THE UNIVERSITY OF WARWICK

Original citation:

Ortner, Christoph and Theil, Florian. (2013) Justification of the Cauchy–Born approximation of elastodynamics. Archive for Rational Mechanics and Analysis, Volume 207 (Number 3). pp. 1025-1073.

JUSTIFICATION OF THE CAUCHY–BORN APPROXIMATION OF ELASTODYNAMICS

C. ORTNER AND F. THEIL

Abstract. We present sharp convergence results for the Cauchy–Born approximation of general classical atomistic interactions, for static problems with small data and for dynamic problems on a macroscopic time interval.

1. Introduction

The Cauchy–Born model (or, approximation) for *Bravais lattices* is the most widely used nonlinear elasticity model of crystal elasticity. It is obtained from the *Cauchy–Born rule*: the stored energy per unit volume under a macroscopically homogeneous deformation equals the energy per unit volume in the corresponding homogeneous crystal. This means that microstructural relaxation effects are ruled out. In some simple cases the Cauchy–Born model for Bravais lattices can be justified as a statement about minimum energy states [11, 6]. In less restricted settings it has been shown to provide a highly accurate approximation of crystal elastostatics [10].

It is highly desirable to obtain comparable results for evolutionary problems because of the importance of phenomena linked to energy transport and dissipation in crystallographic lattices [13, 18, 19]. The main contribution of this article is a rigorous approximation error analysis of the Cauchy–Born wave equation compared to the Newtonian equations of motion in the atomistic model. In this pursuit we are inspired by a recent effort of Blanc, Le Bris and Lions [4] who solve this problem for various one-dimensional examples with different classes of pair interactions.

Our own convergence result is formulated for a general class of multi-body interactions in an infinite lattice, and only requires the assumptions that the "reference lattice" is a "stable" Bravais lattice (see § 5.2) and that the interaction strength decays sufficiently fast. We also provide a rigorous approximation error analysis of the Cauchy–Born approximation for static problems under the same conditions. The lattice stability assumption is essential and cannot be removed (see § C).

Our main dynamic result, Theorem 6.2, is concerned with the Newtonian equations of motion and the nonlinear Cauchy–Born wave equation. In the scaling limit where both spatial and temporal fluctuation are of the order ε (the lattice spacing) we prove that the atomistic solution converges a solution of the Cauchy–Born wave equation. Moreover, difference between the atomistic and the Cauchy-Born solution is of order ε^2. The result for the static case (Theorem 5.4) is analogous.

These strong results are the consequence of sharp quantitative links between particle models and continuum models, which are also useful in a wider context [28, 20, 29]. In particular

Date: April 10, 2012.

2000 *Mathematics Subject Classification.* 65N12, 65N15, 70C20, 35J62, 35L72.

Key words and phrases. atomistic models, coarse graining, Cauchy–Born model, wave equation, approximation error.

This work was supported by the EPSRC Critical Mass Programme "New Frontiers in the Mathematics of Solids" (OxMoS), by the EPSRC grant EP/H003096 "Analysis of atomistic-to-continuum coupling methods".

the localization technique (1.2) provides a continuous representation of discrete objects. A key concept is the notion of atomistic stress, which gives a natural weak form of the first variation. *Pointwise* second-order consistency of the Piola–Kirchhoff stress of the Cauchy–Born model with the atomistic stress is established in Theorem 4.3. Error estimates between local minimizers of the Cauchy–Born and atomistic model are an immediate consequence of consistency. The proof in the dynamic case is based on a similar pointwise consistency result for the divergence of the stresses.

1.1. **Main results.** We assume that the *scaled* total atomistic energy E^ε can be written as

$$E^\varepsilon(u) = \varepsilon^d \sum_{\xi\in\varepsilon\Lambda} V\Big(\Big\{\tfrac{u(\xi+\varepsilon\rho)-u(\xi)}{\varepsilon}\Big\}_{\rho\in\Lambda\setminus\{0\}}\Big),$$

where $\Lambda := \mathbb{Z}^d$, $u : \varepsilon\Lambda \to \mathbb{R}^d$ is a discrete displacement and V a multi-body potential describing the interaction between a site ξ and the rest of the body. The continuum limit is characterized by the Cauchy–Born energy density function $W(\mathsf{F}) = V(\{\mathsf{F}\rho\}_{\rho\in\Lambda\setminus\{0\}})$ and the associated functional $E(u) = \int_{\mathbb{R}^d} W(\nabla u)\,\mathrm{d}x$. We will show that E characterizes the asymptotic behavior of solutions of static and dynamic problems associated with E^ε. We assume throughout this section that $d \le 3$ and that Λ is stable (see § 5.2).

Theorem A (Elastostatics). *There exists constants $C_{\rm stat}, C, \delta_0 > 0$ such that for all $f : \mathbb{R}^d \to \mathbb{R}^d$, $f^\varepsilon : \varepsilon\Lambda \to \mathbb{R}^d$ satisfying*

$$\|f\|_1 \le \delta_0 \quad \textit{and} \quad \|f - f^\varepsilon\|_{-1} \le C_{\rm stat}\varepsilon^2,$$

and for ε sufficiently small, there exist local minimizers u, u^ε of the energies

$$E(u) - \int_{\mathbb{R}^d} f\cdot u\,\mathrm{d}x \quad \textit{and} \quad E^\varepsilon(u) - \varepsilon^d \sum_{\xi\in\varepsilon\Lambda} f^\varepsilon(\xi)\cdot u^\varepsilon(\xi),$$

which also satisfy the bound $\|\nabla u - \nabla u^\varepsilon\|_{L^2} \le C\varepsilon^2$.

The definition of the norms $\|\cdot\|_1$, $\|\cdot\|_{-1}$ and a precise formulation of the result are given in Theorem 5.4.

Theorem B (Elastodynamics). *There exist constants $\kappa, T, C > 0$ such that, for all initial states (u_0, u_1), (u_0^ξ, u_1^ξ) satisfying the bounds*

$$\|\nabla u_0\|_{L^\infty} \le \kappa \qquad \textit{and} \qquad \|\nabla u_0 - \nabla u_0^\xi\|_{L^2} + \|u_1 - u_1^\xi\|_{L^2} \le C_{\rm init}\,\varepsilon^2,$$

where $C_{\rm init}$ is independent of ε, and for all sufficiently small ε, there exist unique solutions $u \in C^2([0,T], H^2(\mathbb{R}^d))$ and $u^\varepsilon \in C^2([0,T], \ell^2(\Lambda))$ of the Cauchy problems

$$\begin{aligned} &\ddot u - \mathrm{div}\mathsf{S}^{\rm c}(\nabla u) = 0, && u(t=0) = u_0, && \dot u(t=0) = u_1,\\ &\ddot u^\varepsilon + \delta E^\varepsilon(u^\varepsilon) = 0, && u^\varepsilon(t=0) = u_0^\xi, && \dot u^\varepsilon(t=0) = u_1^\xi, \end{aligned}$$

where δE^ε denotes the first variation of E^ε, and $\mathsf{S}^{\rm c}_{ij}(F) = \frac{\partial W}{\partial \mathsf{F}_{ij}}(\mathsf{F})$ is the first Piola–Kirchhoff stress tensor in the Cauchy–Born model. The solutions u, u^ε satisfy the estimate

$$\max_{0\le t\le T}\big(\|\nabla u(t) - \nabla\tilde u^\varepsilon(t)\|_{L^2} + \|\dot u - \dot u^\varepsilon(t)\|_{L^2}\big) \le C\varepsilon^2. \tag{1.1}$$

The definition of the norm $\|\cdot\|_3$ and the precise formulation of the result is given in Theorem 6.2. We note that the condition $\|\nabla u_0\|_{L^\infty} \le \kappa$ is a fairly mild condition, which only ensure that u_0 is a “stable configuration”.

We make no statement about the maximal time interval for which the estimate (1.1) holds. Such a statement could be made provided one establishes an atomistic Gårding inequality.

Moreover, such a result would also allow us to treat large deformations in the static case. We stress, however, that our estimates hold for a *macroscopic time interval.*

1.2. **New Concepts.** The comparison of discrete displacements u^ε with continuous displacements u is achieved by the introduction of several approximation operators derived from a nodal basis function ζ with compact support (see § 2.1 for the details). We define the Lipschitz continuous interpolation u^ε and a quasi-interpolation $\tilde{u}^\varepsilon$, which has a Lipschitz-continuous gradient. The key property property of the framework is that it delivers an integral representation of finite differences

$$\frac{\tilde{v}(\xi+\varepsilon\rho)-\tilde{v}(\xi)}{\varepsilon} = \int_{\mathbb{R}^d} \chi^\varepsilon_{\xi,\rho}(x)\nabla_\rho v(x)\,\mathrm{d}x, \quad \text{where} \quad \chi^\varepsilon_{\xi,\rho}(x) := \varepsilon^{-1}\int_0^1 \zeta(\xi+t\varepsilon\rho-x)\,\mathrm{d}t. \tag{1.2}$$

The kernel $\chi^\varepsilon_{\xi,\rho}$ can be understood as a mollified version of the line measure supported on the bond $\{\xi + t\rho \,|\, t \in [0,\varepsilon]\}$.

A version of this technique was proposed by Shapeev [31] for the construction of atomistic-to-continuum coupling schemes. Here we propose an analytically convenient and stable variant of his idea, which is analyzed in detail in [25].

Using (1.2) we can construct an integral represenation of the first variation of the atomistic energy,

$$\big\langle \delta E^\varepsilon(u^\varepsilon), \tilde{v}\big\rangle = \int_{\mathbb{R}^d} \mathsf{S}^\varepsilon(u^\varepsilon;x) : \nabla v(x)\,\mathrm{d}x, \tag{1.3}$$

for all compactly supported virtual displacements v, where S^ε is the *stress* associated with a discrete displacement u^ε,

$$\mathsf{S}^\varepsilon(u^\varepsilon;x) = \sum_{\xi\in\varepsilon\Lambda}\sum_{\xi'\in\varepsilon\Lambda\setminus\{\xi\}} \big[f_{\xi,\xi'}\otimes(\xi'-\xi)\big]\chi^\varepsilon_{\xi,\rho}(x); \tag{1.4}$$

here, $f_{\xi,\xi'}$ is the force acting between atoms ξ and ξ' due to the site-energy associated with atom ξ. A precise definition of the atomistic stress is given in § 4.1. We will prove in § 4.2 that $|\mathsf{S}^{\mathrm{c}} - \mathsf{S}^\varepsilon| = O(\varepsilon^2)$ and in § 6.3 that $|\mathrm{div}(\mathsf{S}^{\mathrm{c}} - \mathsf{S}^\varepsilon)| = O(\varepsilon^2)$, which are the key technical ingredient required for proving Theorems A and B.

Remark 1.1. The tensor S^ε is closely related to the stress defined by Hardy [12]. Indeed, equation (4.5) in that work is essentially an Eulerian version of (1.4), for pair interactions, with a generic weighting function $\chi^\varepsilon_{\xi,\rho}$. A general account of stress in molecular dynamics simulations is given in the recent work of Admal and Tadmor [1].

A concern discussed in [1] is the *non-uniqueness* of stress: note that S^ε is defined by (1.3) only up to a divergence-free tensor. Indeed, it is possible to add "discrete null-Lagrangians" to the atomistic energy, or decompose the atomistic energy in different ways, which would lead to different definitions of the atomistic stress S^ε.

Concerning this question, our work provides a selection mechanism based on comparison with the Cauchy–Born stress. If V is selected to be "as local as possible" (cf. § 2.3.4) and to satisfy an inversion symmetry (cf. § 2.3.3), then the atomistic stress S^ε and the Cauchy–Born stress S^{c} are second-order close. Since there is a natural definition for S^{c}, our version of the atomistic stress is reasonable whenever the atomistic configuration is "close" to an elastic continuum configuration. □

1.3. **Outline.** Since we work in an infinite domain, and admit an infinite interaction range, even the definition of the atomistic energy is non-trivial. Section 2 is devoted to this task. At the same time we establish various auxiliary results that are useful for the subsequent analysis. In Section 3 we define and analyze the Cauchy–Born approximation; in particular, we establish differentiability of the stored energy function and establish a convenient functional analytic setting. In Section 4 we derive and analyze the atomistic stress, which plays a prominent role in our analysis. In Section 5 we present a rigorous approximation error analysis of the static Cauchy–Born approximation. Finally, in Section 6 we establish approximation error estimates between the solutions of Newton's equations of motion and the Cauchy–Born wave equation.

1.4. **Summary of notation.** Throughout, $\mathbb{R}$ denotes the real numbers, and $d \in \mathbb{N}$ the space dimension.

Positions in space are usually denoted by $x, y, z \in \mathbb{R}^d$, while lattice sites are denoted by $\xi, \eta \in \Lambda := \mathbb{Z}^d$. Displacements, either continuous or discrete, are denoted by u, v, w. Lattice directions are denoted by $\rho, \varsigma, \tau \in \Lambda_* := \mathbb{Z}^d \setminus \{0\}$.

Matrices are denoted by capital letters, $\mathsf{A}, \mathsf{F}, \mathsf{G}, \mathsf{S} \in \mathbb{R}^{d\times d}$. In particular, A is reserved for the lattice orientation (beginning of § 2), and S for stress tensors.

If $f : \mathbb{R}^d \to \mathbb{R}^m$ is differentiable in x then we denote its Jacobi matrix by $\nabla f(x)$ and a direction derivative by $\nabla_r f(x) = \nabla f(x) \cdot r$, $r \in \mathbb{R}^d$. Higher derivatives are denoted by $\nabla^j f$ and are understood as j-linear forms with range in $\mathbb{R}^m$.

If $\mathscr{A}, \mathscr{B}$ are Banach spaces and $\mathscr{F} : \mathscr{A} \to \mathscr{B}$ is j times Fréchet differentiable (or simply, differentiable) in a then we denote its j-th derivative (or, variation if $\mathscr{B} = \mathbb{R}$) by $\delta^j \mathscr{F}$, which is understood as a j-linear form with range in $\mathscr{B}$. If $a, a_1, \dots, a_j \in \mathscr{A}$, then we write $\delta^j \mathscr{F}(a)[a_1, \dots, a_j]$ to evaluate this form.

If $\ell : \mathscr{A} \to \mathbb{R}$ is a linear functional, then we write $\ell(a) = \langle \ell, a\rangle$. If $E : \mathscr{A} \to \mathbb{R}$ is differentiable, then we write $\delta E(a)[a_1] = \langle \delta E(a), a_1\rangle$. If it is twice differentiable then we will also write $\delta^2 E(a)[a_1, a_2] = \langle \delta^2 E(a) a_1, a_2\rangle$.

