i_{o}) phonon branches of the crystal [30]. Comparing Assumption A to [6, Assumption A], it thus follows that Assumption A implies the bounds on the acoustic and optical phonon frequencies stated in [6, Assumption A]. Moreover, using the norm equivalence between $\|\cdot\|_{\mathrm{a}_1}, \|\cdot\|_{\mathrm{a}_2}$, and $\|\cdot\|_{\mathrm{a}_3}$ along with [6, Section 6], the same assumptions on the acoustical and optical frequencies can be used to show Assumption A is satisfied so that the two assumptions are in fact equivalent. □

Returning to (4.2), the right-hand side in Fourier space becomes

$$
\begin{aligned}
\langle f, Dv\rangle &= \sum_{(\rho\alpha\beta)\in\mathcal{R}} \sum_{\xi\in\mathcal{L}} f_{(\rho\alpha\beta)}(\xi)\cdot D_{(\rho\alpha\beta)}v(\xi) \\
&= \sum_{(\rho\alpha\beta)\in\mathcal{R}} \int_{\mathcal{B}} \Big[(e^{2\pi i k\cdot\rho}-1)\hat{Z}(k) + e^{2\pi i k\cdot\rho}\hat{q}_\beta(k) - \hat{q}_\alpha(k)\Big]^* \hat{f}_{\rho\alpha\beta}(k) \\
&= \sum_{(\rho\alpha\beta)\in\mathcal{R}} \int_{\mathcal{B}} [(e^{2\pi i k\cdot\rho}-1)\hat{Z}(k)]^* \hat{f}_{(\rho\alpha\beta)}(k) + \sum_{(\rho\alpha\beta)} \int_{\mathcal{B}} [e^{2\pi i k\cdot\rho}\hat{q}_\beta(k) - \hat{q}_\alpha(k)]^* \hat{f}_{(\rho\alpha\beta)}(k) \\
&=: \int_{\mathcal{B}} \begin{bmatrix}\hat{Z}(k)\\ \hat{\boldsymbol{q}}(k)\end{bmatrix}^* \begin{bmatrix}F(k)\\ \boldsymbol{g}(k)\end{bmatrix},
\end{aligned}
$$

where

$$
\begin{aligned}
F(k) &= \sum_{(\rho\alpha\beta)\in\mathcal{R}} (e^{-2\pi i k\cdot\rho}-1)\hat{f}_{(\rho\alpha\beta)}(k), \\
g_\eta(k) &= \sum_{(\rho\alpha\eta)\in\mathcal{R}} e^{-2\pi i k\cdot\rho}\hat{f}_{(\rho\alpha\eta)} - \sum_{(\rho\eta\beta)\in\mathcal{R}} \hat{f}_{(\rho\eta\beta)}.
\end{aligned}
\tag{4.14}
$$

In summary, we have shown the following result.

Theorem 16. *Let $\boldsymbol{u}^\infty = (U^\infty, \boldsymbol{p}^\infty)$ be as in Assumption A. With $H(k), F(k)$, and $\boldsymbol{g}(k)$ as defined in* (4.6) *and* (4.14)*, $(U^\infty, \boldsymbol{p}^\infty)$ satisfies the linear system*

$$
H(k)\begin{bmatrix}\hat{U}^\infty(k)\\ \hat{\boldsymbol{p}}^\infty(k)\end{bmatrix} = \begin{bmatrix}F(k)\\ \boldsymbol{g}(k)\end{bmatrix}. \tag{4.15}
$$

Invertibility of $H(k)$ (except at $k=0$) follows from (4.11) after using either the Schur complement, $Q := H_{00} - H_{0\boldsymbol{p}}H_{\boldsymbol{pp}}^{-1}H_{\boldsymbol{p}0}$, of $H_{\boldsymbol{pp}}$ in H, or the Schur complement, $P := H_{\boldsymbol{pp}} - H_{\boldsymbol{p}0}H_{00}^{-1}H_{0\boldsymbol{p}}$, of H_{00} in H to write the inverse of H as either (c.f. [31])

$$
\begin{aligned}
H^{-1}(k) &= \begin{pmatrix} Q^{-1} & -Q^{-1}H_{0\boldsymbol{p}}H_{\boldsymbol{pp}}^{-1} \\ -H_{\boldsymbol{pp}}^{-1}H_{\boldsymbol{p}0}Q^{-1} & H_{\boldsymbol{pp}}^{-1}H_{\boldsymbol{p}0}Q^{-1}H_{0\boldsymbol{p}}H_{\boldsymbol{pp}}^{-1} + H_{\boldsymbol{pp}}^{-1}\end{pmatrix}, \quad \text{or} \\
H^{-1}(k) &= \begin{pmatrix} H_{00}^{-1} + H_{00}^{-1}H_{0\boldsymbol{p}}P^{-1}H_{\boldsymbol{p}0}H_{00}^{-1} & -H_{00}^{-1}H_{0\boldsymbol{p}}P^{-1} \\ -P^{-1}H_{\boldsymbol{p}0}H_{00}^{-1} & P^{-1}\end{pmatrix}.
\end{aligned}
\tag{4.16}
$$

Setting $\mathcal{G} := (H^{-1})^\vee$ as the atomistic Green's function allows us to write U^∞ and $\boldsymbol{p}^\infty$ as a convolution

$$
\begin{pmatrix}U^\infty\\ \boldsymbol{p}^\infty\end{pmatrix} = \mathcal{G} * \begin{bmatrix}\check{F}\\ \check{\boldsymbol{g}}\end{bmatrix},
$$

or, writing out the individual blocks,

$$
\begin{aligned}
U^\infty(\xi) &= \big[Q^{-1}(k)\big]^\vee * \check{F}(\xi) + \big[-Q^{-1}H_{0\boldsymbol{p}}H_{\boldsymbol{pp}}^{-1}\big]^\vee * \check{\boldsymbol{g}}(\xi) \\
\boldsymbol{p}^\infty(\xi) &= \big[(-Q^{-1}H_{0\boldsymbol{p}}H_{\boldsymbol{pp}}^{-1})^*\big]^\vee * \check{F}(\xi) + \big[H_{\boldsymbol{pp}}^{-1}H_{\boldsymbol{p}0}Q^{-1}H_{0\boldsymbol{p}}H_{\boldsymbol{pp}}^{-1} + H_{\boldsymbol{pp}}^{-1}\big]^\vee * \check{\boldsymbol{g}}(\xi).
\end{aligned}
\tag{4.17}
$$

4.3. **Decay of the Green's Function.** The utility of the expression (4.17) comes from the fact that we can estimate the decay of each of the matrix blocks involved in this formula by comparing them to corresponding blocks in the Cauchy–Born Green's matrix and employing the estimates of Lemma 8.

Theorem 17. *Let $\boldsymbol{\rho} \in (\mathcal{R}_1)^t$, $t \geq 0$ and $|\boldsymbol{\rho}| := t$, then*

$$\big|D_{\boldsymbol{\rho}}[Q^{-1}(k)]^\vee(\xi)\big| \lesssim (1+|\xi|)^{-d-|\boldsymbol{\rho}|+2} \qquad |\boldsymbol{\rho}| \geq 1, \tag{4.18}$$

$$\big|D_{\boldsymbol{\rho}}[-Q^{-1}H_{0\boldsymbol{p}}H_{\boldsymbol{pp}}^{-1}]^\vee(\xi)\big| \lesssim (1+|\xi|)^{-d-|\boldsymbol{\rho}|+1} \qquad |\boldsymbol{\rho}| \geq 0, \tag{4.19}$$

$$\big|D_{\boldsymbol{\rho}}[H_{\boldsymbol{pp}}^{-1}H_{\boldsymbol{p}0}Q^{-1}H_{0\boldsymbol{p}}H_{\boldsymbol{pp}}^{-1}]^\vee\big| + \big|D_{\boldsymbol{\rho}}[H_{\boldsymbol{pp}}^{-1}]^\vee\big| \lesssim (1+|\xi|)^{-d-|\boldsymbol{\rho}|} \qquad |\boldsymbol{\rho}| \geq 0. \tag{4.20}$$

We prove each of the three estimates in Theorem 17 individually. Throughout these proofs, if $\gamma \in \mathbb{N}_0^d$ is a multi-index, then $|\gamma| := \sum_{i=1}^d \gamma_i$ denotes its length and $\partial_\gamma := \partial_{k_1}^{\gamma_1}\cdots\partial_{k_d}^{\gamma_d}$ the associated partial differential operator.

Proof of (4.18) *of Theorem 17.* Let $\hat{\eta} \in C^\infty$ with $\operatorname{supp}(\hat{\eta}) \subset\subset \mathcal{B}$, then arguing similarly as in the proof of [7, Lemma 6.2], we estimate

$$\begin{aligned} |D_{\boldsymbol{\rho}}(Q^{-1})^\vee(\xi)| &\leq |\eta * D_{\boldsymbol{\rho}}(M^{-1})^\vee(\xi)| + |D_{\boldsymbol{\rho}}\big((\eta * M^{-1})^\vee(\xi) - (Q^{-1})^\vee(\xi)\big)| \\ &\lesssim (1+|\xi|)^{2-d-|\rho|} + |D_{\boldsymbol{\rho}}\big((\eta * M^{-1})^\vee(\xi) - (Q^{-1})^\vee(\xi)\big)|, \end{aligned} \tag{4.21}$$

where we have used the estimate in (3.12). Next, we assume that $\hat{\eta} = 1$ on $B_\epsilon(0)$ for some $\epsilon > 0$, then for each multi-index $\gamma \in \mathbb{N}_0^d$, and for $k \in B_\epsilon$,

$$\partial_\gamma(\hat{\eta}M^{-1} - Q^{-1}) = \partial_\gamma(M^{-1}(Q-M)Q^{-1})$$

From the expressions for Q and M, it is clear that $\partial_\gamma(Q-M) = \mathcal{O}(k^{3-|\gamma|})$ and both $\partial_\gamma M^{-1} = \mathcal{O}(k^{-2-|\gamma|})$ and $\partial_\gamma Q^{-1} = \mathcal{O}(k^{-2-|\gamma|})$ so $\partial_\gamma(M^{-1}(Q-M)Q^{-1}) = \mathcal{O}(k^{-1-|\gamma|})$. Outside of B_ϵ, $\partial_\gamma(\hat{\eta}M^{-1} - Q^{-1})$ is bounded. Hence, it follows from Corollary 8 that

$$|D_{\boldsymbol{\rho}}\big((\eta * M^{-1})^\vee(\xi) - (Q^{-1})^\vee(\xi)\big)| \lesssim (1+|\xi|)^{2-d-|\boldsymbol{\rho}|},$$

which, combined with (4.21), completes the proof. □

Proof of (4.19) *of Theorem 17.* Recall the definition of $H_{0\boldsymbol{p}}$ and $J_{0\boldsymbol{p}}$ as

$$[H_{0\boldsymbol{p}}(k)]_\beta := \sum_{\rho\in\mathcal{R}_1}\sum_{\alpha=0}^{S-1}\sum_{(\tau\gamma\delta)\in\mathcal{R}} [(e^{-2\pi i k\cdot\tau}-1)V_{,(\rho\alpha\beta)(\tau\gamma\delta)}(0)(e^{2\pi i k\cdot\rho}) - (e^{-2\pi i k\cdot\tau}-1)V_{,(\rho\beta\alpha)(\tau\gamma\delta)}(0)],$$

$$[J_{0\boldsymbol{p}}(k)]_\beta := \sum_{\rho\in\mathcal{R}_1}\sum_{\alpha=0}^{S-1}\sum_{(\tau\gamma\delta)\in\mathcal{R}} (-2\pi i k\cdot\tau)V_{,(\rho\alpha\beta)(\tau\gamma\delta)}(0) + (-2\pi i k\cdot\tau)V_{,(\rho\beta\alpha)(\tau\gamma\delta)}(0)].$$

To avoid double-subscripts we will write $J_{0\boldsymbol{p}}^\beta(k) := [J_{0\boldsymbol{p}}(k)]_\beta$ to mean the β block of $J_{0\boldsymbol{p}}$ and $[H_{\boldsymbol{pp}}^{-1}]^{\beta\gamma}$ to denote the $\beta\chi$ block of $H_{\boldsymbol{pp}}^{-1}$.

As before let $\hat{\eta} \in C^\infty(\mathcal{B})$ with $\operatorname{supp}(\hat{\eta}) \subset\subset \mathcal{B}$ and $\hat{\eta} = 1$ in a ball B_ϵ contained in $\mathcal{B}$. Our first step will be to show that

$$\big|D_{\boldsymbol{\rho}}\big(\eta * \big[M^{-1}H_{0\boldsymbol{p}}H_{\boldsymbol{pp}}^{-1}\big]^\vee\big)\big| \lesssim |x|^{1-d-|\boldsymbol{\rho}|}, \tag{4.22}$$

after which we will estimate the difference $|\partial_\gamma\big(\hat{\eta}(M^{-1}(H_{0\boldsymbol{p}}-J_{0\boldsymbol{p}})P^{-1})\big)|$. From properties of Fourier transforms

$$\big[[M^{-1}]_{ij}[J^{\beta}_{0\boldsymbol{p}}]_{jm}[H^{-1}_{\boldsymbol{pp}}]^{\beta\chi}_{mn}\big]^{\vee} = \big[[M^{-1}]_{ij}[J^{\beta}_{0\boldsymbol{p}}]_{jm}\big]^{\vee} * \big[[H^{-1}_{\boldsymbol{pp}}]^{\beta\chi}_{mn}\big]^{\vee}. \tag{4.23}$$

We take the *full-space* inverse Fourier transform to find

$$\big[[M^{-1}]_{ij}[J^{\beta}_{0\boldsymbol{p}}]_{jm}\big]^{\vee}(x) = \sum_{s=1}^{d}\frac{\partial}{\partial x_s}\Bigg[\sum_{\tau\delta\gamma}\sum_{\alpha=0}^{S-1}\tau_s[V_{,(\rho\alpha\beta)(\tau\gamma\delta)}(0)+V_{,(\rho\alpha\beta)(\tau\delta\gamma)}(0)]_{jm}[M^{-1}]^{\vee}_{ij}(x)\Bigg],$$

and then use [19, Equation 6.2.15] to deduce that

$$\big|D_{\boldsymbol{\rho}}\big([M^{-1}]_{ij}[J^{\beta}_{0\boldsymbol{p}}]_{jm}\big)^{\vee}(x)\big| \lesssim |x|^{1-d-|\boldsymbol{\rho}|}. \tag{4.24}$$

Furthermore, from the equality (4.23) and the fact that convolution is commutative and associative,

$$\eta * ([M^{-1}]_{ij}[J^{\beta}_{0\boldsymbol{p}}]_{jm})^{\vee} * \big[[H^{-1}_{\boldsymbol{pp}}]^{\beta\chi}_{mn}\big]^{\vee} = ([M^{-1}]_{ij}[J^{\beta}_{0\boldsymbol{p}}]_{jm})^{\vee} * (\eta * \big[[H^{-1}_{\boldsymbol{pp}}]^{\beta\chi}_{mn}\big]^{\vee}). \tag{4.25}$$

Finally, the convolution on the right-hand side of (4.25) will decay at the slower of the two rates involved in the convolution. Because $\eta * \big[[H^{-1}_{\boldsymbol{pp}}]^{\beta\chi}_{mn}\big]^{\vee}$ is the inverse Fourier transform of a smooth function with compact support, it follows that this function is of Schwartz class so decays faster than any polynomial. Since finite differences commute with convolutions, combining (4.25) with (4.24) then yields (4.22).

In the following we will employ the estimates

$$\begin{aligned}\partial_\gamma\big(\hat{\eta}(M^{-1}(J_{0\boldsymbol{p}}-H_{0\boldsymbol{p}})H^{-1}_{\boldsymbol{pp}})\big) &= \mathcal{O}(k^{-|\gamma|}),\\ \partial_\gamma\big(\hat{\eta}(Q^{-1}-M^{-1})H_{0\boldsymbol{p}}H^{-1}_{\boldsymbol{pp}}\big) &= \mathcal{O}(k^{-|\gamma|}),\end{aligned} \tag{4.26}$$

which can be readily established.