We use $L^p, W^{1,p}$, for $p \in [1, \infty]$, to denote the standard Sobolev and Lebesgue spaces, usually on the domain $\mathbb{R}^d$ (and otherwise specified). We will also employ the so-called *homogeneous Sobolev spaces*, $\dot{W}^{j,p}$, which are defined in § 3.1. Negative-norm (dual) spaces are denoted by $W^{-1,p} = (W^{1,p'})^*$ and $\dot{W}^{-1,p} = (\dot{W}^{1,p'})^*$, where $p' := p/(p-1) \in [1, \infty]$ is the dual Sobolev index.

The discrete "Lebesgue space" is denoted by ℓ^p, usually with domain $\mathbb{Z}^d$ and otherwise specified. Since most discrete versions of $W^{1,p}$ would be equivalent to ℓ^p, we will not define such a space. However, we make heavy use of *discrete homogeneous Sobolev spaces* $\dot{\mathscr{W}}^{1,p}$, which are defined in §2.1.

Finally, we make the convention that "$\lesssim$" stands for "$\leq C$", where C is a generic constant that may not depend on any data in the model, nor on any functions involved in the inequality. In particular, we will make explicit all dependence on the interaction potential, which is crucial since we admit an infinite interaction range.

2. The Atomistic Energy

We formulate an atomistic model with classical multi-body interactions on an infinite Bravais lattice. As discrete reference domain, we choose $\Lambda := \mathbb{Z}^d$, where $d \in \mathbb{N}$ (later restricted to $d \leq 3$) is fixed throughout. We admit deformations of the form $y(\xi) = \mathsf{A}\xi + u(\xi)$, where u is an unknown displacement and $\mathsf{A} \in \mathbb{R}^{d\times d}$, $\det \mathsf{A} > 0$, defines the reference state of the system, $\mathsf{A} \cdot \Lambda$, which may be an arbitrary Bravais lattice.

We now present a formal definition of the atomistic potential energy, which we make rigorous throughout the remainder of the section. Let $\Lambda_* := \Lambda \setminus \{0\}$ denote the set of lattice directions. For discrete maps $v : \Lambda \to \mathbb{R}^m$, $m \in \mathbb{N}$, we define the finite differences and finite difference stencils

$$D_\rho v(\xi) := v(\xi+\rho) - v(\xi), \qquad \text{for } \xi \in \Lambda, \rho \in \Lambda_*, \quad \text{and}$$
$$Dv(\xi) := \big(D_\rho v(\xi)\big)_{\rho\in\Lambda_*}, \qquad \text{for } \xi \in \Lambda.$$

A convenient space of finite-difference stencils is

$$\mathscr{D} := \big\{ \boldsymbol{g} = (g_\rho)_{\rho\in\Lambda_*} \,\big|\, g_\rho \in \mathbb{R}^d, \|\boldsymbol{g}\|_{\mathscr{D}} < \infty \big\},$$

equipped with the norm $\|\boldsymbol{g}\|_{\mathscr{D}} := \max_{\rho\in\Lambda_*} |g_\rho|/|\rho|$.

Next, we assume that there exists a site-energy $V : \mathscr{D} \to \mathbb{R} \cup \{\pm\infty\}$, so that the atomistic potential energy of a displacement $u : \Lambda \to \mathbb{R}^d$ can be written, *formally*, as

$$E^{\mathrm{a}}(u) := \sum_{\xi\in\Lambda} \Phi_\xi(u), \quad \text{where } \Phi_\xi(u) := V(Du(\xi)). \tag{2.1}$$

Note that the site-energies are not well-defined for general u, and moreover their sum need not exist. In the remainder of this section, we introduce a discrete function space setting in which we can make (2.1) rigorous.

We remark that V implicitly depends on A, but since A is fixed throughout, we suppress this dependence.

2.1. **Interpolation of lattice functions.** We denote the set of all vector-valued lattice functions by $\mathscr{W}$ and those with compact support by $\mathscr{W}_0$:

$$\mathscr{W} := \big\{ v : \Lambda \to \mathbb{R}^d \big\} \quad \text{and} \quad \mathscr{W}_0 := \big\{ v \in \mathscr{W} \,\big|\, \mathrm{supp}(v) \text{ is compact} \big\}.$$

To facilitate the transition between continuous and discrete maps we introduce two (quasi-) interpolants of lattice functions.

Let $\zeta \in W^{1,\infty}(\mathbb{R}^d;\mathbb{R})$ satisfy $\zeta(\xi) = 0$ for $\xi \in \Lambda \setminus \{0\}$ and $\zeta(0) = 1$. We understand $\zeta(\,\cdot\, - \xi)$ as a nodal basis function associated with the site ξ, and define the *first-order interpolant*

$$v(x) := \sum_{\xi\in\Lambda} v(\xi)\zeta(x-\xi), \qquad \text{for } v \in \mathscr{W}. \tag{2.2}$$

We shall assume throughout that $\zeta \geq 0$, ζ has compact support, ζ is symmetric about the origin $\zeta(-x) = \zeta(x)$, and that the associated interpolation operator reproduces affine functions: $\sum_{\xi\in\Lambda}(a+b\cdot\xi)\zeta(x-\xi) = a+b\cdot x$ for all $a \in \mathbb{R}, b \in \mathbb{R}^d$. The latter property implies, in particular, that $\int_{\mathbb{R}^d} \zeta \,\mathrm{d}x = 1$.

Following [31], we also define a quasi-interpolant obtained through convolution of v with ζ:

$$\tilde{v}(x) := (\zeta * v)(x) = \int_{\mathbb{R}^d} \zeta(x-y)v(y)\,\mathrm{d}y. \tag{2.3}$$

In general, $v(\xi) \neq \tilde{v}(\xi)$ for $\xi \in \Lambda$, hence it is only a quasi-interpolant. The introduction of this second interpolant leads to a set of techniques centered around the *localization formula* [31, 25] (cf. the scaled version in (1.2))

$$D_\rho\tilde{v}(\xi) = \int_{\mathbb{R}^d} \chi_{\xi,\rho}(x)\nabla_\rho v(x)\,\mathrm{d}x, \qquad \text{where} \quad \chi_{\xi,\rho}(x) := \int_0^1 \zeta(\xi+t\rho-x)\,\mathrm{d}t, \tag{2.4}$$

which yield surprisingly strong connections between the atomistic model and its continuum counterpart (in particular, the definition and analysis of the atomistic stress in §4). To prove (2.4), we simply note that

$$D_\rho\tilde{v}(\xi) = \int_0^1 \nabla_\rho\tilde{v}(\xi+t\rho)\,\mathrm{d}t = \int_{\mathbb{R}^d}\int_0^1 \zeta(\xi+t\rho-x)\,\mathrm{d}t\,\nabla_\rho v(x)\,\mathrm{d}x.$$

Remark 2.1. A canonical choice for ζ is the Q1-nodal basis function

$$\zeta(x) := \prod_{i=1}^d \max\big(0, 1 - |x_i|\big),$$

then $\mathrm{supp}(\zeta) = [-1,1]^d$ and ζ is piecewise multi-linear. In this case $\{v \,|\, v \in \mathscr{W}\}$ is the Q1 finite element space, or equivalently, the space of tensor product linear B-splines and $\{\tilde{v} \,|\, v \in \mathscr{W}\}$ is the space of cubic tensor product B-splines [14]. However, other choices are equally possible, and indeed necessary in some situations [28]. Since none of our results require explicit knowledge of the type of interpolant, we admit the most general case. □

We now collect several auxiliary results on the lattice interpolants introduced above, all of which are established in [25].

Lemma 2.2. *Let $v \in \mathscr{W}$, then its first-order interpolant* (2.2) *belongs to $W^{1,\infty}_{\mathrm{loc}}(\mathbb{R}^d;\mathbb{R}^d)$, and $\tilde{v} \in W^{3,\infty}_{\mathrm{loc}}(\mathbb{R}^d;\mathbb{R}^d)$. Moreover, for any $p \in [1,\infty]$,*

$$\|v\|_{\ell^p} \lesssim \|\tilde{v}\|_{\ell^p} \le \|\tilde{v}\|_{L^p} \le \|v\|_{L^p} \lesssim \|v\|_{\ell^p} \qquad \forall v \in \mathscr{W}, \quad \text{and} \tag{2.5}$$

$$\|\nabla v\|_{L^p} \lesssim \|\nabla \tilde{u}\|_{L^p} \le \|\nabla v\|_{L^p} \qquad \forall v \in \mathscr{W}. \tag{2.6}$$

(All constants in the above estimates are independent of p.)

Next, we state a useful embedding result; of particular interest is the case $j = m = 1$ and $q = \infty$, which states (employing (2.6)) that $\|\nabla u\|_{L^\infty} \lesssim \|\nabla u\|_{L^p}$ for all $p \in [1,\infty]$. The proof uses the fact that the "mesh size" in $\mathbb{Z}^d$ is one, and that $\ell^p \subset \ell^\infty$.

Lemma 2.3. *Let $0 \le j \le m \le 3$ and $p \le q \in [1,\infty]$, then $\|\nabla^m \tilde{u}\|_{L^q} \lesssim \|\nabla^j \tilde{u}\|_{L^p}$ for all $u \in \mathscr{W}$.*

2.2. **The space of admissible displacements.** Since the atomistic model is formally translation invariant, we define equivalence classes

$$[u] := \{u + t \,|\, t \in \mathbb{R}^d\}, \qquad \text{for } u \in \mathscr{W},$$

and, for $p \in [1,\infty]$, define corresponding function spaces

$$\dot{\mathscr{W}}^{1,p} := \big\{[u] \,\big|\, u \in \mathscr{W}, \|\nabla u\|_{L^p} < +\infty\big\}. \tag{2.7}$$

We will not make the distinction between u and $[u]$, whenever it is possible to do so without confusion, for example, when a statement or function with argument u is translation invariant.

Proposition 2.4. *$\dot{\mathscr{W}}^{1,p}$ is a Banach space. For $p \in (1,\infty)$, the subspace $\{[v] \,|\, v \in \mathscr{W}_0\}$ is dense in $\dot{\mathscr{W}}^{1,p}$.*

Let $u \in \dot{\mathscr{W}}^{1,p}$, $p < \infty$, be a discrete displacement and $y(\xi) := \mathsf{A}\xi + u(\xi)$ be the associated deformation. It is shown in [25] that $|u(\xi)| \ll |\xi|$ as $|\xi| \to \infty$. Therefore, the discrete deformation satisfies the far-field boundary condition

$$y(\xi) = \mathsf{A}\xi + o(|\xi|) \quad \text{as } |\xi| \to \infty.$$

Aside from satisfying a boundary condition we also require that deformations are injective. Since our main results do not cover arbitrarily large deformations, we will circumvent the question of injectivity by placing an L^∞-bound on the displacement gradient (this will be ensured through conditions on the external forces). Notationally, we fix a constant $\kappa > 0$, and define

$$\mathscr{K} := \big\{u \in \mathscr{W} \,\big|\, |D_\rho u(\xi)| \le \kappa \text{ for all } \xi \in \Lambda, \rho \in \Lambda_*\big\}. \tag{2.8}$$

If κ is chosen sufficiently small, then displacements belonging to $\mathscr{K}$ give rise to injective deformations. Indeed, if $\kappa < \|\mathsf{A}^{-1}\|^{-1}$, where $\|\cdot\|$ denotes the ℓ^2-operator norm, then

$$\big|y(\xi) - y(\eta)\big| \ge \mu\big|\mathsf{A}(\xi - \eta)\big| \qquad \forall \xi, \eta \in \Lambda, \tag{2.9}$$

where $\mu := 1 - \kappa\|\mathsf{A}^{-1}\| > 0$.

To conclude the discussion of discrete function spaces, we note that we can define a smooth nodal interpolant on $\dot{\mathscr{W}}^{1,p}$, which will be useful in interpreting our results.

Lemma 2.5. *Let $u \in \dot{\mathscr{W}}^{1,p}$, $p \in [1,\infty]$, then there exists $w \in \dot{\mathscr{W}}^{1,p}$ such that $u = \tilde{w} =: Iu$. Moreover,*

$$\|\nabla u\|_{L^p} \lesssim \|\nabla Iu\|_{L^p} \lesssim \|\nabla u\|_{L^p} \qquad \forall u \in \dot{\mathscr{W}}^{1,p}. \tag{2.10}$$

2.3. Assumptions on the interaction potential.

2.3.1. *Energy difference.* We assume throughout that $V(\mathbf{0}) = 0$. Physically, this condition means that E^{a} is an energy difference between the deformed state $y(\xi) = \mathsf{A}\xi + u(\xi)$ and the reference state $y(\xi) = \mathsf{A}\xi$, which may have infinite energy.

2.3.2. *Smoothness.* We assume that V is "smooth" at injective configurations; more precisely, we define $\mathscr{D}_\kappa := \{\boldsymbol{g} \in \mathscr{D} \,|\, \|\boldsymbol{g}\|_{\mathscr{D}} \le \kappa\}$, and assume that $V \in C^k(\mathscr{D}_\kappa)$, for some $k \ge 2$ and for all κ that are sufficiently small.

For $\boldsymbol{g} \in \mathscr{D}_\kappa$ and for any "multi-index" $\boldsymbol{\rho} \in \Lambda_*^j, 1 \le j \le k$, the partial derivative

$$V_{\boldsymbol{\rho}}(\boldsymbol{g}) := \frac{\partial^j V(\boldsymbol{g})}{\partial g_{\rho_1} \dots \partial g_{\rho_j}} \in \mathbb{R}^{d^j}$$

exists; $V_{\boldsymbol{\rho}}(\boldsymbol{g})$ is understood as a multilinear form acting on families of vectors $\boldsymbol{h} = (h_1, \dots, h_j)$; $V_{\boldsymbol{\rho}}(\boldsymbol{g})[\boldsymbol{h}] = V_{\rho_1 \cdots \rho_j}(\boldsymbol{g})[h_1, \dots, h_j]$.

We also define the associated partial derivatives of the site-energies by $\Phi_{\xi,\boldsymbol{\rho}}(u) := V_{\boldsymbol{\rho}}(Du(\xi))$, or,

$$\Phi_{\xi,\boldsymbol{\rho}}(u)[D_{\boldsymbol{\rho}}\boldsymbol{v}(\xi)] = \Phi_{\xi,\rho_1\cdots\rho_j}[D_{\rho_1}v_1(\xi), \dots, D_{\rho_j}v_j(\xi)] = V_{\boldsymbol{\rho}}(Du(\xi))[D_{\boldsymbol{\rho}}\boldsymbol{v}(\xi)],$$

where $D_{\boldsymbol{\rho}}\boldsymbol{v}(\xi) = (D_{\rho_1}v_1(\xi), \dots, D_{\rho_j}v_j(\xi))$ for $\rho_i \in \Lambda_*, v_i \in \dot{\mathscr{W}}$, $i = 1, \dots, j$.

2.3.3. *Symmetry.* We assume throughout that V satisfies the following inversion symmetry:

$$V\big((-g_{-\rho})_{\rho \in \Lambda_*}\big) = V(\boldsymbol{g}) \qquad \forall \boldsymbol{g} \in \mathscr{D}. \tag{2.11}$$

This condition is physically motivated by the fact that permutations of atoms and isometries should not change the energy of a system. The requirement (2.11) then assumes that the global energy was partitioned in a way that preserves this symmetry.