We now split

$$\begin{aligned}|D_{\boldsymbol{\rho}}\big(Q^{-1}H_{0\boldsymbol{p}}H^{-1}_{\boldsymbol{pp}}\big)^{\vee}(\xi)| \le\ &\Big|D_{\boldsymbol{\rho}}\big(Q^{-1}H_{0\boldsymbol{p}}H^{-1}_{\boldsymbol{pp}}\big)^{\vee}(\xi) - D_{\boldsymbol{\rho}}\big(\eta*(M^{-1}J_{0\boldsymbol{p}}H^{-1}_{\boldsymbol{pp}})^{\vee}\big)(\xi)\Big|\\ &+\Big|D_{\boldsymbol{\rho}}\big(\eta*(M^{-1}J_{0\boldsymbol{p}}H^{-1}_{\boldsymbol{pp}})\big)^{\vee}(\xi)\Big|.\end{aligned} \tag{4.27}$$

We already know the decay of the second term from (4.22), hence we focus on the first term on the right-hand side of (4.27). We take its Fourier transform and then a derivative of order $\gamma \in \mathbb{N}_0^d$ with the goal being to apply Corollary 8:

$$\begin{aligned}&\partial_\gamma\Big(\big(Q^{-1}H_{0\boldsymbol{p}}H^{-1}_{\boldsymbol{pp}}\big) - \hat{\eta}(M^{-1}J_{0\boldsymbol{p}}H^{-1}_{\boldsymbol{pp}})\Big)\\ &\quad= \partial_\gamma\Big(\big(Q^{-1}H_{0\boldsymbol{p}}H^{-1}_{\boldsymbol{pp}}\big) - \hat{\eta}M^{-1}H_{0\boldsymbol{p}}H^{-1}_{\boldsymbol{pp}} + \hat{\eta}M^{-1}H_{0\boldsymbol{p}}H^{-1}_{\boldsymbol{pp}} - \hat{\eta}(M^{-1}J_{0\boldsymbol{p}}H^{-1}_{\boldsymbol{pp}})\Big)\\ &\quad= \partial_\gamma\Big(\big(Q^{-1}H_{0\boldsymbol{p}}H^{-1}_{\boldsymbol{pp}}\big) - \hat{\eta}M^{-1}H_{0\boldsymbol{p}}H^{-1}_{\boldsymbol{pp}}\Big) + \partial_\gamma\Big(\hat{\eta}M^{-1}\big[H_{0\boldsymbol{p}}-J_{0\boldsymbol{p}}\big]H^{-1}_{\boldsymbol{pp}})\Big).\end{aligned} \tag{4.28}$$

Combining (4.26) and the properties of $\hat{\eta}$ we obtain

$$\partial_\gamma\left(\big(Q^{-1}H_{0\boldsymbol{p}}H^{-1}_{\boldsymbol{pp}}\big) - \hat{\eta}M^{-1}H_{0\boldsymbol{p}}H^{-1}_{\boldsymbol{pp}}\right) = \mathcal{O}(k^{-|\gamma|}). \tag{4.29}$$

Applying Corollary 8 to the estimates in (4.28), (4.26) and (4.29) yields

$$\begin{aligned} \Big|D_{\boldsymbol{\rho}}\Big(\hat{\eta}\big(M^{-1}(J_{0\boldsymbol{p}}-H_{0\boldsymbol{p}})H_{\boldsymbol{pp}}^{-1}\big)\Big)^{\vee}(\xi)\Big| &\lesssim\ (1+|\xi|)^{1-d-|\boldsymbol{\rho}|} \\ \Big|D_{\boldsymbol{\rho}}\Big(\big(Q^{-1}H_{0\boldsymbol{p}}H_{\boldsymbol{pp}}^{-1}-\hat{\eta}M^{-1}H_{0\boldsymbol{p}}H_{\boldsymbol{pp}}^{-1}\big)\Big)^{\vee}(\xi)\Big| &\lesssim\ (1+|\xi|)^{1-d-|\boldsymbol{\rho}|}. \end{aligned} \tag{4.30}$$

Combining the estimates in (4.30) and (4.22) and using them in the decomposition (4.27) gives the desired decay estimate (4.19). □

Proof of (4.20) *of Theorem 17.* To prove the second part of the estimate,

$$\big|D_{\boldsymbol{\rho}}(H_{\boldsymbol{pp}}^{-1})^{\vee}\big| \lesssim\ (1+|\xi|)^{-d-|\boldsymbol{\rho}|},$$

we simply note that $D_{\gamma}(H_{\boldsymbol{pp}}^{-1})^{\vee}\in L^1(\mathcal{B})$ for any γ. (In fact the decay is at least super-algebraic, but this will be dominated by other $(1+|\xi|)^{-d-|\boldsymbol{\rho}|}$ terms later in the proof.)

The first part of the estimate,

$$\big|D_{\boldsymbol{\rho}}(H_{\boldsymbol{pp}}^{-1}H_{\boldsymbol{p}0}Q^{-1}H_{0\boldsymbol{p}}H_{\boldsymbol{pp}}^{-1})^{\vee}\big| \lesssim\ (1+|\xi|)^{-d-|\boldsymbol{\rho}|},$$

can be obtained using a procedure very similar to that in the proof of (4.20), that is, by comparing Q^{-1} with M^{-1} and $H_{0\boldsymbol{p}}$ with $J_{0\boldsymbol{p}}$. Briefly, while $\partial_\gamma Q^{-1}=\mathcal{O}(k^{-2-|\gamma|})$, the blocks $H_{\boldsymbol{p}0}$ and $H_{0\boldsymbol{p}}$ contribute two additional powers of k which in real-space terms translates to the improvement of the decay estimate (4.20) over (4.18). □

4.4. **Decay of Displacement and Shifts.** Using the decay estimates on the Hessian from the previous section and the residual decay estimates on the linearized equation (4.15), we now establish the desired decay rates for the displacement field U^∞ and shift fields $\boldsymbol{p}^\infty$. Recall that from the linearized equation (4.15), we have

$$\begin{aligned} \hat{U}^\infty &= Q^{-1}F - Q^{-1}H_{0\boldsymbol{p}}H_{\boldsymbol{pp}}^{-1}\boldsymbol{g} \\ \hat{\boldsymbol{p}}^\infty &= -H_{\boldsymbol{pp}}^{-1}H_{\boldsymbol{p}0}Q^{-1}F + H_{\boldsymbol{pp}}^{-1}H_{\boldsymbol{p}0}Q^{-1}H_{0\boldsymbol{p}}H_{\boldsymbol{pp}}^{-1}\boldsymbol{g} + H_{\boldsymbol{pp}}^{-1}\boldsymbol{g}. \end{aligned}$$

Observe also that $F=\mathcal{O}(k)$ and $g_\eta=\mathcal{O}(1)$ from (4.14). By taking inverse Fourier transforms, we obtain

$$\begin{aligned} U^\infty &= (Q^{-1})^{\vee} * \check{F} - (Q^{-1}H_{0\boldsymbol{p}}H_{\boldsymbol{pp}}^{-1})^{\vee} * \check{\boldsymbol{g}} \\ \boldsymbol{p}^\infty &= (-H_{\boldsymbol{pp}}^{-1}H_{\boldsymbol{p}0}Q^{-1})^{\vee} * \check{F} + (H_{\boldsymbol{pp}}^{-1}H_{\boldsymbol{p}0}Q^{-1}H_{0\boldsymbol{p}}H_{\boldsymbol{pp}}^{-1})^{\vee} * \check{\boldsymbol{g}} + (H_{\boldsymbol{pp}}^{-1})^{\vee} * \check{\boldsymbol{g}} \end{aligned}$$

For notational convenience, we set $A := Q^{-1}$ and $B = Q^{-1}H_{0\boldsymbol{p}}H_{\boldsymbol{pp}}^{-1}$ and rewrite the first of these as

$$\begin{aligned}
U^\infty(\ell) = &\ A * \check{F} - B * \check{\boldsymbol{g}} = \sum_{\xi\in\mathcal{L}} \bigg(A(\ell-\xi)\check{F}(\xi) + \sum_{\alpha=0}^{S-1} B_\alpha(\ell-\xi)\check{g}_\alpha(\xi) \bigg) \\
= &\ \sum_{\xi\in\mathcal{L}} \sum_{(\rho\alpha\beta)\in\mathcal{R}} A(\ell-\xi) D_\rho f_{(\rho\alpha\beta)}(\xi) \\
&\qquad + \sum_{\xi\in\mathcal{L}} \sum_{\alpha=0}^{S-1} B_\alpha(\ell-\xi) \Bigg[\sum_{\rho\in\mathcal{R}_0} \sum_{\beta=0}^{S-1} \big(f_{(\rho\beta\alpha)}(\xi+\rho) - f_{(\rho\alpha\beta)}(\xi) \big) \Bigg] \\
= &\ \sum_{\xi\in\mathcal{L}} \sum_{(\rho\alpha\beta)\in\mathcal{R}} A(\ell-\xi) D_\rho f_{(\rho\alpha\beta)}(\xi) \\
&\qquad + \sum_{\xi\in\mathcal{L}} \Bigg[\sum_{(\rho\alpha\beta)\in\mathcal{R}} B_\alpha(\ell-\xi) \big(f_{(\rho\beta\alpha)}(\xi+\rho) - f_{(\rho\alpha\beta)}(\xi) \big) \Bigg].
\end{aligned}$$

In a similar manner, we may rewrite the second of these as

$$\begin{aligned}
p_\alpha^\infty(\ell) = &\ \sum_\beta \sum_{\xi\in\mathcal{L}} (-B^*)^\vee_\beta(\ell-\xi) \sum_{(\tau\gamma\delta)} D_\tau f_{(\tau\gamma\delta)}(\xi) \\
&+ \sum_\beta \sum_{\xi\in\mathcal{L}} (H_{\boldsymbol{pp}}^{-1} H_{\boldsymbol{p}0} Q^{-1} H_{0\boldsymbol{p}} H_{\boldsymbol{pp}}^{-1})^\vee_\beta(\ell-\xi)\check{g}_\beta(\xi) + \sum_\beta \sum_{\xi\in\mathcal{L}} (H_{\boldsymbol{pp}}^{-1})^\vee_\beta * \check{g}_\beta(\xi).
\end{aligned}$$

We are now ready to prove our main result, Theorem 4.