Lemma 2.6. *Let $\mathsf{F} \in \mathbb{R}^{d\times d}$, $|\mathsf{F}| \le \kappa$, then*

$$V_{-\boldsymbol{\rho}}(\mathsf{F}\cdot\Lambda_*) = (-1)^j V_{\boldsymbol{\rho}}(\mathsf{F}\cdot\Lambda_*) \qquad \forall \boldsymbol{\rho} \in \Lambda_*^j, \quad 1 \le j \le k. \tag{2.12}$$

Proof. Let $\boldsymbol{g}_{\mathsf{F}} := \mathsf{F}\cdot\Lambda_*$, then $\boldsymbol{g}_{\mathsf{F}}' := (-\mathsf{F}(-\rho))_{\rho\in\Lambda_*} = \boldsymbol{g}_{\mathsf{F}}$. Since V is k times differentiable in $\mathscr{D}_\kappa$, we can differentiate (2.11) at $\boldsymbol{g}_{\mathsf{F}}$. Evaluating the first and second derivatives gives the stated result. □

2.3.4. *Decay Hypothesis.* Sufficiently rapid decay of the interatomic interaction is a crucial ingredient in our analysis. We define the following basic bounds on the interaction potential: With this notation, we define the bounds

$$m(\boldsymbol{\rho}) := \prod_{i=1}^{j} |\rho_i| \sup_{\boldsymbol{g}\in\mathscr{D}_\kappa} \|V_{\boldsymbol{\rho}}(\boldsymbol{g})\| \qquad \text{for } \boldsymbol{\rho}\in\Lambda_*^j, \quad 1\le j\le k,$$

where $\|\ell\| := \sup_{\boldsymbol{h}\in(\mathbb{R}^d)^j, |h_1|=\dots=|h_j|=1} \ell[h_1,\dots,h_j]$ for a j-linear form ℓ. We shall assume throughout that V and κ are such, that

$$M^{(j)} := \sum_{\boldsymbol{\rho}\in\Lambda_*^j} m(\boldsymbol{\rho}) < +\infty, \qquad \text{for } 1\le j\le k, \tag{2.13}$$

which will ensure that E^{a} is k times Fréchet differentiable (cf. Theorem 2.8).

In order to describe the class of admissible potentials, we also discuss the decay assumption we will require in the static and dynamic approximation error analysis. To simplify the following expressions, we define $|\boldsymbol{\rho}| := \sum_{i=1}^{j} |\rho_i|$, for $\boldsymbol{\rho}\in\Lambda_*^j$, $j\in\mathbb{N}$.

Let $p\in[1,\infty]$ and $2\le j\le k$. In the static analysis, we will assume finiteness of certain

$$M_{\mathrm{s}}^{(j,p)} := \sum_{\boldsymbol{\rho}\in\Lambda_*^j} m_{\mathrm{s}}^{(p)}(\boldsymbol{\rho}), \quad \text{where}$$

$$m_{\mathrm{s}}^{(p)}(\boldsymbol{\rho}) := m(\boldsymbol{\rho})|\boldsymbol{\rho}|^2 \Big(\sum_{i=2}^{j} \big(|\rho_1\times\rho_i| + |\rho_1| + |\rho_i|\big)\Big)^{\frac{1}{(j-1)p}}, \quad \text{for } \boldsymbol{\rho}\in\Lambda_*^j.$$

In the dynamic analysis we will assume finiteness of certain constants of the form

$$M_{\mathrm{d}}^{(j,p)} := \sum_{\boldsymbol{\rho}\in\Lambda_*^j} m_{\mathrm{d}}^{(p)}(\boldsymbol{\rho}), \quad \text{where}$$

$$m_{\mathrm{d}}^{(p)}(\boldsymbol{\rho}) := \frac{m(\boldsymbol{\rho})|\boldsymbol{\rho}|^3}{|\rho_1|} \Big(\sum_{i=2}^{j} \big(|\rho_1\times\rho_i| + |\rho_1| + |\rho_i|\big)\Big)^{\frac{1}{(j-1)p}}, \quad \text{for } \boldsymbol{\rho}\in\Lambda_*^j.$$

These constants naturally arise in the modeling error estimates established in §4.3 and §6.3.

We stress that, while finiteness of $M^{(j)}$, $1\le j\le k$, is a standing assumption, we will assume finiteness of $M_{\mathrm{s}}^{(j,p)}$ and $M_{\mathrm{d}}^{(j,p)}$, for certain choices of j and p, only when required.

Remark 2.7. If E^{a} contains only pair interactions, then we can write V in the form

$$V(\boldsymbol{g}) = \frac{1}{2}\sum_{\rho\in\Lambda_*} \big[\varphi(|g_\rho|) - \varphi(|\mathsf{A}\rho|)\big],$$

which clearly satisfies the symmetry (2.11). Moreover, we show in §B.1 that, if $\varphi^{(j)}(r) \lesssim r^{-\alpha-j}$ for $r\ge 1$, $1\le j\le k$, then

$$M^{(j)} \lesssim \sum_{\rho\in\Lambda_*} |\rho|^{-\alpha}, \quad \text{and} \quad M_{\mathrm{s}}^{(j,2)} + M_{\mathrm{d}}^{(j,2)} \lesssim \sum_{\rho\in\Lambda_*} |\rho|^{5/2-\alpha}.$$

It therefore follows that the constants $M^{(j)}$ are finite provided that $\alpha > d$ and that $M_{\mathrm{s}}^{(j,2)}, M_{\mathrm{d}}^{(j,2)}$ are finite provided that $\alpha > d+5/2$. In particular, this implies that the Lennard-Jones potential, $\varphi(r) = r^{-12} - 2r^{-6}$, is included in our analysis.

In §B we discuss other commonly employed potentials and show that they fall within our assumptions. □

2.4. **Definition of the atomistic energy.** We mentioned at the beginning of §2 that, due to the infinite domain and the infinite interaction range, the definition of the energy (2.1) is non-trivial. The purpose of this section is to give (2.1) a rigorous interpretation.

Theorem 2.8 (Regularity of E^{a}). *(i) If $u \in \mathscr{W}_0 \cap \mathscr{K}$, then $(\Phi_\xi(u))_{\xi\in\Lambda} \in \ell^1$; that is, $E^{\mathrm{a}}(u)$ given by* (2.1) *is well-defined.*

(ii) $E^{\mathrm{a}} : (\mathscr{W}_0 \cap \mathscr{K}, \|\cdot\|_{\dot{\mathscr{W}}^{1,2}}) \to \mathbb{R}$ is continuous; that is, there exists a unique continuous extension to $\dot{\mathscr{W}}^{1,2} \cap \mathscr{K}$, which we still denote by E^{a}.

(iii) $E^{\mathrm{a}} \in C^k(\dot{\mathscr{W}}^{1,2} \cap \mathscr{K})$, with

$$\delta^j E^{\mathrm{a}}(u)[\boldsymbol{v}] = \sum_{\xi\in\Lambda} \sum_{\boldsymbol{\rho}\in\Lambda_*^j} \Phi_{\xi,\boldsymbol{\rho}}(u)[D_{\boldsymbol{\rho}}\boldsymbol{v}(\xi)] \tag{2.14}$$

for $j = 1, \dots, k$, for all $u \in \dot{\mathscr{W}}^{1,2}$ and $\boldsymbol{v} \in \mathscr{W}_0^j$. Moreover, if $1 \le j \le k$ and $\sum_{i=1}^j \frac{1}{p_i} = 1$, $p_i \in [1,\infty]$, then

$$\big|\delta^j E^{\mathrm{a}}(u)[\boldsymbol{v}]\big| \lesssim M^{(j)} \prod_{i=1}^j \|\nabla v_i\|_{L^{p_i}}. \tag{2.15}$$

The proof of Theorem 2.8 is established throughout the remainder of the section. We begin by establishing a simple bound on finite differences, which gives a first glimpse of the localisation technique used at crucial steps throughout the paper.

Lemma 2.9. *Let $\rho \in \Lambda_*$ and $p \in [1,\infty]$, then*

$$\|D_\rho \tilde{u}\|_{\ell^p} \le \|\nabla_\rho u\|_{L^p} \le |\rho| \|\nabla u\|_{L^p} \qquad \forall u \in \dot{\mathscr{W}}^{1,p}.$$

Proof. The case $p = \infty$ is trivial, hence suppose that $p < \infty$. Using the localisation formula (2.4), the fact that $\{\zeta(\,\cdot\, - \xi) \,|\, \xi \in \Lambda\}$ is a partition of unity (and hence $\int_{\mathbb{R}^d} \zeta(x-\xi)\,\mathrm{d}x = 1$), we can estimate

$$\begin{aligned}
\sum_{\xi\in\Lambda} \big|D_\rho \tilde{u}(\xi)\big|^p &= \sum_{\xi} \Big| \int_{t=0}^1 \int_{\mathbb{R}^d} \zeta(\xi + t\rho - x) \nabla_\rho u(x)\,\mathrm{d}x\,\mathrm{d}t \Big|^p \\
&\le \sum_{\xi} \int_{t=0}^1 \int_{\mathbb{R}^d} \zeta(\xi + t\rho - x) \big|\nabla_\rho u(x)\big|^p \,\mathrm{d}x\,\mathrm{d}t \\
&= \int_{\mathbb{R}^d} \big|\nabla_\rho u(x)\big|^p \,\mathrm{d}x \le |\rho|^p \|\nabla u\|_{L^2}^p.
\end{aligned}$$

□

Lemma 2.10. *Let $\boldsymbol{g}_\xi \in \mathscr{D}_\kappa$, $\xi \in \Lambda$, and $v_i \in \dot{\mathscr{W}}^{1,p_i}, 1 \le i \le j \le k$, with $\sum_{i=1}^j \frac{1}{p_i} = 1$, then*

$$\sum_{\xi\in\Lambda} \sum_{\boldsymbol{\rho}\in\Lambda_*^j} \big|V_{\boldsymbol{\rho}}(\boldsymbol{g}_\xi)[D_{\boldsymbol{\rho}}\boldsymbol{v}(\xi)]\big| \lesssim M^{(j)} \prod_{i=1}^j \|\nabla v_i\|_{L^{p_i}}.$$

Proof. Let $w_i \in \dot{\mathscr{W}}^{1,p_i}$ such that $\tilde{w}_i = I v_i$, then

$$\big|V_{\boldsymbol{\rho}}(\boldsymbol{g}_\xi)[D_{\boldsymbol{\rho}}\boldsymbol{v}(\xi)]\big| \le \frac{m(\boldsymbol{\rho})}{\prod_{i=1}^j |\rho_i|} \prod_{i=1}^j |D_{\rho_i} \tilde{w}_i(\xi)|.$$

Summing over $\xi \in \Lambda$, $\boldsymbol{\rho} \in \Lambda_*^j$, applying the generalized Hölder inequality, followed by Lemma 2.9, yields

$$\sum_{\boldsymbol{\rho}\in\Lambda_*^j}\sum_{\xi\in\Lambda}\big|V_{\boldsymbol{\rho}}(\boldsymbol{g}_\xi)[D_{\boldsymbol{\rho}}\boldsymbol{v}(\xi)]\big| \le \sum_{\boldsymbol{\rho}\in\Lambda_*^j}\frac{m(\boldsymbol{\rho})}{\prod_{i=1}^j|\rho_i|}\sum_{\xi\in\Lambda}\prod_{i=1}^j|D_{\rho_i}\tilde{w}_i(\xi)|$$
$$\le \sum_{\boldsymbol{\rho}\in\Lambda_*^j}\frac{m(\boldsymbol{\rho})}{\prod_{i=1}^j|\rho_i|}\prod_{i=1}^j\|D_\rho\tilde{w}_i\|_{\ell^{p_i}} \le \sum_{\boldsymbol{\rho}\in\Lambda_*^j} m(\boldsymbol{\rho})\|\nabla w_i\|_{L^p}.$$

Applying (2.10) yields the stated result. □

Remark 2.11. Lemma 2.10 implies, in particular, that we can interchange the summation in series of the form $\sum_{\xi\in\Lambda}\sum_{\boldsymbol{\rho}\in\Lambda_*^j}V_{\boldsymbol{\rho}}(\boldsymbol{g}_\xi)[D_{\boldsymbol{\rho}}\boldsymbol{v}(\xi)]$, provided that $\boldsymbol{g}_\xi \in \mathscr{D}_\kappa$ and ∇v_i have sufficient integrability. We will henceforth perform interchanges of summations without further comment. □

Lemma 2.12. *If $u \in \mathscr{W}_0$, then*

$$\sum_{\xi\in\Lambda}\sum_{\rho\in\Lambda_*}\Phi_{\xi,\rho}(0)\cdot D_\rho u(\xi) = 0. \tag{2.16}$$

Proof. According to Lemma 2.10, the sum on the right-hand side of (2.16) is well-defined, the summand belonging to ℓ^1.

Since $\Phi_{\xi,\rho}(0) = V_\rho(\mathbf{0})$, and interchanging the order of summation, we obtain

$$\sum_{\xi\in\Lambda}\sum_{\rho\in\Lambda_*}\Phi_{\xi,\rho}(\mathbf{0})\cdot D_\rho u(\xi) = \sum_{\rho\in\Lambda_*}V_\rho(\mathbf{0})\sum_{\xi\in\Lambda}D_\rho u(\xi).$$

For $u \in \mathscr{W}_0$ the right-hand side clearly vanishes. □

Motivated by the previous lemma, we define

$$\hat{E}^{\rm a}(u) := \sum_{\xi\in\Lambda}\hat{\Phi}_\xi(u), \qquad \text{where } \hat{\Phi}_\xi(u) := \Phi_\xi(u) - \sum_{\rho\in\Lambda_*}\Phi_{\xi,\rho}(0)\cdot D_\rho u(\xi), \tag{2.17}$$

then we immediately obtain the following result.