Proof of Theorem 4. Part I: proof of lowest-order decay. We begin by proving the conclusion of the theorem for $D_\tau U^\infty$ (that is, $\boldsymbol{\rho} = \rho$ with $|\boldsymbol{\rho}| = 1$) and p_α^∞ ($|\boldsymbol{\rho}| = 0$) and will follow the same method as [7, Section 6]. The main idea is to prove the result similar to how one would prove that the convolution of two functions with known decay will decay at the slower of the two rates: we split the convolution over an inner set and an outer set and then use the relevant decay properties on each set. Here, the decay of the Green's functions is governed by Theorem 17, and the decay of the residual is governed by Corollary 14.

To this end define the translation operator $T_\rho q_\beta(\xi) := q_\beta(\xi+\rho)$, and set

$$w(r) = \sup_{|\ell|\geq r} |DU^\infty(\ell)|, \quad q_\beta(r) = \sup_{|\ell|\geq r} \max_{\rho\in\mathcal{R}_1} |T_\rho p_\beta^\infty(\ell)|, \quad q(r) = \sup_\beta q_\beta(r),$$

and note that

$$\begin{aligned}
w(2r) &= \sup_{|\ell|\geq 2r} \max_{\tau\in\mathcal{R}_1} |D_\tau U^\infty(\ell)| \\
&= \sup_{|\ell|\geq 2r} \max_{\tau\in\mathcal{R}_1} \Bigg| \sum_{\xi\in\mathcal{L}} \sum_{(\rho\alpha\beta)\in\mathcal{R}} \bigg(D_\tau D_\rho A(\ell-\xi) f_{(\rho\alpha\beta)}(\xi) \\
&\qquad\qquad + D_\tau B_\alpha(\ell-\xi) \big(f_{(\rho\beta\alpha)}(\xi+\rho) - f_{(\rho\alpha\beta)}(\xi) \big) \bigg) \Bigg| \qquad (4.31) \\
&= \sup_{|\ell|\geq 2r} \max_{\tau\in\mathcal{R}_0} \Bigg| \sum_{\xi\in\mathcal{L}} \sum_{(\rho\alpha\beta)\in\mathcal{R}} \bigg(D_\tau D_\rho A(\xi) f_{(\rho\alpha\beta)}(\ell-\xi) \\
&\qquad\qquad + D_\tau B_\alpha(\xi+\rho) f_{(\rho\beta\alpha)}(\ell-\xi) - D_\tau B_\alpha(\xi) f_{(\rho\alpha\beta)}(\ell-\xi) \bigg) \Bigg|.
\end{aligned}$$

By Theorem 17, $|D_\tau D_\rho A(\xi)| \lesssim (1+|\xi|)^{-d}$ and $|D_\tau B_\alpha(\xi)| \lesssim (1+|\xi|)^{-d}$, and by Corollary 14, $|f(\xi)| \lesssim |D\boldsymbol{u}^\infty(\xi)|^2$. Employing these estimates in (4.31), we then get

$$\begin{aligned} w(2r) &\lesssim \sup_{|\ell|\geq 2r}(1+|r|)^{-d}\sum_{|\xi|\geq r}|D\boldsymbol{u}^\infty(\ell-\xi)|^2 + \sup_{|\ell|\geq 2r}\sum_{|\xi|\leq r}(1+|\xi|)^{-d}|D\boldsymbol{u}^\infty(\ell-\xi)|^2 \\ &\lesssim (1+|r|)^{-d}\|\boldsymbol{u}^\infty\|_{\mathrm{a}}^2 + \big(w(r)^{3/2}+q(r)^{3/2}\big)\sum_{\xi\in\mathcal{L}}(1+|\xi|)^{-d}|D\boldsymbol{u}^\infty(\ell-\xi)|^{1/2}. \end{aligned}$$

Since $|D\boldsymbol{u}^\infty| \in \ell^2$ it follows that $(1+|\xi|)^{-d}|D\boldsymbol{u}^\infty(\ell-\xi)|^{1/2}$ is summable, hence we obtain

$$w(2r) \lesssim (1+|r|)^{-d} + w(r)\sqrt{w(r)} + q(r)\sqrt{q(r)}. \tag{4.32}$$

By analogous computations and employing the remaining decay rates of Theorem 17,

$$\begin{aligned} q_\beta(2r) &= \sup_{|\ell|\geq 2r}\max_{\rho\in\mathcal{R}_1}|T_\rho p_\beta^\infty(\ell)| \\ &= \sup_{|\ell|\geq 2r}\sum_\beta\sum_{\xi\in\mathcal{L}}T_\rho(-H_{\boldsymbol{pp}}^{-1}H_{\boldsymbol{p}0}H_{00}^{-1})_\beta^\vee(\xi)\check{F}(\ell-\xi) \\ &\qquad + \sup_{|\ell|\geq 2r}\sum_\beta\sum_{\xi\in\mathcal{L}}T_\rho(H_{\boldsymbol{pp}}^{-1}H_{\boldsymbol{p}0}H_{00}^{-1}H_{0\boldsymbol{p}}H_{\boldsymbol{pp}}^{-1})_\beta^\vee(\xi)\check{g}_\beta(\ell-\xi) \\ &\qquad + \sup_{|\ell|\geq 2r}\sum_\beta\sum_{\xi\in\mathcal{L}}T_\rho(H_{\boldsymbol{pp}}^{-1})_\beta^\vee(\xi)\check{g}_\beta(\ell-\xi) \\ &\lesssim (1+|r|)^{-d} + w(r)\sqrt{w(r)} + q(r)\sqrt{q(r)}. \end{aligned} \tag{4.33}$$

Combining equations (4.32) and (4.33), we have

$$\begin{aligned} w(2r) &\leq C_1(1+|r|)^{-d} + C_1 w(r)\sqrt{w(r)} + C_1 q(r)\sqrt{q(r)}, \\ q(2r) &\leq C_2(1+|r|)^{-d} + C_2 w(r)\sqrt{w(r)} + C_2 q(r)\sqrt{q(r)}. \end{aligned}$$

Applying Step 2 of [7, Lemma 6.3] to $v(r) = r^d(w(r)+q(r))$ we deduce that there exists a constant C such that

$$|r^d(w(r)+q(r))| \leq \ C \quad \forall\, r > 0.$$

which completes the proof for the lowest-order decay,

$$|D_\rho U^\infty(\xi)| \lesssim (1+|\xi|)^{-d} \qquad \text{and} \qquad |p_\alpha^\infty(\xi)| \lesssim (1+|\xi|)^{-d}.$$

Part II: proof of higher-order decay. Let $\boldsymbol{\rho} \in \mathcal{R}_0^t, t \in \{2,3\}$, then we have

$$D_{\boldsymbol{\rho}}U^\infty(\ell) = \sum_{\xi\in\mathcal{L}}\bigg(D_{\boldsymbol{\rho}}A(\xi)\check{F}(\ell-\xi) + \sum_{\alpha=0}^{S-1}D_{\boldsymbol{\rho}}B_\alpha(\xi)\check{g}_\alpha(\ell-\xi)\bigg).$$

The decay rates established in *Part I* of the proof in particular entail that

$$|DU^\infty(\xi)| \lesssim (1+|\xi|)^{-d}$$

hence Theorems 14 implies that

$$|\check{F}(\xi)| + |\check{\mathbf{g}}(\xi)| \lesssim |f(\xi)| \lesssim (1+|\xi|)^{-2d}. \tag{4.34}$$

Using also the decay estimates for the Green's matrix, from Theorem 17, we continue to estimate

$$\begin{aligned}\big|D_{\boldsymbol{\rho}}U^\infty(\ell)\big| &\lesssim \sum_{|\xi|\le 1/2|\ell|}(1+|\xi|)^{1-d-|\rho|}(1+|\ell-\xi|)^{-2d} \\ &\qquad + \sum_{|\xi|\ge 1/2|\ell|}(1+|\xi|)^{1-d-|\rho|}(1+|\ell-\xi|)^{-2d} \\ &\lesssim (1+|\ell|)^{-2d}\sum_{|\xi|\le 1/2|\ell|}(1+|\xi|)^{1-d-|\rho|} \\ &\qquad + (1+|\ell|)^{1-d-|\rho|}\sum_{|\xi|\ge 1/2|\ell|}(1+|\ell-\xi|)^{-2d} \\ &\lesssim (1+|\ell|)^{-2d} + (1+|\ell|)^{1-d-|\rho|}, \end{aligned} \tag{4.35}$$

which completes the proof of the first estimate in (2.7).

To establish the corresponding higher-order decay for the shifts, let $\boldsymbol{\rho} \in \mathcal{R}_0^t, t \in \{1,2\}$, then

$$\begin{aligned} D_{\boldsymbol{\rho}} p_\alpha^\infty(\ell) = &\sum_\beta \sum_{\xi\in\mathcal{L}} D_{\boldsymbol{\rho}}(-H_{\boldsymbol{pp}}^{-1}H_{\boldsymbol{p}0}Q^{-1})_\beta^\vee(\xi)\check{F}(\ell-\xi) \\ + &\sum_\beta\sum_{\xi\in\mathcal{L}} D_{\boldsymbol{\rho}}(H_{\boldsymbol{pp}}^{-1}H_{\boldsymbol{p}0}Q^{-1}H_{0\boldsymbol{p}}H_{\boldsymbol{pp}}^{-1})_\beta^\vee(\xi)\check{g}_\beta(\ell-\xi) + \sum_\beta\sum_{\xi\in\mathcal{L}} D_{\boldsymbol{\rho}}(H_{\boldsymbol{pp}}^{-1})_\beta^\vee * \check{g}_\beta(\ell-\xi). \end{aligned}$$

As in the estimate for $D_\rho U^\infty$, we insert the Green's matrix decay estimate from Theorem 17 and (4.34), and then argue precisely as in (4.35) to obtain the second estimate in (2.7). ☐

5. Discussion

We have extended the model formulation and analysis (decay of discrete elastic fields) for point defects embedded in a homogeneous crystalline solid from the Bravais lattice case [7] to multilattices. While, at a conceptual level, the arguments remained fairly similar, numerous modifications were required in accounting for the shift degrees of freedom, in particular an extension of the decay estimates for the lattice Green's matrix to the multilattice case. Our results build a foundation for the numerical analysis of coarse-graining schemes for multilattices, in particular an analysis of atomistic/continuum blending schemes [21].

To conclude we briefly mention some important extensions: (1) To include dislocations we need to replace the reference lattice as the predictor configuration with a linearised elasticity solution. We anticipate that following the ideas from [7] but replacing the simple lattice Cauchy–Born model for the computation of the predictor displacement with the classical multilattice Cauchy–Born model (3.3) should be sufficient to carry out this extension.

(2) A second problem of interest is the extension of our analysis to ionic crystals. Here, long-range interactions play a crucial role, and it is at this point largely unclear to what extent our results generalise.

(3) Finally, a problem of current interest is the application of our results to defects in bilayer materials [1], where two or more multilattice crystals are stacked on top of each other. By considering the top layer to be shifted relative to the bottom layer, our current results extend to that case as long as the multilattices in each layer are the same (or, more generally, have a common periodic cell). However, this does not allow for important effects such as disregistry to be modeled where the lattice constants in each layer differ by an irrational

factor [5]. These effects would require a different analysis due to lack of periodicity and lack of continuum model to compare the atomistic Green's function too.

Appendix A. Proofs and Additional Results

A.1. **Density of Test Functions.** Here we prove density of the test function space.

Lemma 18. *The quotient space* $\boldsymbol{\mathcal{U}}_0$ *is dense in* $\boldsymbol{\mathcal{U}} = \mathcal{U}/\mathbb{R}^n$.

Proof. The proof is a slight modification of [23, Theorem 2.1] taking into account both the interpolation operator and additional shift vectors. We only provide a brief sketch of the proof; for a related proof in the context of a simple lattice, see [22, Lemma 1.8].

Let η be a smooth bump function with support in $B_1(0)$ and equal to one on $B_{3/4}(0)$, and for $R > 0$, let $\eta_R(x) := \eta(x/R)$ and $A_R := \operatorname{supp}(\nabla(I\eta_R))$. Next, for $\boldsymbol{u} \in \boldsymbol{\mathcal{U}}$, define the truncation operator $T_R\boldsymbol{u} = (T_R u_\alpha)_{\alpha=0}^{S-1}$ by

$$T_R u_\alpha(x) = \eta_R(x)\big(Iu_\alpha - \frac{1}{|A_R|}\int_{A_R} Iu_0\,dx\big),$$

where $|A_R|$ represents the measure of A_R. Then define

$$\begin{aligned}\Pi_R\boldsymbol{u} &:= (\Pi_R u_\alpha)_{\alpha=0}^{S-1},\\ \Pi_R u_\alpha &:= I(T_R u_\alpha).\end{aligned}$$

Clearly $\Pi_R\boldsymbol{u} \in \boldsymbol{\mathcal{U}}_0$, and so we need to show $\Pi_R\boldsymbol{u} - \boldsymbol{u} \to 0$ as $R \to \infty$. Using the definition of Π_R, it is straightforward to show

$$\begin{aligned}
&\|\nabla\Pi_R u_\alpha - \nabla I u_\alpha\|_{L^2(\mathbb{R}^d)} = \|\nabla I T_R u_\alpha - \nabla I u_\alpha\|_{L^2(\mathbb{R}^d)}\\
&\lesssim \|\nabla(I(\eta_R(Iu_\alpha - \frac{1}{|A_R|}\int_{A_R} Iu_0\,dx))) - \nabla(I\eta_R(Iu_\alpha - \frac{1}{|A_R|}\int_{A_R} Iu_0\,dx))\\
&\qquad + \nabla(I\eta_R(Iu_\alpha - \frac{1}{|A_R|}\int_{A_R} Iu_0\,dx)) - \nabla I u_\alpha\|_{L^2(\mathbb{R}^d)}\\
&\lesssim \|\nabla(I(\eta_R u_\alpha)) - \nabla(I\eta_R I u_\alpha)\|_{L^2(A_R)}\\
&\quad + \|(Iu_\alpha - \frac{1}{|A_R|}\int_{A_R} Iu_0\,dx)\nabla I\eta_R^\top\|_{L^2(A_R)} + \|(I\eta_R - 1)\nabla I u_\alpha\|_{L^2(A_R)}\\
&\qquad + \|\nabla I u_\alpha\|_{L^2(\mathbb{R}^d\setminus B_R)}.
\end{aligned} \tag{A.1}$$

Clearly, the latter two terms tend to zero as $R \to \infty$ since $\nabla u_\alpha \in L^2(\mathbb{R}^d)$.

By splitting the first term into a sum over triangles and using standard interpolation estimates on each triangle, the first term in (A.1) can also be seen to go to zero as $R \to \infty$:

$$\begin{aligned}
\|\nabla(I(\eta_R u_\alpha)) - \nabla(I\eta_R I u_\alpha)\|^2_{L^2(A_R)} &= \|\nabla I(I\eta_R I u_\alpha) - \nabla(I\eta_R I u_\alpha)\|^2_{L^2(A_R)} \\
&= \sum_{T\in\mathcal{T}_{\rm a}, T\cap A_R\neq\emptyset} \|\nabla I(I\eta_R I u_\alpha) - \nabla(I\eta_R I u_\alpha)\|^2_{L^2(T)} \\
&\lesssim \sum_{T\in\mathcal{T}_{\rm a}, T\cap A_R\neq\emptyset} \|\nabla^2(I\eta_R I u_\alpha)\|^2_{L^2(T)} = 2 \sum_{T\in\mathcal{T}_{\rm a}, T\cap A_R\neq\emptyset} \|\nabla I\eta_R \nabla I u_\alpha^\top\|^2_{L^2(T)} \\
&\lesssim \frac{1}{R^2} \sum_{T\in\mathcal{T}_{\rm a}, T\cap A_R\neq\emptyset} \|\nabla I u_\alpha\|^2_{L^2(T)} \lesssim \frac{1}{R^2}\|\nabla I u_\alpha\|^2_{L^2(A_R)} \to 0 \quad \text{as } R\to\infty,
\end{aligned}$$

where we used $\|\nabla I\eta_R\|_{L^\infty} \lesssim \|\nabla \eta_R\|_{L^\infty} \lesssim R^{-1}$ in the second inequality.

The second term in (A.1) can also be seen to converge to zero after using the Poincaré inequality and the fact that the Poincaré constant for A_R is bounded by a constant multiple of R. Specifically,

$$\|(Iu_\alpha - \frac{1}{|A_R|}\int_{A_R} Iu_0\,dx)\nabla(I\eta(x/R))^T\|_{L^2(A_R)} \lesssim \|\nabla I u_\alpha\|_{L^2(A_R)} + \frac{1}{R}\|Iu_\alpha - Iu_0\|_{L^2(A_R)},$$

which clearly tends to zero. □

A.2. **Proof of Theorem 1.** As the summations defining $\mathcal{E}^{\rm a}_{\rm hom}(\boldsymbol{u})$ and $\mathcal{E}^{\rm a}(\boldsymbol{u})$ differ only on the finite set where $V_\xi \not\equiv V$, we need only show that $\mathcal{E}^{\rm a}_{\rm hom}(\boldsymbol{u})$ is well-defined. We prove this along the lines of [24][Theorem 2.8]; we will construct an auxiliary energy functional $\bar{\mathcal{E}}^{\rm a}_{\rm hom}$ which is C^3 and show that $\mathcal{E}^{\rm a}_{\rm hom}$ and $\bar{\mathcal{E}}^{\rm a}_{\rm hom}$ are equal on the dense subset $\boldsymbol{\mathcal{U}}_0$.