Lemma 2.13. *$\hat{\Phi}_\xi \in C^k(\dot{\mathscr{W}}^{1,p}\cap\mathscr{K})$, for all $p\in[1,\infty]$, with*

$$\hat{\Phi}_{\xi,\rho}(u) = \Phi_{\xi,\rho}(u) - \Phi_{\xi,\rho}(0), \quad \text{for } \rho\in\Lambda_*, \quad \text{and}$$
$$\hat{\Phi}_{\xi,\boldsymbol{\rho}}(u) = \Phi_{\xi,\boldsymbol{\rho}}(u), \quad \text{for } \boldsymbol{\rho}\in\Lambda_*^j, 2\le j\le k.$$

Proof. This result follows immediately from the fact that $\Phi_\xi \in C^k(\dot{\mathscr{W}}^{1,p}\cap\mathscr{K})$ and the estimate

$$\sum_{\rho\in\Lambda_*}|\Phi_{\xi,\rho}(0)|\,|D_\rho u(\xi)| \lesssim \sum_{\rho\in\Lambda_*}|\rho|m(\rho)\|\nabla u\|_{L^p} = M^{(1)}\|\nabla u\|_{L^p}.$$ □

Lemma 2.14. *Let $u \in \dot{\mathscr{W}}^{1,2}\cap\mathscr{K}$, then $\hat{\Phi}_\xi(u)\in\ell^1$; that is, (2.17) is well-defined for all $u\in\dot{\mathscr{W}}^{1,2}\cap\mathscr{K}$. Moreover, $\hat{E}^{\rm a}\in C^k(\dot{\mathscr{W}}^{1,2}\cap\mathscr{K})$ with variations given by (2.14) (with $E^{\rm a}$ replaced by $\hat{E}^{\rm a}$).*

Proof. Fix $u \in \dot{\mathscr{W}}^{1,2} \cap \mathscr{K}$, then $\theta Du(\xi) \in \mathscr{D}_\kappa$ for all $\xi \in \Lambda$ and $\theta \in [0,1]$. Hence, we can expand

$$\hat{\Phi}_\xi(u) = \hat{\Phi}_\xi(0) + \sum_{\rho \in \Lambda_*} \hat{\Phi}_{\xi,\rho}(0) \cdot D_\rho u(\xi) + \sum_{\rho,\varsigma \in \Lambda_*} V_{\rho\varsigma}(\boldsymbol{g}_\xi)[D_\rho u(\xi), D_\varsigma u(\xi)], \tag{2.18}$$

where $\boldsymbol{g}_\xi = \theta_\xi Du(\xi) \in \mathscr{D}_\kappa$ for some $\theta_\xi \in (0,1)$. By definition, $\hat{\Phi}_\xi(0) = \hat{\Phi}_{\xi,\rho}(0) = 0$, and hence,

$$\hat{\Phi}_\xi(u) = \sum_{\rho,\varsigma \in \Lambda_*} V_{\rho\varsigma}(\boldsymbol{g}_\xi)[D_\rho u(\xi), D_\varsigma u(\xi)] \qquad \forall \xi \in \Lambda.$$

It now follows from Lemma 2.9 that $\hat{\Phi}_\xi(u) \in \ell^1$, that is, $\hat{E}^{\rm a}(u)$ is well-defined.

The differentiability of $\hat{\Phi}$ can be shown using analogous arguments. □

Proof of Theorem 2.8. (i) If $u \in \mathscr{W}_0 \cap \mathscr{K}$ then Lemma 2.14 implies that $\hat{\Phi}_\xi(u) \in \ell^1$, while Lemma 2.12 ensures that $(\hat{\Phi}_\xi(u) - \Phi_\xi(u)) \in \ell^1$.

(ii) For $u \in \mathscr{W}_0 \cap \mathscr{K}$, Lemma 2.12 implies that $E^{\rm a}(u) = \hat{E}^{\rm a}(u)$. Since $\hat{E}^{\rm a}$ is continuous on $\dot{\mathscr{W}}^{1,2} \cap \mathscr{K}$, and $\mathscr{W}_0$ is dense in $\dot{\mathscr{W}}^{1,2}$, it follows that $\hat{E}^{\rm a}$ is the continuous extension of $E^{\rm a}$ to $\dot{\mathscr{W}}^{1,2} \cap \mathscr{K}$.

(iii) Since $\hat{E}^{\rm a} = E^{\rm a}$, this statement follows from Lemma 2.14. The simplified representation of $\delta E^{\rm a}$ (replacing $\hat{\Phi}_{\xi,\rho}$ with $\Phi_{\xi,\rho}$) follows from Lemma 2.12. For $j > 1$ and $\boldsymbol{\rho} \in \Lambda_*^j$ we have $\hat{\Phi}_{\xi,\boldsymbol{\rho}} = \Phi_{\xi,\boldsymbol{\rho}}$. □

Remark 2.15. 1. From the proof of Lemma 2.14 is becomes apparent why we assumed in §2.3.2 that $k \geq 2$. Only in that case are able to show that $\hat{E}^{\rm a}$ is well-defined on $\dot{\mathscr{W}}^{1,2} \cap \mathscr{K}$. We note, however, that if we only assume $k = 1$, then the the definition (2.1) still yields $E^{\rm a} \in C^1(\dot{\mathscr{W}}^{1,1} \cap \mathscr{K})$.

2. To define $E^{\rm a}(u)$ it is not necessary to assume a bound on $\|\nabla u\|_{L^\infty}$. Indeed, if we require that V is smooth at all configurations $Du(\xi)$ for displacements u satisfying the injectivity requirement (2.9), then Theorem 2.8 can be extended to this class of deformations.

The key observation is that $|\rho|^{-1}|D_\rho u(\xi)| \to 0$ uniformly in ρ as $|\xi| \to \infty$, and also $|\rho|^{-1}|D_\rho u(\xi)| \to 0$ uniformly in ξ as $|\rho| \to \infty$. (The first statement follows from the fact that $\xi \mapsto D_\rho u(\xi) \in \ell^2$; the second statement follows from the inequality $|\rho|^{-1}|D_\rho u(\xi)| \lesssim |\rho|^{-1/2}\|\nabla u\|_{L^2}$, which is easily established from (2.4).) In particular, this implies that $Du(\xi) \in \mathscr{D}_\kappa$ for $|\xi|$ sufficiently large. One can now apply the expansion (2.18) in the far-field. □

3. The Cauchy–Born Approximation

The Cauchy–Born elastic energy density function $W : \mathbb{R}^{d\times d} \to \mathbb{R} \cup \{\pm\infty\}$ is defined by

$$W(\mathsf{F}) := V(\mathsf{F} \cdot \Lambda_*). \tag{3.1}$$

In the regime of "smooth elastic" deformations, the *Cauchy–Born* model is a popular approximation to the atomistic model $E^{\rm a}$ [3, 10, 32, 15].

Formally, if $u : \mathbb{R}^d \to \mathbb{R}^d$ is smooth, then $V(Du(\xi)) \approx V(\nabla u(\xi) \cdot \Lambda_*) = W(\nabla u(\xi))$ and hence we can approximate $E^{\rm a}(u)$ by

$$E^{\rm c}(u) := \int_{\mathbb{R}^d} W(\nabla u)\,{\rm d}x. \tag{3.2}$$

In the remainder of this section we introduce a function space setting to make (3.2) rigorous, and establish associated auxiliary results.

3.1. **Homogeneous Sobolev spaces.** The formal Euler–Lagrange equation associated with $E^{\rm c}$ is a second-order elliptic system in $\mathbb{R}^d$. Due to the translation invariance, convenient function spaces for equations of this type are the *homogeneous Sobolev spaces* (or, *Beppo-Levi spaces* [8]). Here, we use a variant of spaces of equivalence classes:

$$\dot W^{m,2} := \big\{[u] \,\big|\, u \in W^{m,2}_{\rm loc}(\mathbb{R}^d;\mathbb{R}^d), \nabla u \in W^{m-1,2}\big\}, \qquad \text{for } m = 1, 2, \dots.$$

The space $\dot W^{m,2}$ is equipped with the norm

$$\|u\|_{\dot W^{m,2}} := \big(\textstyle\sum_{1\le j\le m}\|\nabla^j u\|^2_{L^2}\big)^{1/2}.$$

It is easy to see (see [27] for a proof of the case $m = 1$; the general case is analogous) that $\dot W^{m,2}$ is a Banach space, and that the subspace $\{[v] \,|\, v \in C_0^\infty\}$ is dense, where $C_0^\infty := \{u \in C^\infty(\mathbb{R}^d;\mathbb{R}^d) \,|\, \mathrm{supp}(u) \text{ compact}\}$.

The natural space of continuous displacements is $\dot W^{1,2}$. In order to avoid non-interpenetration of matter we shall assume that all displacement gradients satisfy a uniform bound. To that end we define

$$K := \big\{u \in W^{1,\infty} \,\big|\, \|\nabla u\|_{L^\infty} \le \kappa\big\},$$

where κ is the same constant as in the definition of $\mathscr{K}$ (2.8).

A straightforward extension of [27, Thm. 2.2] shows that $|u(x)| \ll |x|$ as $|x| \to \infty$ for all $u \in \dot W^{1,2} \cap K$, hence the associated *deformation* $y(x) = \mathsf{A}x + u(x)$ again satisfies the far-field boundary condition $y(x) \sim \mathsf{A}x$ as $|x| \to \infty$.

3.2. **Definition of the Cauchy–Born energy.** In this section we make the definition of the Cauchy–Born energy (3.2) rigorous. We first analyze the stored energy function W of the Cauchy–Born model.

Lemma 3.1. *$W \in C^k(\{\mathsf{F} \in \mathbb{R}^{d\times d} \,|\, |\mathsf{F}| \le \kappa\})$. For $|\mathsf{F}| \le \kappa$ and $(\mathsf{G}_1, \dots, \mathsf{G}_j) \in (\mathbb{R}^{d\times d})^j$, $1 \le j \le k$, we have*

$$\delta^j W(\mathsf{F})[\mathsf{G}_1, \dots, \mathsf{G}_j] = \sum_{\boldsymbol\rho\in\Lambda_*^j} V_{\boldsymbol\rho}(\mathsf{F}\cdot\Lambda_*)[\mathsf{G}_1\rho_1, \dots, \mathsf{G}_j\rho_j].$$

Proof. This result follows immediately from the fact that, for $|\mathsf{F}| \le \kappa$, $\mathsf{F}\cdot\Lambda_* \in \mathscr{D}_\kappa$. ☐

The derivative of W can be represented by the first Piola–Kirchhoff stress tensor,

$$\mathsf{S}^{\rm c}_{i\alpha}(u;x) := \frac{\partial W(\mathsf{F})}{\partial \mathsf{F}_{i\alpha}}\bigg|_{\mathsf{F}=\nabla u(x)} \qquad \text{for } i, \alpha = 1\dots d,\ u \in K. \tag{3.3}$$

Then we can write $\delta W(\nabla u)[\mathsf{G}] = \mathsf{S}^{\rm c}(u) : \mathsf{G}$, where ':' denotes the usual Frobenius inner product.

Following the arguments in §2.4, we obtain that $E^{\rm c}$ is well-defined in $C_0^\infty \cap K$ and has a continuous extension to $\dot W^{1,2} \cap K$. The proof is analogous to the proof of Theorem 2.8.

Proposition 3.2 (Definition of $E^{\rm c}$). *(i) If $u \in C_0^\infty \cap K$, then $W(\nabla u) \in L^1$; hence $E^{\rm c}(u)$ is well-defined by* (3.2).

(ii) $E^{\rm c} : (C_0^\infty \cap K, \|\cdot\|_{\dot W^{1,2}}) \to \mathbb{R}$ is continuous; hence there exists a unique continuous extension to $\dot W^{1,2} \cap K$, which we still denote by $E^{\rm c}$.

(iii) $E^{\rm c} \in C^k(\dot W^{1,2} \cap K; \|\cdot\|_{\dot W^{1,2}} + \|\cdot\|_{\dot W^{1,\infty}})$ with

$$\delta^j E^{\rm c}(u)[\boldsymbol v] = \int_{\mathbb{R}^d} \delta^j W(\nabla u)[\nabla v_1, \dots, \nabla v_j]\,{\rm d}x, \qquad \textit{for } \boldsymbol v \in (C_0^\infty)^j, \quad 1 \le j \le k. \tag{3.4}$$

Moreover, for $\sum_{i=1}^{j} \frac{1}{p_i} = 1$*, we have*

$$\delta^j E^{\mathrm{c}}(u)[\boldsymbol{v}] \leq M^{(j)} \prod_{i=1}^{j} \|\nabla v_i\|_{L^{p_i}}. \tag{3.5}$$

4. Stress

For $u \in \dot{W}^{1,2} \cap K$ the canonical representation of $\delta E^{\mathrm{c}}(u)$ is (cf. (3.4) with $j = 1$)

$$\big\langle \delta E^{\mathrm{c}}(u), v \big\rangle = \int_{\mathbb{R}^d} \mathsf{S}^{\mathrm{c}}(u) : \nabla v \, \mathrm{d}x, \qquad \text{for } v \in C_0^\infty. \tag{4.1}$$

The *first Piola–Kirchhoff stress* S^{c} is dual to the virtual displacement gradient ∇v. By contrast, the first variation of the atomistic energy is more commonly expressed in terms of forces, which are dual to v. The purpose of this section is to derive and analyze an atomistic concept of stress that yields a representation of δE^{a} analogous to (4.1). This will then be employed in a sharp consistency analysis of the Cauchy–Born approximation in § 4.2, § 4.3, and § 6.3.

4.1. **An atomistic stress function.** The "canonical weak form" of δE^{a}, given in (2.14), is

$$\big\langle \delta E^{\mathrm{a}}(u), v \big\rangle = \sum_{\xi \in \Lambda} \sum_{\rho \in \Lambda_*} \Phi_{\xi,\rho}(u) \cdot D_\rho v(\xi), \qquad \text{for } v \in \mathscr{W}_0. \tag{4.2}$$

To proceed, we fix $v \in \mathscr{W}_0$ but test $\delta E^{\mathrm{a}}(u)$ with $\tilde{v}$ instead of v. We apply the localization formula (2.4) to obtain

$$\begin{aligned} \big\langle \delta E^{\mathrm{a}}(u), \tilde{v} \big\rangle &= \sum_{\xi \in \Lambda} \sum_{\rho \in \Lambda_*} \Phi_{\xi,\rho}(u) \cdot \int_{\mathbb{R}^d} \chi_{\xi,\rho}(x) \, \nabla_\rho v(x) \, \mathrm{d}x \\ &= \int_{\mathbb{R}^d} \bigg\{ \sum_{\xi \in \Lambda} \sum_{\rho \in \Lambda_*} \big[\Phi_{\xi,\rho}(u) \otimes \rho\big] \chi_{\xi,\rho}(x) \bigg\} : \nabla v \, \mathrm{d}x. \end{aligned} \tag{4.3}$$

Using the decay assumption (2.13) one can apply Fubini's theorem to justify the interchange of integral and sums, and thus obtain the following result.

Proposition 4.1. *Let* $u \in \dot{\mathscr{W}}^{1,2} \cap \mathscr{K}$*, then*

$$\begin{aligned} \big\langle \delta E^{\mathrm{a}}(u), \tilde{v} \big\rangle &= \int_{\mathbb{R}^d} \mathsf{S}^{\mathrm{a}}(u; x) : \nabla v(x) \, \mathrm{d}x \qquad \forall v \in \mathscr{W}_0, \\ \text{where} \quad \mathsf{S}^{\mathrm{a}}(u; x) &:= \sum_{\xi \in \Lambda} \sum_{\rho \in \Lambda_*} \big[\Phi_{\xi,\rho}(u) \otimes \rho\big] \chi_{\xi,\rho}(x), \end{aligned} \tag{4.4}$$

and $\chi_{\xi,\rho}$ *is defined in* (2.4).

Remark 4.2. The fact that the test function in the left-hand side and right-hand side of (4.4) differ may seem counter-intuitive at first. Allowing this seeming discrepancy makes the rather simple definition of atomistic stress possible, and will lead to sharp consistency estimates requiring only modest analytical effort while the subsequent error analysis in §5 and §6 requires only minor adjustments. □

4.2. **Second-order accuracy of the Cauchy–Born stress.** In this section we prove the following pointwise second-order consistency estimate between the Cauchy–Born and atomistic stress functions.

Theorem 4.3. *Let $u \in \dot{W}^{3,\infty} \cap K$, and $x \in \mathbb{R}^d$, then*

$$\big|\mathsf{S}^{\rm a}(u;x) - \mathsf{S}^{\rm c}(u;x)\big| \lesssim \sum_{\boldsymbol{\rho}\in\Lambda_*^2} m_{\rm s}^{(\infty)}(\boldsymbol{\rho})\, \|\nabla^3 y\|_{L^\infty(x+\nu_{\rho_1,\rho_2})} + \sum_{\boldsymbol{\rho}\in\Lambda_*^3} m_{\rm s}^{(\infty)}(\boldsymbol{\rho})\, \|\nabla^2 y\|_{L^\infty(x+\nu_{\rho_1,\rho_2})} \|\nabla^2 y\|_{L^\infty(x+\nu_{\rho_1,\rho_3})}, \tag{4.5}$$

where $m_{\rm s}^{(\infty)}$ is defined in §2.3.4, and for each $\rho, \varsigma \in \Lambda_*$ the set $\nu_{\rho\varsigma}$ satisfies $\nu_{\rho\varsigma} \subset B(0, c(|\rho|+|\varsigma|))$, for some constant $c > 0$, $-\nu_{\rho\varsigma} = \nu_{\rho\varsigma}$, and

$$\mathrm{vol}(\nu_{\rho\varsigma}) \lesssim |\rho \times \varsigma| + |\rho| + |\varsigma|. \tag{4.6}$$

Before we embark on the proof of Theorem 4.3, we establish two useful identities for the weights $\chi_{\xi,\rho}$, which will enable us to exploit the inversion symmetry (2.11).

Lemma 4.4. *Let $x, \rho \in \mathbb{R}^d$; then*

$$\sum_{\xi\in\Lambda} \chi_{\xi,\rho}(x) = 1, \qquad \text{and} \tag{4.7}$$

$$\sum_{\xi\in\Lambda} \chi_{\xi,\rho}(x)\,(\xi - x) = -\tfrac{1}{2}\rho. \tag{4.8}$$

Proof. Both results rely on the assumption that affine functions are invariant under the first-order interpolant. Clearly, this is still true on a shifted grid: if $v : \mathbb{R}^d \to \mathbb{R}^d$ is affine, then for any $z, x \in \mathbb{R}^d$ we have

$$v(x) = \sum_{\eta\in(\Lambda+z)} \zeta(x-\eta) v(\eta). \tag{4.9}$$

To prove (4.7) we write out the left-hand side, and employ (4.9) with $v(x) = 1$:

$$\sum_{\xi\in\Lambda} \chi_{\xi,\rho}(x) = \int_{s=0}^1 \sum_{\xi\in\Lambda} \zeta\big(\xi + (s\rho - x)\big)\,\mathrm{d}s = \int_{s=0}^1 1\,\mathrm{d}s = 1.$$

To prove (4.8), let $s \in [0,1]$ be fixed; then

$$\sum_{\xi\in\Lambda} \zeta\big((\xi - x) + s\rho\big)(\xi - x) = \sum_{\eta\in(x+\Lambda)} \zeta(s\rho - \eta)(-\eta),$$

were we substituted $\eta = -(\xi - x)$, and hence sum over $-(\Lambda - x) = (x + \Lambda)$. Employing again (4.9) with $v(x') = -x'$, we obtain

$$\sum_{\xi\in\Lambda} \zeta\big((\xi - x) + s\rho\big)(\xi - x) = -s\rho,$$

and integrating with respect to s gives

$$\sum_{\xi\in\Lambda} \chi_{\xi,\rho}(x)(\xi - x) = \int_{s=0}^1 \sum_{\xi\in\Lambda} \zeta\big((\xi - x) + s\rho\big)(\xi - x)\,\mathrm{d}s = \int_{s=0}^1 (-s\rho)\,\mathrm{d}s = -\tfrac{1}{2}\rho. \qquad \square$$

Proof of Theorem 4.3. Throughout this proof, let $\nu_{\xi,\varsigma} := \mathrm{conv}\{x, \xi, \xi + \varsigma\}$, and

$$\varepsilon_{\xi,\varsigma} := \|\nabla^2 u\|_{L^\infty(\nu_{\xi,\varsigma})} \quad \text{and} \quad \delta_{\xi,\varsigma} := \|\nabla^3 u\|_{L^\infty(\nu_{\xi,\varsigma})}.$$

We will suppress all arguments where it is possible to do so without confusion, for example, $\mathsf{S}^{\mathrm{a}} = \mathsf{S}^{\mathrm{a}}(u; x)$ and $\mathsf{S}^{\mathrm{c}} = \mathsf{S}^{\mathrm{c}}(u; x)$.

Defining the symbols

$$V_{\boldsymbol{\rho}} := V_{\boldsymbol{\rho}}(x) := V_{\boldsymbol{\rho}}\big(\nabla u(x) \cdot \Lambda_*\big), \qquad \text{for } \boldsymbol{\rho} \in \Lambda_*^j, \quad j = 1, 2.$$

we can rewrite $\mathsf{S}^{\mathrm{c}} = \sum_{\rho \in \Lambda_*} V_\rho \otimes \rho$. In (4.7) we have established that $\sum_{\xi \in \Lambda} \chi_{\xi,\rho}(x) = 1$, which implies

$$\begin{aligned} \mathsf{S}^{\mathrm{a}} - \mathsf{S}^{\mathrm{c}} &= \sum_{\rho \in \Lambda_*} \bigg\{ \sum_{\xi \in \Lambda} \big[\Phi_{\xi,\rho} \otimes \rho\big] \chi_{\xi,\rho}(x) - \big[V_\rho \otimes \rho\big] \bigg\} \\ &= \sum_{\rho \in \Lambda_*} \sum_{\xi \in \Lambda} \Big\{ \big[\Phi_{\xi,\rho} - V_\rho\big] \otimes \rho \Big\} \chi_{\xi,\rho}(x). \end{aligned} \tag{4.10}$$

Since ζ has compact support, there exists a constant $c > 0$ such that $\chi_{\xi,\rho}(x) = 0$ for all $\xi \in \Lambda$ with $|\xi - x| > c|\rho|$. Hence, we will assume throughout the rest of the proof that $|\xi - x| \lesssim |\rho|$.

We Taylor expand the term $[\Phi_{\xi,\rho} - V_\rho]$ as follows:

$$\Phi_{\xi,\rho} - V_\rho = \sum_{\varsigma \in \Lambda_*} V_{\rho\varsigma}[\,\cdot\,, D_\varsigma u(\xi) - \nabla_\varsigma u(x)] + E_1, \tag{4.11}$$

$$\text{where} \quad |E_1| \lesssim \sum_{\tau\varsigma \in \Lambda_*} (|\tau| + |\varsigma| + |\rho|)^2 \tfrac{m(\rho,\varsigma,\tau)}{|\rho|}\, \varepsilon_{\xi,\varsigma} \varepsilon_{\xi,\tau}$$

The details of the estimates for the remainder E_1 are easily established, the key observation being that

$$|D_\varsigma u(\xi) - \nabla_\varsigma u(x)| \le (\tfrac{1}{2}|\varsigma| + |\xi - x|)|\varsigma| \varepsilon_{\xi,\varsigma} \lesssim (|\varsigma| + |\rho|)|\varsigma|\, \varepsilon_{\xi,\varsigma},$$

which is obtained by expanding along the segments $\mathrm{conv}\{x, \xi\}$ and $\mathrm{conv}\{\xi, \xi + \varsigma\}$. Here, and in the following, we skip the details required for estimating the remainders.

Expanding $D_\varsigma u(\xi) - \nabla_\varsigma u(x)$,

$$\begin{aligned} D_\varsigma u(\xi) - \nabla_\varsigma u(x) &= \nabla_\varsigma u(\xi) + \tfrac{1}{2} \nabla_\varsigma^2 u(\xi) - \nabla_\varsigma u(x) + E_2' \\ &= \nabla_{\xi - x} \nabla_\varsigma u(x) + \tfrac{1}{2} \nabla_\varsigma^2 u(x) + E_2, \end{aligned} \tag{4.12}$$

$$\text{where} \quad |E_2| \lesssim |\varsigma|(|\varsigma| + |\rho|)^2\, \delta_{\xi,\varsigma},$$

and combining (4.12) with (4.11) yields

$$\Phi_{\xi,\rho} - V_\rho = \sum_{\varsigma \in \Lambda_*} V_{\rho\varsigma}\big[\,\cdot\,, \nabla_{\xi - x} \nabla_\varsigma u(x) + \tfrac{1}{2} \nabla_\varsigma^2 u(x)\big] + E_1 + E_3, \tag{4.13}$$

$$\text{where} \quad |E_3| \le \sum_{\varsigma \in \Lambda_*} \frac{m(\rho, \varsigma)}{|\rho||\varsigma|} |E_2| \lesssim \sum_{\varsigma \in \Lambda_*} \frac{m(\rho, \varsigma)}{|\rho|} (|\varsigma| + |\rho|)^2\, \delta_{\xi,\varsigma},$$

which we insert into (4.10) to obtain

$$\mathsf{S}^{\mathrm{a}} - \mathsf{S}^{\mathrm{c}} = \sum_{\rho \in \Lambda_*} \sum_{\xi \in \Lambda} \sum_{\varsigma \in \Lambda_*} \Big\{ V_{\rho\varsigma}\big[\,\cdot\,, \nabla_{\xi - x} \nabla_\varsigma u + \tfrac{1}{2} \nabla_\varsigma^2 u\big] \otimes \rho \Big\} \chi_{\xi,\rho}(x) + E_4, \tag{4.14}$$

$$\text{where} \quad E_4 = \sum_{\rho \in \Lambda_*} \sum_{\xi \in \Lambda} \big[(E_1 + E_3) \otimes \rho\big] \chi_{\xi,\rho}(x).$$

Rearranging the sums, we arrive at the expression

$$\mathsf{S}^{\mathrm{a}} - \mathsf{S}^{\mathrm{c}} = \sum_{\rho\in\Lambda_*}\sum_{\varsigma\in\Lambda_*} \Big\{ V_{\rho\varsigma}\big[\,\cdot\,, \textstyle\sum_{\xi\in\Lambda}\chi_{\xi,\rho}(x)(\nabla_{\xi-x}\nabla_\varsigma u + \frac12 \nabla_\varsigma^2 u)\big]\otimes\rho\Big\} + E_4. \qquad (4.15)$$

Using (4.7) we see that

$$\sum_{\xi\in\Lambda}\chi_{\xi,\rho}\,\nabla_\varsigma^2 u = \nabla_\varsigma^2 u, \quad \text{and} \quad \sum_{\xi\in\Lambda}\chi_{\xi,\rho}\,\nabla_{\xi-x}\nabla_\varsigma u = -\tfrac12 \nabla_\rho\nabla_\varsigma u. \qquad (4.16)$$

Combining (4.16) with (4.15), we arrive at the identity

$$\mathsf{S}^{\mathrm{a}} - \mathsf{S}^{\mathrm{c}} = \frac12 \sum_{\rho\in\Lambda_*}\sum_{\varsigma\in\Lambda_*} V_{\rho\varsigma}\big[\,\cdot\,, \nabla_\varsigma^2 y - \nabla_\varsigma\nabla_\rho y\big]\otimes\rho + E_4.$$

Applying the symmetry $V_{\rho\varsigma} = V_{-\rho,-\varsigma}$ (cf. §2.3.3), yields

$$V_{\rho\varsigma}\big[\,\cdot\,, \nabla_\varsigma^2 y - \nabla_\varsigma\nabla_\rho y\big]\otimes\rho + V_{-\rho,-\varsigma}\big[\,\cdot\,, \nabla_{-\varsigma}^2 y - \nabla_{-\varsigma}\nabla_{-\rho} y\big]\otimes(-\rho) = 0,$$

and hence we deduce that $\mathsf{S}^{\mathrm{a}} - \mathsf{S}^{\mathrm{c}} = E_4$.

It remains to bound E_4. Using its definition (4.14), and the bounds (4.11) for E_1 and (4.13) for E_3, and the estimate $\sum_{\xi\in\Lambda}\chi_{\xi,\rho} f_\xi \le \max_{\xi\in\Lambda,\chi_{\xi,\rho}(x)\neq 0} f_\xi$ we estimate

$$\begin{aligned} |E_4| &\le \sum_{\rho\in\Lambda_*}|\rho| \sum_{\xi\in\Lambda}(|E_1| + |E_3|)\chi_{\xi,\rho} \\ &\lesssim \sum_{\rho,\varsigma,\tau\in\Lambda_*} (|\rho| + |\varsigma| + |\tau|)^2 m(\rho,\varsigma,\tau) \max_{\substack{\xi\in\Lambda \\ \chi_{\xi,\rho}(x)\neq 0}} \varepsilon_{\xi,\varsigma}\varepsilon_{\xi,\tau} \\ &\quad + \sum_{\rho,\varsigma\in\Lambda_*} (|\rho| + |\varsigma|)^2 m(\rho,\varsigma) \max_{\substack{\xi\in\Lambda \\ \chi_{\xi,\rho}(x)\neq 0}} \delta_{\xi,\varsigma}. \end{aligned} \qquad (4.17)$$

There exists a constant $c > 0$ such that, if $\chi_{\xi,\rho}(x) \neq 0$, then $|\xi + t\rho - x| \le c$ for some $t \in [0,1]$ and one readily checks that this implies

$$\nu_{\xi,\varsigma} - x \subset \nu_{\rho,\varsigma} := \big\{ y \in \mathbb{R}^d \,\big|\, \mathrm{dist}(y, \mathrm{conv}\{\pm 2\rho \pm \varsigma\}) \le 2c \big\}.$$

Hence, we obtain

$$\max_{\substack{\xi\in\Lambda \\ \chi_{\xi,\rho}(x)\neq 0}} \varepsilon_{\xi,\varsigma}\varepsilon_{\xi,\tau} \le \|\nabla^2 u\|_{L^\infty(x+\nu_{\rho,\varsigma})}\|\nabla^2 u\|_{L^\infty(\nu_{\rho,\tau})} \quad \text{and} \quad \max_{\substack{\xi\in\Lambda \\ \chi_{\xi,\rho}(x)\neq 0}} \delta_{\xi,\varsigma} \le \|\nabla^3 u\|_{L^\infty(x+\nu_{\rho,\varsigma})}.$$

Inserting these bounds into (4.17), and recalling that $\mathsf{S}^{\mathrm{a}} - \mathsf{S}^{\mathrm{c}} = E_4$, we obtain the stated estimate.