To that end, define

$$\bar{\mathcal{E}}^{\rm a}_{\rm hom}(\boldsymbol{u}) := \sum_{\xi\in\mathcal{L}} \big[V(D\boldsymbol{u}(\xi)) - \sum_{(\rho\alpha\beta)\in\mathcal{R}} V_{,(\rho\alpha\beta)}(D\boldsymbol{y}(\xi))\cdot D_{(\rho\alpha\beta)}\boldsymbol{u}(\xi)\big].$$

Using a Taylor expansion of the site potential about $D\boldsymbol{y}(\xi)$ and a bound on the second derivatives of V,

$$\begin{aligned}
|\bar{\mathcal{E}}^{\rm a}_{\rm hom}(\boldsymbol{u})| &\lesssim \sum_{\xi\in\mathcal{L}} \sum_{(\rho\alpha\beta)\in\mathcal{R}} \sum_{(\tau\gamma\delta)\in\mathcal{R}} |D_{(\rho\alpha\beta)}\boldsymbol{u}(\xi)|\cdot|D_{(\tau\gamma\delta)}\boldsymbol{u}(\xi)| \\
&\lesssim \Big\{\sum_{\xi\in\mathcal{R}} \sum_{(\rho\alpha\beta)\in\mathcal{R}} |D_{(\rho\alpha\beta)}\boldsymbol{u}(\xi)|^2\Big\}^{1/2} \Big\{\sum_{\xi\in\mathcal{R}} \sum_{(\tau\gamma\delta)\in\mathcal{R}} |D_{(\tau\gamma\delta)}\boldsymbol{u}(\xi)|^2\Big\}^{1/2} \le \|\boldsymbol{u}\|^2_{\rm a_1}.
\end{aligned}$$

Since $\bar{\mathcal{E}}^{\rm a}_{\rm hom}$ is clearly invariant with respect to addition by constants, this shows $\bar{\mathcal{E}}^{\rm a}_{\rm hom}$ is well-defined on the quotient space $\boldsymbol{\mathcal{U}}$.

To show $\bar{\mathcal{E}}^{\rm a}_{\rm hom}(\boldsymbol{u})$ is differentiable, we again use a Taylor expansion and bound on the second derivative of V to observe

$$\begin{aligned}
\bar{\mathcal{E}}^{\rm a}_{\rm hom}(\boldsymbol{u}+\boldsymbol{v}) - \bar{\mathcal{E}}^{\rm a}_{\rm hom}(\boldsymbol{u}) - \sum_{\xi\in\mathcal{L}} \sum_{(\rho\alpha\beta)\in\mathcal{R}} \big[&V_{,(\rho\alpha\beta)}(D\boldsymbol{u}(\xi))\cdot D_{(\rho\alpha\beta)}\boldsymbol{v}(\xi) \\
&+ V_{,(\rho\alpha\beta)}(D\boldsymbol{y}(\xi))\cdot D_{(\rho\alpha\beta)}\boldsymbol{v}(\xi)\big] \\
\lesssim \sum_{\xi\in\mathcal{L}} \sum_{(\rho\alpha\beta)\in\mathcal{R}} \sum_{(\tau\gamma\delta)\in\mathcal{R}} |D_{(\rho\alpha\beta)}\boldsymbol{v}(\xi)|\cdot|D_{(\tau\gamma\delta)}\boldsymbol{v}(\xi)| \lesssim \|\boldsymbol{v}\|^2_{\rm a_1}.
\end{aligned}$$

The first Fréchet derivative of $\bar{\mathcal{E}}^{\rm a}_{\rm hom}$ is thus defined by

$$\langle \delta\bar{\mathcal{E}}^{\rm a}_{\rm hom}(\boldsymbol{u}), \boldsymbol{v}\rangle = \sum_{\xi\in\mathcal{L}} \sum_{(\rho\alpha\beta)\in\mathcal{R}} \big[V_{,(\rho\alpha\beta)}(D\boldsymbol{u}(\xi))\cdot D_{(\rho\alpha\beta)}(\boldsymbol{v}(\xi)) + V_{,(\rho\alpha\beta)}(D\boldsymbol{y}(\xi))\cdot D_{(\rho\alpha\beta)}\boldsymbol{v}(\xi)\big].$$

To prove that $\delta\bar{\mathcal{E}}^{\rm a}_{\rm hom}(\boldsymbol{u})$ is differentiable, we again employ a Taylor expansion and a bound on the third derivative of V

$$\begin{aligned}
&\langle \delta\bar{\mathcal{E}}^{\rm a}_{\rm hom}(\boldsymbol{u}+\boldsymbol{w}) - \delta\bar{\mathcal{E}}^{\rm a}_{\rm hom}(\boldsymbol{u}), \boldsymbol{v}\rangle \\
&\qquad - \sum_{\xi\in\mathcal{L}} \sum_{(\rho\alpha\beta)\in\mathcal{R}} \sum_{(\tau\gamma\delta)\in\mathcal{R}} \big[D_{(\tau\gamma\delta)}(\boldsymbol{w}(\xi))\big]^\top V_{,(\rho\alpha\beta)(\tau\gamma\delta)}(D\boldsymbol{u}(\xi))\big[D_{(\rho\alpha\beta)}\boldsymbol{v}(\xi)\big] \\
&\lesssim \sum_{\xi\in\mathcal{L}} \sum_{(\rho\alpha\beta)\in\mathcal{R}} \sum_{(\tau\gamma\delta)\in\mathcal{R}} \sum_{(\sigma\iota\chi)\in\mathcal{R}} |D_{(\rho\alpha\beta)}\boldsymbol{v}(\xi)|\cdot|D_{(\tau\gamma\delta)}\boldsymbol{w}(\xi)|\cdot|D_{(\sigma\iota\chi)}\boldsymbol{w}(\xi)| \\
&\lesssim \|\boldsymbol{v}\|_{\rm a_1}\cdot \sum_{\xi\in\mathcal{L}} \sum_{(\tau\gamma\delta)\in\mathcal{R}} \sum_{(\sigma\iota\chi)\in\mathcal{R}} |D_{(\tau\gamma\delta)}\boldsymbol{w}(\xi)|\cdot|D_{(\sigma\iota\chi)}\boldsymbol{w}(\xi)| \lesssim \|\boldsymbol{v}\|_{\rm a_1}\|\boldsymbol{w}\|^2_{\rm a_1}.
\end{aligned}$$

Consequently, $\bar{\mathcal{E}}^{\rm a}_{\rm hom}(\boldsymbol{u})$ is twice differentiable with

$$\langle \delta^2\bar{\mathcal{E}}^{\rm a}_{\rm hom}(\boldsymbol{u})\boldsymbol{v}, \boldsymbol{w}\rangle = \sum_{\xi\in\mathcal{L}} \sum_{(\rho\alpha\beta)\in\mathcal{R}} \sum_{(\tau\gamma\delta)\in\mathcal{R}} V_{,(\rho\alpha\beta)(\tau\gamma\delta)}(D\boldsymbol{u}(\xi)) : D_{(\rho\alpha\beta)}(\boldsymbol{v}(\xi)) : D_{(\tau\gamma\delta)}(\boldsymbol{w}(\xi)).$$

In a similar fashion, a Taylor expansion and a bound on the fourth derivative of V can be used to show that $\bar{\mathcal{E}}^{\rm a}_{\rm hom}(\boldsymbol{u})$ is three times differentiable with

$$\begin{aligned}
&\langle \delta^3\bar{\mathcal{E}}^{\rm a}_{\rm hom}(\boldsymbol{u})[\boldsymbol{v},\boldsymbol{w},\boldsymbol{z}]\rangle = \\
&\sum_{\xi\in\mathcal{L}} \sum_{(\rho\alpha\beta)\in\mathcal{R}} \sum_{(\tau\gamma\delta)\in\mathcal{R}} \sum_{(\sigma\iota\chi)\in\mathcal{R}} V_{,(\rho\alpha\beta)(\tau\gamma\delta)(\sigma\iota\chi)}(D\boldsymbol{u}(\xi))[D_{(\rho\alpha\beta)}(\boldsymbol{v}(\xi)), D_{(\tau\gamma\delta)}(\boldsymbol{w}(\xi)), D_{(\sigma\iota\chi)}(\boldsymbol{z}(\xi))].
\end{aligned}$$

Now for $\boldsymbol{u}\in\boldsymbol{\mathcal{U}}_0$, we see that $\mathcal{E}^{\rm a}_{\rm hom}(\boldsymbol{u})$ is well defined (finite) and $\mathcal{E}^{\rm a}_{\rm hom}(\boldsymbol{u}) = \bar{\mathcal{E}}^{\rm a}_{\rm hom}(\boldsymbol{u})$ due to (2.4). Since $\boldsymbol{\mathcal{U}}_0$ is dense in $\boldsymbol{\mathcal{U}}$, it follows that $\bar{\mathcal{E}}^{\rm a}_{\rm hom}$ is the unique, continuous extension of $\mathcal{E}^{\rm a}_{\rm hom}$ to $\boldsymbol{\mathcal{U}}$, which we have also proven to be C^3 on $\boldsymbol{\mathcal{U}}$. This completes the proof of Theorem 1.