The statements about the sets $\nu_{\rho,\varsigma}$ are easy to establish. □

4.3. **Global modeling error estimate.** We present a modeling error estimate that is a natural corollary of Theorem 4.3. For our subsequent analysis we only require the case $p = 2$, however, we give a more general statement since the same proof applies verbatim for general p. Earlier results this direction have been obtained in [21, 10].

Lemma 4.5. *Let $u \in \dot W^{3,p} \cap K$, $p \in (1,\infty]$, and let $\tilde u := \zeta * u$; then, for all $v \in \dot{\mathscr{W}}^{1,p'}$,*

$$\big|\big\langle \delta E^{\mathrm{a}}(\tilde u), \tilde v\big\rangle - \big\langle \delta E^{\mathrm{c}}(u), v\big\rangle\big| \lesssim \big(M_{\mathrm{s}}^{(2,p)}\|\nabla^3 u\|_{L^p} + M_{\mathrm{s}}^{(3,p)}\|\nabla^2 u\|_{L^{2p}}^2\big)\|\nabla v\|_{L^{p'}}, \qquad (4.18)$$

where the constants $M_{\mathrm{s}}^{(j,p)}$ are defined in §2.3.4.

Proof. The case $p = \infty$ follows immediately from Theorem 4.3, hence we assume that $p \in (1, \infty)$. Further, we assume that $v \in \mathscr{W}_0$, and apply a density argument to obtain the general statement.

First, we need to show that $w := \tilde{u}|_\Lambda \in \mathscr{K}$. To that end, we estimate

$$|D_\rho w(\xi)| = \left| \int_{t=0}^{1} \nabla_\rho \tilde{u}(\xi + t\rho)\,\mathrm{d}t \right| \le |\rho| \|\nabla \tilde{u}\|_{L^\infty} \le |\rho| \|\zeta\|_{L^1} \|\nabla u\|_{L^\infty}.$$

Since $u \in K$ and $\|\zeta\|_{L^1} = \int \zeta \,\mathrm{d}x = 1$, we obtain that $|D_\rho w(\xi)| \le \kappa|\rho|$ and hence $w = \tilde{u}|_\Lambda \in \mathscr{K}$. Hence it follows that the first variations on the left-hand side are well-defined.

From Proposition 4.1 it follows that

$$\begin{aligned} \big|\big\langle \delta E^{\mathrm{a}}(\tilde{u}), \tilde{v} \big\rangle - \big\langle \delta E^{\mathrm{c}}(u), v \big\rangle\big| &= \int_{\mathbb{R}^d} \big[\mathsf{S}^{\mathrm{a}}(\tilde{u}) - \mathsf{S}^{\mathrm{c}}(u)\big] : \nabla v \,\mathrm{d}x \\ &\le \big\|\mathsf{S}^{\mathrm{a}}(\tilde{u}) - \mathsf{S}^{\mathrm{c}}(u)\big\|_{L^p} \|\nabla v\|_{L^{p'}}. \end{aligned} \tag{4.19}$$

We apply the triangle inequality,

$$\big\|\mathsf{S}^{\mathrm{a}}(\tilde{u}) - \mathsf{S}^{\mathrm{c}}(u)\big\|_{L^p} \le \big\|\mathsf{S}^{\mathrm{a}}(\tilde{u}) - \mathsf{S}^{\mathrm{c}}(\tilde{u})\big\|_{L^p} + \big\|\mathsf{S}^{\mathrm{c}}(\tilde{u}) - \mathsf{S}^{\mathrm{c}}(u)\big\|_{L^p}, \tag{4.20}$$

to separately estimate the two terms on the right-hand side.

Applying (3.5) and Lemma A.2, we can bound the second term by

$$\big\|\mathsf{S}^{\mathrm{c}}(\nabla\tilde{u}) - \mathsf{S}^{\mathrm{c}}(\nabla u)\big\|_{L^p} \lesssim M^{(2)} \|\nabla\tilde{u} - \nabla u\|_{L^p} \lesssim M^{(2)} \|\nabla^3 u\|_{L^p}. \tag{4.21}$$

To estimate the first term on the right-hand side of (4.20) we first apply Theorem 4.3 to obtain

$$\begin{aligned} \big|\mathsf{S}^{\mathrm{a}}(\tilde{u};x) - \mathsf{S}^{\mathrm{c}}(\tilde{u};x)\big| \lesssim& \sum_{\rho,\varsigma\in\Lambda_*} m_{\mathrm{s}}^{(\infty)}(\rho,\varsigma) \|\nabla^3 \tilde{u}\|_{L^\infty(x+\nu_{\rho,\varsigma})} \\ &+ \sum_{\rho,\varsigma,\tau\in\Lambda_*} m_{\mathrm{s}}^{(\infty)}(\rho,\varsigma,\tau) \|\nabla^2\tilde{u}\|_{L^\infty(x+\nu_{\rho,\varsigma})} \|\nabla^2\tilde{u}\|_{L^\infty(x+\nu_{\rho,\tau})}. \end{aligned} \tag{4.22}$$

Next, we estimate the L^p-norm of the first term on the right-hand side. To that end, we first recall the definition of $\nu_{\rho,\varsigma}$ from Theorem 4.3 as well as the enlarged sets $\nu'_{\rho,\varsigma}$ defined in Lemma A.4. Let $(w_{\rho\varsigma}) \in \ell^p(\Lambda_*^2)$, and let $w := (\sum_{\rho,\varsigma\in\Lambda_*} w_{\rho\varsigma}^{p'} m_{\mathrm{s}}^{(\infty)}(\rho,\varsigma))^{p'/p}$, then applying first Hölder's inequality and then Lemma A.4, gives

$$\begin{aligned} \int_{\mathbb{R}^d} \bigg| \sum_{\rho,\varsigma\in\Lambda_*} m_{\mathrm{s}}^{(\infty)}(\rho,\varsigma) \|\nabla^3\tilde{u}\|_{L^\infty(\nu_{\rho,\varsigma})} \bigg|^p \mathrm{d}x &\le w \sum_{\rho,\varsigma\in\Lambda_*} w_{\rho\varsigma}^{-p} m_{\mathrm{s}}^{(\infty)}(\rho,\varsigma) \int_{\mathbb{R}^d} \|\zeta * \nabla^3 u\|_{L^\infty(x+\nu_{\rho,\varsigma})}^p \,\mathrm{d}x \\ &\le w \sum_{\rho,\varsigma\in\Lambda_*} w_{\rho\varsigma}^{-p} m_{\mathrm{s}}^{(\infty)}(\rho,\varsigma) \mathrm{vol}(\nu'_{\rho,\varsigma}) \, \|\nabla^3 u\|_{L^p}^p. \end{aligned}$$

Choosing $w_{\rho\varsigma}$ to balance w with $\sum_{\rho,\varsigma\in\Lambda_*} w_{\rho\varsigma}^{-p} \bar{M}_\mu^{(\rho,\varsigma)} \,\mathrm{vol}(\nu'_{\rho,\varsigma})$, and noting that $\mathrm{vol}(\nu'_{\rho\varsigma}) \lesssim \mathrm{vol}(\nu_{\rho\varsigma})$ (this follows immediately from the definition of $\nu_{\rho\varsigma}$) yields

$$\bigg(\int_{\mathbb{R}^d} \bigg| \sum_{\rho,\varsigma\in\Lambda_*} m_{\mathrm{s}}^{(\infty)}(\rho,\varsigma) \|\nabla^3\tilde{u}\|_{L^\infty(\nu_{\rho,\varsigma})} \bigg|^p \mathrm{d}x \bigg)^{1/p} \lesssim M_{\mathrm{s}}^{(2,p)} \|\nabla^3 u\|_{L^p}. \tag{4.23}$$

With an analogous argument we obtain

$$\bigg(\int_{\mathbb{R}^d} \bigg| \sum_{\rho,\varsigma,\tau\in\Lambda_*} m_{\mathrm{s}}^{(\infty)}(\rho,\varsigma,\tau) \|\nabla^2\tilde{u}\|_{L^\infty(x+\nu_{\rho,\varsigma})} \|\nabla^2\tilde{u}\|_{L^\infty(x+\nu_{\rho,\tau})} \bigg|^{2p} \mathrm{d}x \bigg)^{1/p} \lesssim M_{\mathrm{s}}^{(3,p)} \|\nabla^2 u\|_{L^{2p}}^2. \tag{4.24}$$

Combining (4.22), (4.23) and (4.24) with (4.21), and noting that $M^{(2)} \le M_{\mathrm{s}}^{(2,p)}$, completes the proof. □

5. Elastostatic problems

In this section we present error estimates for local minimizers of the Cauchy–Born model. We essentially recover the result of E and Ming [10, Thm. 2.3] for a more general class of interactions, and in the more challenging setting of an infinite domain and infinite interaction range. Moreover, due to our new consistency estimates in §4, we obtain sharper and more explicit estimates.

5.1. **The variational problems.**

5.1.1. *Continuous external forces.* For $f, g \in L^1_{\rm loc}$ with $f \cdot g \in L^1$ we define the inner product

$$(f, g)_{\mathbb{R}^d} := \int_{\mathbb{R}^d} f \cdot g \,\mathrm{d}x.$$

We say that $f \in L^1_{\rm loc} \cap \dot{W}^{-1,2}$ if there exists a constant $\|f\|_{\dot{W}^{-1,2}}$ such that

$$(f, v)_{\mathbb{R}^d} \leq \|f\|_{\dot{W}^{-1,2}} \|\nabla v\|_{L^2} \qquad \forall v \in C_0^\infty.$$

In this case there exists a unique continuous extension of $(f, \,\cdot\,)_{\mathbb{R}^d}$ to $\dot{W}^{1,2}$.

5.1.2. *The Cauchy–Born Problem.* In the Cauchy–Born model, given $f^{\rm c} \in L^1_{\rm loc} \cap \dot{W}^{-1,2}$, we seek

$$u^{\rm c} \in \arg\min \big\{ E^{\rm c}(u) - (f^{\rm c}, u)_{\mathbb{R}^d} \,\big|\, u \in \dot{W}^{1,2} \big\}. \tag{5.1}$$

We understand (5.1) as a *local* minimization problem with respect to the $(\dot{W}^{1,2} \cap \dot{W}^{1,\infty})$-topology. If $u^{\rm c} \in K$ is a solution to (5.1), then it satisfies the first-order optimality condition

$$\big\langle \delta E^{\rm c}(u^{\rm c}), v \big\rangle = (f^{\rm c}, v)_{\mathbb{R}^d} \qquad \forall v \in \dot{W}_0. \tag{5.2}$$

We call a solution $u^{\rm c}$ of (5.2) *stable* if there exists $c_0 > 0$ such that

$$\big\langle \delta^2 E^{\rm c}(u^{\rm c}) v, v \big\rangle \geq c_0 \|\nabla v\|_{L^2}^2 \qquad \forall v \in \dot{W}_0. \tag{5.3}$$

From Proposition 3.2 it follows that, if $u^{\rm c}$ is a stable solution of (5.2), then it is a strict $(\dot{W}^{1,2} \cap \dot{W}^{1,\infty})$-local minimizer of $E^{\rm c} - (f^{\rm c}, \,\cdot\,)_{\mathbb{R}^d}$, and hence a solution of (5.1).

5.1.3. *External forces in the atomistic problem.* For $f, g \in \mathscr{W}$ with $f \cdot g \in \ell^1$ we define the inner product

$$(f, g)_\Lambda := \sum_{\xi \in \Lambda} f(\xi) \cdot g(\xi).$$

We say that $f \in \dot{\mathscr{W}}^{-1,2}$ if $f \in \mathscr{W}$ and there exists a constant $\|f\|_{\dot{\mathscr{W}}^{-1,2}}$ such that

$$(f, v)_\Lambda \leq \|f\|_{\dot{\mathscr{W}}^{-1,2}} \|\nabla v\|_{L^2} \qquad \forall v \in \mathscr{W}_0.$$

In this case there exists a unique continuous extension of $(f, \,\cdot\,)_\Lambda$ to $\dot{\mathscr{W}}^{1,2}$.

5.1.4. *The atomistic problem.* Given $f^{\rm a} \in \dot{\mathscr{W}}^{-1,2}$ we seek

$$u^{\rm a} \in \arg\min \big\{ E^{\rm a}(u) - (f^{\rm a}, u)_\Lambda \,\big|\, u \in \dot{\mathscr{W}}^{1,2} \big\}. \tag{5.4}$$

We understand (5.4) as a *local* minimization problem. If $u^{\rm a} \in \mathscr{K}$ is a solution to (5.4), then it satisfies the first-order optimality condition

$$\big\langle \delta E^{\rm a}(u^{\rm a}), v \big\rangle = (f^{\rm a}, v)_\Lambda \qquad \forall v \in \mathscr{W}_0. \tag{5.5}$$

We call a solution $u^{\rm a}$ of (5.5) *stable* if there exists $c_0 > 0$ such that

$$\big\langle \delta^2 E^{\rm a}(u^{\rm a}) v, v \big\rangle \geq c_0 \|\nabla v\|_{L^2}^2 \qquad \forall v \in \mathscr{W}_0. \tag{5.6}$$

From Proposition 2.8 it follows that, if $u^{\rm a}$ is a stable solution of (5.5) then $u^{\rm a}$ is a strict $\dot{\mathscr{W}}^{1,2}$-local minimizer of $E^{\rm a} - (f^{\rm a}, \,\cdot\,)_\Lambda$ and hence a solution of (5.4).

5.2. **Stability of small displacements.** We say that the lattice $\mathsf{A}\cdot\Lambda$ is stable if

$$\gamma := \inf_{\substack{v\in\mathscr{W}_0\\ \|\nabla v\|_{L^2}=1}} \big\langle \delta^2 E^{\rm a}(0)v, v\big\rangle > 0. \tag{5.7}$$

Physically, (5.7) states that small distortions of the Lattice $\mathsf{A}\cdot\Lambda$ *increase* its energy.

For simple interactions (5.7) can be proven analytically [26, 9]. In practise one checks this stability condition by block-diagonalising $\delta^2 E^{\rm a}(0)$ using Fouriers series [32, 10, 15], that is, one checks whether the dispersion relation satisfies $\omega(k) \geq c|k|$. The condition is discussed in more detail in [15] and in Appendix C.

Assuming only (5.7) we can deduce stability of "small" displacements both in the atomistic and Cauchy–Born models. The factor $\frac12$ in the following result is arbitrary and may be replaced with any number between zero and one.

Proposition 5.1. *Let $\mathsf{A}\cdot\Lambda$ be stable, then there exists $\kappa_1 > 0$ such that, for $\kappa \leq \kappa_1$,*

$$\big\langle \delta^2 E^{\rm a}(u)v, v\big\rangle \geq \tfrac12\gamma\|\nabla v\|_{L^2}^2 \qquad \forall v\in\dot{\mathscr{W}}^{1,2}, \quad \forall u\in\mathscr{K}, \quad \textit{and}$$
$$\big\langle \delta^2 E^{\rm c}(u)v, v\big\rangle \geq \tfrac12\gamma\|\nabla v\|_{L^2}^2 \qquad \forall v\in\dot{W}^{1,2}, \quad \forall u\in K.$$

Before we prove Proposition 5.1 we state a variant of a classical intermediate result (see, e.g., [32, p. 89]; the following proof is adapted from [15, Thm. 3.1]).

Lemma 5.2. *Let γ be defined by* (5.7), *then*

$$\big\langle \delta^2 E^{\rm c}(0)v, v\big\rangle \geq \gamma\|\nabla v\|_{L^2}^2 \qquad \forall v\in\dot{W}^{1,2}.$$

Proof. Fix $v\in\dot{W}_0\setminus\{0\}$ and set $v_N(x) := Nv(N^{-1}x)$ for any $N\in\mathbb{N}$, and let $w_N := v_N|_\Lambda$; then we have

$$\langle\delta^2 E^{\rm c}(0)v, v\rangle = N^{-d}\langle\delta^2 E^{\rm c}(0)v_N, v_N\rangle.$$

Taking into account [15, Remark 1.1.1], and using the fact that v is smooth, Lemma 3.2 in [15] yields

$$N^{-d}\big|\langle\delta^2 E^{\rm c}(0)v_N, v_N\rangle - \langle\delta^2 E^{\rm a}(0)w_N, w_N\rangle\big| \to 0 \quad \text{as } N\to\infty.$$

We remark, that [15, Lemma 3.2] is formulated for finite-range interactions only, however, under the assumption that $M^{(2)}$ is finite a straightforward approximation argument extends it to the present case.

Using the smoothness of v it is also easy to see that $N^{-d/2}\|\nabla w_N\|_{L^2} \to \|\nabla v\|_{L^2}$. Hence, we obtain

$$\gamma \leq \frac{\langle\delta^2 E^{\rm a}(0)w_N, w_N\rangle}{\|\nabla w_N\|_{L^2}^2} \xrightarrow{N\to\infty} \frac{\langle\delta^2 E^{\rm c}(0)v, v\rangle}{\|\nabla v\|_{L^2}^2}.$$

Taking the infimum over all $v\in\dot{W}_0$ yields the stated result. □

Proof of Proposition 5.1. We first consider the atomistic case. A simple variation of the proof of (2.15) with $j = 3$ (replacing $\|\nabla u\|_{L^\infty}$ with $\max_{\xi\in\Lambda}\max_{\rho\in\Lambda_*}|D_\rho u(\xi)|$) gives the Lipschitz bound

$$\big|\big\langle(\delta^2 E^{\rm a}(u) - \delta^2 E^{\rm a}(0))v, v\big\rangle\big| \leq cM^{(3)}\kappa\|\nabla v\|_{L^2}^2 \qquad \forall v\in\dot{\mathscr{W}}^{1,2},$$

where c is a generic positive constant. Hence, choosing $\kappa \leq \gamma/(2cM^{(3)})$ yields the atomistic stability result.

After employing Lemma 5.2, the proof for the continuous case is analogous. □

Remark 5.3. We have shown that stability of the atomistic model implies stability of the continuum model, using only pointwise convergence of the atomistic hessian to the continuum hessian (this is in fact a consequence of convergence of the energy) and scale-invariance of the continuum limit. Conversely, one can construct examples [9, 15] where the continuum limit is stable (in 1D, convex) while the atomistic model is not stable in the sense of (5.7). In this case, we would still expect that atomistic solutions of both the static and dynamic problem exist (in a suitable extended framework), however, we can no longer expect them to be "close" to the solutions of the Cauchy–Born equations. We give a more detailed discussion in Appendix C, from which can conclude that (5.7) (or a similar assumption) is also *necessary* to obtain the results we seek. □

5.3. **Main result.** We first restate the Cauchy–Born equation (5.1) at a macroscopic scale

$$X = \varepsilon x, \quad U = \varepsilon u, \quad \text{and} \quad F^{\rm c} = \varepsilon^{-1} f^{\rm c}, \tag{5.8}$$

where $X \in \mathbb{R}^d, U, F^{\rm c} : \mathbb{R}^d \to \mathbb{R}^d$, and ε is the atomic spacing in the X-scale. In these *macroscopic variables*, the Cauchy–Born equation (5.2) reads, formally

$$-\operatorname{div}_X \mathsf{S}^{\rm c}(\nabla_X U^{\rm c}) = F^{\rm c}, \tag{5.9}$$

By assuming that $F^{\rm c}$ is small, more precisely, that

$$\|F^{\rm c}\|_{\dot W^{-1,2}} + \|\nabla F^{\rm c}\|_{L^2} =: \delta \tag{5.10}$$

is sufficiently small, we will be able to prove that there exists a solution $U^{\rm c}$ to (5.9). Reversing the scaling (5.8), we obtain a solution $u^{\rm c}(x) := \varepsilon^{-1} U^{\rm c}(\varepsilon x)$ of the atomic scale equation (5.2), with external force $f^{\rm c}(x) := \varepsilon F^{\rm c}(\varepsilon x)$. We note that

$$\|\nabla^3 u^{\rm c}\|_{L^2} + \|\nabla^2 u^{\rm c}\|_{L^4}^2 = \varepsilon^{2-d/2}\big(\|\nabla_X^3 U^{\rm c}\|_{L^2} + \|\nabla_X^2 U^{\rm c}\|_{L^4}^2\big), \tag{5.11}$$

which implies that the atomistic/Cauchy–Born modelling error in the internal forces is of order $O(\varepsilon^{2-d/2}$ (cf. Lemma 4.5). To ensure that the modelling error in the external forces is of the same order of magnitude, we shall assume that

$$\big|(f^{\rm c}, v)_{\mathbb{R}^d} - (f^{\rm a}, v)_\Lambda\big| \le C_f \delta \varepsilon^{2-d/2}. \tag{5.12}$$

As a concrete example, we show in Lemma A.5 that, if $F^{\rm c} \in \dot W^{-1,2} \cap W^{1,2}$, $f^{\rm c}$ is defined by (5.8), and $f^{\rm a}$ is defined by $f^{\rm a}(\xi) := \int \zeta(x-\xi) f^{\rm c}(x)\,{\rm d}x$, then $f^{\rm a} \in \dot{\mathscr{W}}^{-1,2}$ and (5.12) holds.

Theorem 5.4. *Let $d \le 3, k \ge 4$, and suppose that $\mathsf{A}\cdot\Lambda$ is stable and that $M_{\rm s}^{(2,2)}$ and $M_{\rm s}^{(3,2)}$ are finite (cf. § 2.3.4).*

There exist constants $\delta_0, \varepsilon_0 > 0$ such that, for $F^{\rm c} \in \dot W^{-1,2} \cap W^{1,2}$ satisfying (5.10)*, $f^{\rm c}$ defined by* (5.8) *and $f^{\rm a} \in \dot{\mathscr{W}}^{-1,2}$ satisfying* (5.12)*, and for $\delta \le \delta_0$ and $\varepsilon \le \varepsilon_0$, there exist stable solutions $u^{\rm c}$ and $u^{\rm a}$ of, respectively,* (5.2) *and* (5.5)*, such that*

$$\varepsilon^{d/2}\|\nabla u^{\rm c} - \nabla I u^{\rm a}\|_{L^2} \le C\frac{\delta\varepsilon^2}{\gamma},$$

where $C = C_f C(M_{\rm s}^{(2,2)}/\gamma, M_{\rm s}^{(3,2)}/\gamma)$.

Remark 5.5. 1. Formally, Theorem 5.4 states that, if the external forces are sufficiently small and of a "macroscopic nature" (encoded in the assumption that $f^{\rm c}(x) = \varepsilon F^{\rm c}(\varepsilon x)$, which implies that $\nabla f^{\rm a} \approx \nabla f^{\rm c} = O(\varepsilon^2)$), then the atomistic solution may be approximated to second-order accuracy by a solution of the Cauchy–Born model.

2. The conclusion of Theorem 5.4 may also be stated as

$$\|\nabla u^{\rm c} - \nabla I u^{\rm a}\|_{L^2} \lesssim C' \tfrac{\delta}{\gamma}\big(M_{\rm s}^{(2,2)}\|\nabla^3 u^{\rm c}\|_{L^2} + M_{\rm s}^{(3,2)}\|\nabla^2 u^{\rm c}\|_{L^4}^2\big),$$

where $C' = C'(\delta_0)$. In macroscopic units, with $U^{\rm a}_\varepsilon(X) := \varepsilon I u^{\rm a}(\varepsilon^{-1}X)$ the estimate reads

$$\|\nabla U^{\rm c} - \nabla U^{\rm a}_\varepsilon\|_{L^2} \le C' \tfrac{\delta}{\gamma} \varepsilon^2 \big(M_{\rm s}^{(2,2)} \|\nabla^3 U^{\rm c}\|_{L^2} + M_{\rm s}^{(3,2)} \|\nabla^2 U^{\rm c}\|_{L^4}^2\big).$$

On the right-hand sides of both of these estimates we may also replace $u^{\rm c}$ with $Iu^{\rm a}$, respectively $U^{\rm c}$ with $U^{\rm a}$, which effectively turns them into *a priori* error estimates.

3. The factor δ in these estimates shows that the error is $O(\varepsilon^2)$ *relative* to the magnitude of the external force and hence the displacement; that is, our estimates are in fact relative error estimates. □

The proof of this result uses a quantitative version of the inverse function theorem. The following version is taken from [24, Thm. 2.1].

Lemma 5.6 (Inverse Function Theorem). *Let $\mathscr{A}, \mathscr{B}$ be Banach spaces, $\mathscr{O}$ an open subset of $\mathscr{A}$, and let $\mathscr{F} : \mathscr{O} \to \mathscr{B}$ be Fréchet differentiable. Suppose also that there exist $\eta, \sigma > 0$ and a monotone function $\omega : [0, +\infty) \to [0, +\infty]$ such that*

$$\begin{aligned}
&\overline{B_{\mathscr{A}}(0, 2\eta\sigma)} \subset \mathscr{O}, \quad \|\mathscr{F}(0)\|_{\mathscr{B}} \le \eta, \quad \|\delta\mathscr{F}(0)^{-1}\|_{L(\mathscr{B},\mathscr{A})} \le \sigma, \\
&\|\mathscr{F}'(U) - \mathscr{F}'(V)\|_{L(\mathscr{A},\mathscr{B})} \le \omega\big(\|U - V\|_{\mathscr{A}}\big) \quad \text{for} \quad \|U\|_{\mathscr{A}}, \|V\|_{\mathscr{A}} \le 2\eta\sigma, \\
&2\sigma\omega(2\eta\sigma) \le 1, \quad \text{and} \quad \sigma\omega(2\eta\sigma) < 1.
\end{aligned}$$

Then, there exists a unique $U \in \mathscr{A}$ such that $\mathscr{F}(U) = 0$ and $\|U\|_{\mathscr{A}} \le 2\eta\sigma$.

Proof. The result follows from [24, Thm. 2.1], upon replacing σ with σ^{-1}, taking $\bar\omega(t) = t\omega(t)$ (admissible since ω is monotone), and $R = 2\eta\sigma$. □

Proof of Theorem 5.4. Part 1: Existence of a Cauchy–Born solution: Since $\mathsf{A} \cdot \Lambda$ is stable, Lemma 5.1 implies that $\delta^2 E^{\rm c}(0)$ is positive definite, which is equivalent to the statement that $\nabla^2 W(\mathsf{0})$ satisfies the strong Legendre–Hadamard condition. Under this condition it is proven in [27] that $\delta^2 E^{\rm c}(0) : \dot W^{3,2} \to \dot W^{1,2} \cap \dot W^{-1,2}$ is an isomorphism. Hence, we can hope to apply Lemma 5.6 with

$$\begin{aligned}
&\mathscr{A} := \dot W^{3,2}, \quad \mathscr{B} := \dot W^{1,2} \cap \dot W^{-1,2}, \\
&\mathscr{F}(U) := \delta E^{\rm c}(U) - F^{\rm c}, \quad \text{and} \quad \mathscr{O} := \{U \in \mathscr{A} \mid \|U\|_{\dot W^{3,2}} \le \delta\}.
\end{aligned}$$

Since $d \le 3$, $\mathscr{A}$ is embedded in $\dot W^{1,\infty}$ and hence, for δ sufficiently small, we have $\mathscr{O} \subset K$. Hence, (3.5) implies that, for $U, V \in \mathscr{O}$,

$$\big\|\mathscr{F}(U+V) - \mathscr{F}(U) - \delta^2 E^{\rm c}(U)[V, \,\cdot\,]\|_{\dot W^{-1,2}} \le M^{(3)} \|\nabla V\|_{L^2}^2 \le M^{(3)} \|V\|_{\mathscr{A}}^2.$$

A tedious but straightforward computation also shows that

$$\begin{aligned}
&\big\|\mathscr{F}(U+V) - \mathscr{F}(U) - \delta^2 E^{\rm c}(U)[V, \,\cdot\,]\|_{\dot W^{1,2}} \\
&= \big\|\nabla \mathrm{div}\big[\nabla W(\nabla U + \nabla V) - \nabla W(\nabla U) - \nabla^2 W(\nabla U) : \nabla V\big]\big\|_{L^2} \\
&\lesssim o_1(\|V\|_{\mathscr{A}}) \qquad \text{for } U \in \mathscr{O}, \text{ and for } \|V\|_{\mathscr{A}} \text{ sufficiently small,}
\end{aligned}$$

where $o_1(t) \ll t$ as $t \to 0$. (The function $o_1(t)$ depends on $M^{(3)}$ and $M^{(4)}$ and on the modulus of continuity of $\nabla^4 W$ in the set $\{\mathsf{F} \,|\, |\mathsf{F}| \le \kappa\}$; if $k = 5$, then $o_1(t) = \sum_{j=3}^5 M^{(j)} t^2$.) This shows that $\mathscr{F}$ is Fréchet differentiable and $\delta\mathscr{F}(U) = \delta^2 E^{\rm c}(U)$.

Similarly, we can also show that

$$\|\delta\mathscr{F}(U) - \delta\mathscr{F}(U')\|_{L(\mathscr{A},\mathscr{B})} \le o_0(\|U - U'\|_{\mathscr{A}}),$$

where $o_0(t) \to 0$ as $t \to 0$. (In fact, $o_0(t) = o_1(t)/t$.)