A.3. **Lattice Stability.** Here we prove that if there exists any displacement $\boldsymbol{u}\in\boldsymbol{\mathcal{U}}$ such that

$$\langle \delta^2\mathcal{E}^{\rm a}(\boldsymbol{u})\boldsymbol{v}, \boldsymbol{v}\rangle \geq \gamma_{\rm a}\|\boldsymbol{v}\|^2_{\rm a_1}, \quad \forall\, \boldsymbol{v}\in\boldsymbol{\mathcal{U}}_0,$$

then the stability assumption of Assumption A is met.

Lemma 19. *Suppose that there exists a displacement $\boldsymbol{u}\in\boldsymbol{\mathcal{U}}$ such that*

$$\langle \delta^2\mathcal{E}^{\rm a}(\boldsymbol{u})\boldsymbol{v}, \boldsymbol{v}\rangle \geq \gamma_{\rm a}\|\boldsymbol{v}\|^2_{\rm a_1}, \quad \forall\, \boldsymbol{v}\in\boldsymbol{\mathcal{U}}_0.$$

Then the reference configuration satisfies (2.6)

Proof. The proof is a straightforward extension of [7, Lemma 2.2]. Fix a test pair $\boldsymbol{v}$ and let r be large enough so that $D\boldsymbol{v}$ has support in the ball of radius r. Our goal is to find a suitable sequence of test pairs $\boldsymbol{v}_n$ which satisfy

$$\lim_{n\to\infty}\langle \delta^2\mathcal{E}^{\rm a}(\boldsymbol{u}^\infty)\boldsymbol{v}_n, \boldsymbol{v}_n\rangle = \langle \delta^2\mathcal{E}^{\rm a}_{\rm hom}(0)\boldsymbol{v}, \boldsymbol{v}\rangle.$$

Take $\xi_n \in \mathcal{L}$ such that $|\xi_n| < |\xi_{n+1}|$ and $|\xi_n| \to \infty$, and further define $\boldsymbol{v}_n(\xi) = \boldsymbol{v}(\xi - \xi_n)$, which shifts the support of $D\boldsymbol{v}_n$ to $B_r(\xi_n)$. Consequently,

$$\begin{aligned}
\gamma_{\rm a}\|\boldsymbol{v}\|_{\rm a}^2 \leq \lim_{n\to\infty}\langle\delta^2\mathcal{E}^{\rm a}(\boldsymbol{u})\boldsymbol{v}_n,\boldsymbol{v}_n\rangle &= \lim_{n\to\infty}\sum_{\xi\in\mathcal{L}}\langle\delta^2V_\xi(D\boldsymbol{u})D\boldsymbol{v}_n(\xi),D\boldsymbol{v}_n(\xi)\rangle \\
&= \lim_{n\to\infty}\sum_{\xi\in\mathcal{L}\cap B_r(\xi_n)}\langle\delta^2V_\xi(D\boldsymbol{u})D\boldsymbol{v}(\xi-\xi_n),D\boldsymbol{v}(\xi-\xi_n)\rangle \\
&= \lim_{n\to\infty}\sum_{\xi\in\mathcal{L}\cap B_r(0)}\langle\delta^2V_{\xi+\xi_n}(D\boldsymbol{u}(\xi+\xi_n))D\boldsymbol{v}(\xi),D\boldsymbol{v}(\xi)\rangle \\
&= \sum_{\xi\in\mathcal{L}\cap B_r(0)}\lim_{n\to\infty}\langle\delta^2V_{\xi+\xi_n}(D\boldsymbol{u}(\xi+\xi_n))D\boldsymbol{v}(\xi),D\boldsymbol{v}(\xi)\rangle \\
&= \sum_{\xi\in\mathcal{L}\cap B_r(0)}\langle\delta^2V(0)D\boldsymbol{v}(\xi),D\boldsymbol{v}(\xi)\rangle,
\end{aligned}$$

by virtue of $V_\xi(D\boldsymbol{u}(\xi+\xi_n)) \to V(0)$ in ℓ^∞ which itself is due to $D\boldsymbol{u}^\infty \in \ell^2$. $\square$

A.4. **Proof of (3.4).**

Proof. Without loss of generality, we assume that

$$(\rho\alpha\beta) \in \mathcal{R} \quad \text{if and only if} \quad (-\rho\beta\alpha) \in \mathcal{R}.$$

This condition can always be met by enlarging the interaction range if necessary.

To prove (3.4), we then observe that

$$\begin{aligned}
&\langle\mathcal{E}^{\rm a}_{\rm hom}(0),\boldsymbol{v}\rangle \\
&= \sum_{(\rho\gamma\beta)\in\mathcal{R}}\hat{V}_{,(\rho\gamma\beta)}(D\boldsymbol{y}(\zeta))\cdot\big[v_\beta(\zeta+\rho)-v_\gamma(\zeta)\big] + \sum_{(\rho\beta\gamma)\in\mathcal{R}}\hat{V}_{,(\rho\beta\gamma)}(D\boldsymbol{y}(\zeta))\cdot\big[v_\gamma(\zeta+\rho)-v_\beta(\zeta)\big] \\
&- \sum_{(\rho\gamma\gamma)\in\mathcal{R}}\hat{V}_{,(\rho\gamma\gamma)}(D\boldsymbol{y}(\zeta))\cdot\big[v_\gamma(\zeta+\rho)-v_\gamma(\zeta)\big] + \sum_{\substack{(\sigma\iota\chi)\in\mathcal{R}\\ \sigma\neq0}}\sum_{(\rho\alpha\beta)\in\mathcal{R}}\hat{V}_{,(\rho\alpha\beta)}(D\boldsymbol{y}(\zeta+\sigma))\cdot D_{(\rho\alpha\beta)}\boldsymbol{v}(\zeta+\sigma) \\
&= -\sum_{(\rho\gamma\beta)\in\mathcal{R}}\hat{V}_{,(\rho\gamma\beta)}(D\boldsymbol{y}(\zeta)) + \sum_{(0\beta\gamma)\in\mathcal{R}}\hat{V}_{,(0\beta\gamma)}(D\boldsymbol{y}(\zeta)) - \sum_{(\rho\gamma\gamma)\in\mathcal{R}}\hat{V}_{,(\rho\gamma\gamma)}(D\boldsymbol{y}(\zeta)) \\
&+ \sum_{(\rho\gamma\gamma)\in\mathcal{R}}\hat{V}_{,(\rho\gamma\gamma)}(D\boldsymbol{y}(\zeta)) + \sum_{\substack{(\sigma\iota\chi)\in\mathcal{R}\\ \sigma\neq0}}\sum_{(\rho\alpha\beta)\in\mathcal{R}}\hat{V}_{,(\rho\alpha\beta)}(D\boldsymbol{y}(\zeta+\sigma))\cdot\big[v_\beta(\zeta+\sigma+\rho)-v_\alpha(\zeta+\sigma)\big] \\
&= -\sum_{(\rho\gamma\beta)\in\mathcal{R}}\hat{V}_{,(\rho\gamma\beta)}(D\boldsymbol{y}(\zeta)) + \sum_{(0\beta\gamma)\in\mathcal{R}}\hat{V}_{,(0\beta\gamma)}(D\boldsymbol{y}(\zeta)) + \sum_{\substack{(\sigma\beta\gamma)\in\mathcal{R}\\ \sigma\neq0}}\hat{V}_{,(-\sigma\beta\gamma)}(D\boldsymbol{y}(\zeta+\sigma)) \\
&= -\sum_{(\rho\gamma\beta)\in\mathcal{R}}\hat{V}_{,(\rho\gamma\beta)}(D\boldsymbol{y}(\zeta)) + \sum_{(\rho\beta\gamma)\in\mathcal{R}}\hat{V}_{,(\rho\beta\gamma)}(D\boldsymbol{y}(\zeta)) \\
&= -\sum_{(\rho\gamma\beta)\in\mathcal{R}}\hat{V}_{,(\rho\gamma\beta)}\big((\mathsf{G}\sigma+p_\chi-p_\iota)_{(\sigma\iota\chi)\in\mathcal{R}}\big) + \sum_{(\rho\beta\gamma)\in\mathcal{R}}\hat{V}_{,(\rho\beta\gamma)}\big((\mathsf{G}\sigma+p_\chi-p_\iota)_{(\sigma\iota\chi)\in\mathcal{R}}\big).
\end{aligned}$$

Meanwhile, straightforward computations yield

$$\partial_{p_\gamma}\hat{W}(\mathsf{G},\boldsymbol{p}) = \sum_{(\rho\beta\gamma)\in\mathcal{R}}\hat{V}_{,(\rho\beta\gamma)}\big((\mathsf{G}\sigma+p_\chi-p_\iota)_{(\sigma\iota\chi)\in\mathcal{R}}\big) - \sum_{(\rho\gamma\beta)\in\mathcal{R}}\hat{V}_{,(\rho\gamma\beta)}\big((\mathsf{G}\sigma+p_\chi-p_\iota)_{(\sigma\iota\chi)\in\mathcal{R}}\big).$$

□

A.5. **Proof of (3.11).** Applying the chain rule, and repeatedly using the fact that G satisfies $\partial_{\boldsymbol{p}}\hat{W}((\mathsf{G},\boldsymbol{p}))=0$, we obtain

$$\partial^2_{\mathsf{G}}\bar{W}(\mathsf{G})=\partial^2_{\mathsf{GG}}W(\mathsf{G},\boldsymbol{p})-\partial^2_{\mathsf{G}\boldsymbol{p}}W(\mathsf{G},\boldsymbol{p})[\partial^2_{\boldsymbol{pp}}W(\mathsf{G},\boldsymbol{p})]^{-1}\partial^2_{\boldsymbol{p}\mathsf{G}}W(\mathsf{G},\boldsymbol{p}).$$

From straightforward computations, we have

$$\begin{aligned}
\partial^2_{\boldsymbol{pp}}W(\mathsf{G},\boldsymbol{p}) &= J_{\boldsymbol{pp}}\\
\partial^2_{\mathsf{G}_{mn}\boldsymbol{p}^l_\beta}W(\mathsf{G},\boldsymbol{p}) &= \sum_{(\rho\alpha\beta)\in\mathcal{R}}\sum_{(\tau\gamma\delta)\in\mathcal{R}}V^{lm}_{,(\rho\alpha\beta)(\tau\gamma\delta)}(0)\tau_n-\sum_{(\rho\beta\alpha)\in\mathcal{R}}\sum_{(\tau\gamma\delta)\in\mathcal{R}}V^{lm}_{,(\rho\beta\alpha)(\tau\gamma\delta)}(0)\tau_n\\
\partial^2_{\mathsf{G}_{mn}\mathsf{G}_{rs}} &= \sum_{(\rho\alpha\beta)\in\mathcal{R}}\sum_{(\tau\gamma\delta)\in\mathcal{R}}V^{mr}_{,(\rho\alpha\beta)(\tau\gamma\delta)}(0)\rho_n\tau_s
\end{aligned}$$

so that

$$\begin{aligned}
\int_{\mathbb{R}^d}\mathrm{A}:\nabla Z:\nabla Z\,dx &= \int_{\mathbb{R}^d}\partial^2_{\mathsf{GG}}W(\mathsf{G},\boldsymbol{p}):\nabla Z:\nabla Z\,dx\\
&\quad-\int_{\mathbb{R}^d}\partial^2_{\mathsf{G}\boldsymbol{p}}W(\mathsf{G},\boldsymbol{p})[\partial^2_{\boldsymbol{pp}}W(\mathsf{G},\boldsymbol{p})]^{-1}\partial^2_{\boldsymbol{p}\mathsf{G}}W(\mathsf{G},\boldsymbol{p}):\nabla Z:\nabla Z\,dx\\
&=\int_{\mathbb{R}^d}\partial^2_{\mathsf{G}_{mn}\mathsf{G}_{rs}}W(\mathsf{G},\boldsymbol{p})\frac{\partial}{\partial x_n}Z_m(x)\frac{\partial}{\partial x_s}Z_r(x)\,dx\\
&\quad-\int_{\mathbb{R}^d}\partial^2_{\mathsf{G}_{rs}\boldsymbol{p}^\alpha_i}W(\mathsf{G},\boldsymbol{p})[J_{\boldsymbol{pp}}]^{-1}_{\alpha i\beta j}\partial^2_{\boldsymbol{p}^\beta_j\mathsf{G}_{mn}}W(\mathsf{G},\boldsymbol{p})\frac{\partial}{\partial x_n}Z_m(x)\frac{\partial}{\partial x_s}Z_r(x)\,dx\\
&=\int_{\mathbb{R}^d}4\pi^2\partial^2_{\mathsf{G}_{mn}\mathsf{G}_{rs}}W(\mathsf{G},\boldsymbol{p})k_nk_s\hat{Z}^*_m(k)\hat{Z}_r(x)\,dk\\
&\quad-\int_{\mathbb{R}^d}4\pi^2\hat{Z}^*_m(k)\partial^2_{\mathsf{G}_{rs}\boldsymbol{p}^\alpha_i}W(\mathsf{G},\boldsymbol{p})k_s[J_{\boldsymbol{pp}}]^{-1}_{\alpha i\beta j}\partial^2_{\boldsymbol{p}^\beta_j\mathsf{G}_{mn}}W(\mathsf{G},\boldsymbol{p})k_n\hat{Z}_r(k)\,dk\\
&=\int_{\mathbb{R}^d}\hat{Z}^*_m(k)J^{mr}_{00}(k)\hat{Z}_r(k)\,dk-\int_{\mathbb{R}^d}\hat{Z}^*_m(k)[J_{0\boldsymbol{p}}J^{-1}_{\boldsymbol{pp}}J_{\boldsymbol{p}0}]_{mr}\hat{Z}_r(k)\,dk\\
&=\int_{\mathbb{R}^d}\hat{Z}^*(k)M(k)\hat{Z}(k)\,dk\ \gtrsim\|\nabla Z\|^2_{L^2(\mathbb{R}^d)}.
\end{aligned}$$

This completes the proof of (3.11).

A.6. **Norm Equivalence. Lemma 20.** *The norms defined for $\boldsymbol{v}=(Z,\boldsymbol{q})$ by*

$$\|\boldsymbol{v}\|^2_{\mathrm{a}_3}=\|(Z,\boldsymbol{q})\|^2_{\mathrm{a}_3}:=\|2\pi|k|\hat{Z}\|^2_{L^2(\mathcal{B})}+\sum_{\alpha=1}^{S-1}\|\hat{q}_\alpha\|^2_{L^2(\mathcal{B})}$$

and

$$\|\boldsymbol{v}\|^2_{\mathrm{a}_2}:=\|\nabla IZ\|^2_{L^2(\mathbb{R}^d)}+\sum_\alpha\|Iq_\alpha\|^2_{L^2(\mathbb{R}^d)}.$$

are equivalent on $\boldsymbol{\mathcal{U}}$.

Proof. Note

$$\sum_{i=1}^{d}\sum_{\xi\in\mathcal{L}}|D_{e_i}v_0(\xi)|^2 \lesssim \|\nabla IZ\|^2_{L^2(\mathbb{R}^d)} \lesssim \sum_{i=1}^{d}\sum_{\xi\in\mathcal{L}}|D_{e_i}v_0(\xi)|^2$$

and

$$\begin{aligned}\sum_{i=1}^{d}\sum_{\xi\in\mathcal{L}}|D_{e_i}v_0(\xi)|^2 &= \sum_{i=1}^{d}\int_{\mathcal{B}}\widehat{D_{e_i}Z}^*\widehat{D_{e_i}Z}\\ &= \sum_{i=1}^{d}\int_{\mathcal{B}}4\sin^2(\pi k_i)|\hat{Z}|^2(k)\end{aligned}$$

Since

$$\|2\pi|k|Z\|^2_{L^2(\mathcal{B})} \lesssim \sum_{i=1}^{d}\int_{\mathcal{B}}4\sin^2(\pi k_i)|\hat{Z}|^2(k) \lesssim \|2\pi|k|\hat{Z}\|^2_{L^2(\mathcal{B})}$$

we see that

$$\|2\pi|k|\hat{Z}\|_{L^2(\mathcal{B})} \lesssim \|\nabla IZ\|^2_{L^2(\mathbb{R}^d)} \lesssim \|2\pi|k|\hat{Z}\|_{L^2(\mathcal{B})}.$$

Similarly,

$$\int_{\mathcal{B}}|\hat{q_\alpha}|^2 = \|q_\alpha\|_{\ell^2(\mathcal{L})} \lesssim \|Iq_\alpha\|^2_{L^2(\mathbb{R}^d)} \lesssim \|q_\alpha\|_{\ell^2(\mathcal{L})} = \int_{\mathcal{B}}|\hat{q_\alpha}|^2.$$

□

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