We have in particular established that $\delta\mathscr{F}(0) = \delta^2 E^{\rm c}(0)$, which we already know to be an isomorphism from $\mathscr{A}$ to $\mathscr{B}$. Moreover, by assumption we have

$$\|\mathscr{F}(0)\|_{\mathscr{B}} = \|F^{\rm c}\|_{\dot W^{-1,2}\cap \dot W^{1,2}} \le \delta.$$

Hence, Lemma 5.6 guarantees that, for δ sufficiently small, there exists $U^{\rm c} \in \dot W^{1,2} \cap \dot W^{3,2}$ satisfying (5.9) in the strong sense, and

$$\|U^{\rm c}\|_{\mathscr{A}} \le c\delta/\gamma, \tag{5.13}$$

where c is a generic constant. (The factor $1/\gamma$ is due to the fact that $\|\delta\mathscr{F}(0)^{-1}\|_{L(\mathscr{B},\mathscr{A})} \lesssim 1/\gamma$.)

Let $u^{\rm c}(x) := \varepsilon^{-1}U^{\rm c}(\varepsilon x)$, then the arguments given before the statement of the theorem, and Proposition 5.1, show that $u^{\rm c}$ is a stable solution of (5.2) with $f^{\rm c}$ given by (5.8).

Upon noting that $\|\nabla^3 U^{\rm c}\|_{L^2} + \|\nabla^2 U^{\rm c}\|_{L^4}^2 \lesssim \|U^{\rm c}\|_{\mathscr{A}} \lesssim \delta/\gamma$, and that $\|\nabla U^{\rm c}\|_{L^\infty} \lesssim \|U^{\rm c}\|_{\mathscr{A}} \lesssim \delta/\gamma$, we obtain the bounds

$$\|\nabla^3 u^{\rm c}\|_{L^2} + \|\nabla^2 u^{\rm c}\|_{L^4}^2 \lesssim \varepsilon^{2-d/2}\delta/\gamma, \quad \text{and} \quad \|\nabla u^{\rm c}\|_{L^\infty} \lesssim \delta/\gamma. \tag{5.14}$$

Part 2: existence of an atomistic solution. Recall the definition of $\tilde u^{\rm c} := \zeta * u^{\rm c}$ from Lemma 4.5. We apply Lemma 5.6 with $\mathscr{A} = \dot{\mathscr{W}}^{1,2}$, $\mathscr{B} = \dot{\mathscr{W}}^{-1,2}$, $\mathscr{O} := \{w \in \dot{\mathscr{W}}^{1,2} \,|\, \|\nabla w\|_{L^2} < \delta_1\}$ for some constant $\delta_1 > 0$ that remains to be chosen. If δ_1 is chosen sufficiently small, then $\tilde u^{\rm c}|_\Lambda + \mathscr{O} \subset \dot{\mathscr{W}}^{1,2} \cap \mathscr{K}$, hence we can define

$$\big\langle \mathscr{F}(w), v\big\rangle := \big\langle \delta E^{\rm a}(\tilde u^{\rm c} + w), v\big\rangle - (f^{\rm a}, v)_\Lambda \qquad \text{for } w \in \mathscr{O}, \quad v \in \dot{\mathscr{W}}^{1,2}.$$

By Theorem 2.8, $\mathscr{F}$ is Fréchet differentiable in $\mathscr{O}$, and $\delta\mathscr{F}$ is Lipschitz continuous in $\mathscr{O}$, that is we can choose $\omega(t) = cM^{(3)}t$ in Lemma 5.6.

To obtain a stability estimate, we use (5.14) and Proposition 5.1 to deduce that, if δ and δ_1 are chosen sufficiently small, then

$$\big\langle \delta^2 E^{\rm a}(\tilde u^{\rm c})v, v\big\rangle \ge \tfrac12 \gamma \|\nabla v\|_{L^2}^2 \qquad \forall v \in \dot{\mathscr{W}}^{1,2},$$

that is, $\|\delta\mathscr{F}(0)^{-1}\|_{L(\mathscr{B},\mathscr{A})} \le \big(\tfrac12\gamma\big)^{-1} =: \sigma$.

To obtain a residual bound, we apply Lemmas 4.5 and A.5, to estimate

$$\begin{aligned}
\big\langle \mathscr{F}(0), \tilde v\big\rangle &= \big\langle \delta E^{\rm a}(\tilde u^{\rm c}), \tilde v\big\rangle - (f^{\rm a}, \tilde v)_\Lambda \\
&= \Big\{\big\langle \delta E^{\rm a}(\tilde u^{\rm c}), \tilde v\big\rangle - \big\langle \delta E^{\rm c}(u^{\rm c}), v\big\rangle\Big\} - \Big\{(f^{\rm a}, \tilde v)_\Lambda - (f^{\rm c}, v)_{\mathbb{R}^d}\Big\} \\
&\lesssim \big(M_{\rm s}^{(2,2)}\|\nabla^3 u^{\rm c}\|_{L^2} + M_{\rm s}^{(3,2)}\|\nabla^2 u^{\rm c}\|_{L^4}^2 + \|\nabla f^{\rm c}\|_{L^2}\big)\|\nabla v\|_{L^2}.
\end{aligned}$$

that is,

$$\|\mathscr{F}(0)\|_{\mathscr{B}} \le \eta := C\left[1 + \gamma^{-1}(M_{\rm s}^{(2,2)} + M_{\rm s}^{(3,2)})\right]\delta\varepsilon^{2-d/2}.$$

Lemma 5.6 states that, if

$$C\frac{M^{(3)}}{\gamma}\left(1 + \frac{M_{\rm s}^{(2,2)} + M_{\rm s}^{(3,2)}}{\gamma}\right)\frac{\delta}{\gamma}\varepsilon^{2-d/2} < 1, \tag{5.15}$$

then there exists a locally unique solution v of $\mathscr{F}(v) = 0$. This can be guaranteed provided that $\delta\varepsilon^{2-d/2}/\gamma < \varepsilon_0 = \varepsilon_0(M_{\rm s}^{(2,2)}/\gamma, M_{\rm s}^{(3,2)}/\gamma)$. (Recall that $M^{(3)} \le M_{\rm s}^{(3,2)}$.)

Let $w^{\rm c} := \tilde u^{\rm c}|_\Lambda$. Setting $u^{\rm a}(\xi) := w^{\rm c}(\xi) + v(\xi)$, and applying (2.10) we obtain the estimate

$$\|\nabla u^{\rm a} - \nabla w^{\rm c}\|_{L^2} \le 2\sigma\eta \lesssim \left[1 + \tfrac{1}{\gamma}(M_{\rm s}^{(2,2)} + M_{\rm s}^{(3,2)})\right]\tfrac{\delta}{\gamma}\varepsilon^{2-d/2}.$$

Applying the interpolation error estimate given in Corollary A.3 and (2.10), we obtain

$$\begin{aligned}\|\nabla u^{\rm c} - \nabla I u^{\rm a}\|_{L^2} &\le \|\nabla I(w^{\rm c} - u^{\rm a})\|_{L^2} + \|\nabla u^{\rm c} - \nabla I w^{\rm c}\|_{L^2} \\ &\lesssim \|\nabla(u^{\rm c} - u^{\rm a})\|_{L^2} + \|\nabla^3 u^{\rm c}\|_{L^2} \\ &\lesssim \big[1 + \tfrac{1}{\gamma}(M_{\rm s}^{(2,2)} + M_{\rm s}^{(3,2)})\big]\tfrac{\delta}{\gamma}\varepsilon^{2-d/2}.\end{aligned}$$

This concludes the proof of the theorem. □

6. Convergence to solutions of the Wave Equation

In this section we consider the dynamic problem

$$\begin{aligned}&(\ddot u^{\rm a}(t), v)_\Lambda + \langle \delta E^{\rm a}(u^{\rm a}(t)), v\rangle = 0 \qquad \forall v \in \mathscr{W}_0, \quad t > 0, \\ &u^{\rm a}(0) = u^{\rm a}_0, \quad \dot u^{\rm a}(0) = u^{\rm a}_1.\end{aligned} \tag{6.1}$$

We will prove that, if the initial condition is "macroscopic", then there exists a unique solution to (6.1), which remains close to a solution of the corresponding Cauchy–Born wave equation for a "macroscopic time interval".

For simplicity, we do not consider external forces in the the dynamic problem.

6.1. **The macroscopic wave equation.** Formally, the continuum limit of (6.1) is the Cauchy–Born wave equation

$$\ddot u^{\rm c}(t) - {\rm div}\mathsf{S}^{\rm c}(\nabla u^{\rm c}(t)) = 0,$$

subject to initial conditions. Upon rescaling

$$X := \varepsilon x, \quad U := \varepsilon u, \quad T := \varepsilon t, \tag{6.2}$$

we formally obtain

$$\tfrac{{\rm d}^2}{{\rm d}T^2} U^{\rm c}(T) - {\rm div}_X \mathsf{S}^{\rm c} \nabla_X U^{\rm c}(T)) = 0, \tag{6.3}$$

which we supply with the initial condition

$$U^{\rm c}(0) = U^{\rm c}_0, \quad \text{and} \quad \nabla_T U^{\rm c}(0) = U^{\rm c}_1. \tag{6.4}$$

To establish well-posedness of (6.3), (6.4), we apply the well-established theory. In our context, Theorem III in [16] reads as follows. Note that, from here on, we employ again the standard Sobolev spaces instead of homogeneous Sobolev spaces.

Proposition 6.1. *Let $d \in \{1,2,3\}$, $k \ge 4$, and suppose that $\mathsf{A}\cdot\Lambda$ is stable. Let $U^{\rm c}_0 \in W^{4,2}, U^{\rm c}_1 \in W^{3,2}$ with $\|\nabla U^{\rm c}_0\|_{L^\infty} < \kappa$, then there exists $T^{\rm c} > 0$ such that the system* (6.3), (6.4) *has a unique solution $U^{\rm c} \in C^2([0,T^{\rm c}]; W^{2,2}) \cap C^1([0,T^{\rm c}]; W^{3,2}) \cap C([0,T^{\rm c}]; W^{4,2})$, satisfying $\max_{T\in[0,T^{\rm c}]} \|\nabla U^{\rm c}(T)\|_{L^\infty} < \kappa$.*

Proof. The symbol Ω, and the conditions (a1), (a2), (a3), (3.1), (3.2) in this proof refer to [16].

In the notation of [16], (6.3) reads

$$a_{00}\frac{\partial^2 U}{\partial T^2} = \sum_{\alpha,\beta=1}^{d} a_{\alpha\beta}\frac{\partial^2 U}{\partial X_\alpha \partial X_\beta} + b,$$

where $a_{00} = I, a_{\alpha\beta} = (\mathbb{C}^{j\beta}_{i\alpha}(\nabla U))^d_{i,j=1}$, where $\mathbb{C}(\mathsf{F}) = \nabla^2_{\mathsf{F}} W(\mathsf{F})$, $b_i = \sum_{\alpha,\beta,j=1}^d \frac{\partial \mathbb{C}^{j\beta}_{i\alpha}}{\partial X_\alpha}\frac{\partial U_j}{\partial X_\beta}$, and $a_{0,i} = a_{i,0} = 0$, for $i = 1,\dots,d$. Condition (a1) is trivially satisfied and condition (a2) follows from the fact that $W \in C^2$. Condition (a3) is the Legendre–Hadamard condition for $\mathbb{C}(\mathsf{F})$, which we know from Proposition 5.1 to be satisfied for $|\mathsf{F}| \le \kappa$. Hence, choosing $\Omega = \mathbb{R}^d \times \mathbb{R}^d \times B_{\mathbb{R}^{d\times d}}(\mathsf{0}, \kappa)$ we obtain (a3).

Condition (3.1) is satisfied for $s = 3$. Condition (3.2) is satisfied since we assumed that $\|\nabla_X U_0\|_{L^\infty} < \kappa$. The requirement that $s \geq d/2 + 1$ holds since we have restricted $d \leq 3$. This ensures the existence of a solution with the stated regularity.

Since $U^{\rm c} \in C^1([0, T^{\rm c}]; W^{3,2}) \subset C^1([0, T^{\rm c}]; W^{1,\infty})$ and since $\|\nabla U^{\rm c}(0)\|_{L^\infty} < \kappa$ it follows that $\|\nabla U^{\rm c}(T)\|_{L^\infty} \leq \kappa$ for sufficiently short time. Thus choosing $T^{\rm c}$ sufficiently small, we obtain that $\max_{T\in[0,T^{\rm c}]} \|\nabla U^{\rm c}(T)\|_{L^\infty} < \kappa$. □

Upon reverting the scaling (6.2), we obtain the existence of a trajectory $u^{\rm c}(x, t) := \varepsilon^{-1}U^{\rm c}(\varepsilon x, \varepsilon t)$, defined for $x \in \mathbb{R}^d, t \in [0, t^{\rm c}]$, where $t^{\rm c} := T^{\rm c}/\varepsilon$, satisfying the following conditions:

$$(\ddot{u}^{\rm c}, u)_{\mathbb{R}^d} + \langle \delta E^{\rm c}(u^{\rm c}), u\rangle = 0 \qquad \forall\, u \in W^{1,2}, \quad t \in (0, t^{\rm c}], \tag{6.5}$$

$$u^{\rm c}(x, 0) = \varepsilon^{-1}U^{\rm c}_0(\varepsilon x), \quad \dot{u}^{\rm c}(x, 0) = U^{\rm c}_1(\varepsilon x), \qquad \text{and} \tag{6.6}$$

$$\|\nabla^m_x \nabla^l_t u^{\rm c}\|_{L^\infty([0,t^{\rm c}],L^2)} \leq C_{m,l}\varepsilon^{m+l-1-d/2} \quad \text{for } m, l \in \mathbb{N}, 1 \leq m + l \leq 4, \tag{6.7}$$

where $C_{m,l} = \|\nabla^m_X \nabla^l_T U^{\rm c}\|_{L^\infty([0,T^{\rm c}],L^2)}$.

We also imposed in Proposition 6.1 that $T^{\rm c}$ is chosen sufficiently small to ensure that $U^{\rm c}(T) \in K$ for all $T \in [0, T^{\rm c}]$. This implies that $u^{\rm c}(t) \in K$ for all $t \in [0, t^{\rm c}]$, and hence we may conclude that

$$\langle \delta^2 E^{\rm a}(u^{\rm c}(t))v, v\rangle \geq \tfrac{1}{2}\gamma\|\nabla v\|^2_{L^2} \qquad \forall\, v \in \ell^2, \quad t \in [0, t^{\rm c}_1].$$

6.2. **Main result.** After the preparation we can state our result on the convergence of solutions of (6.1).

Theorem 6.2. *Suppose that* $d \in \{1, 2, 3\}, k \geq 4$, *and* $\mathsf{A}\cdot\Lambda$ *is stable. Let* $\|\nabla U^{\rm c}_0\|_{L^\infty} < \kappa$, *where* κ *is chosen sufficiently small so that Proposition 5.1 applies. Finally, suppose that* $M^{(j,2)}_{\rm d}$ *is finite for* $j = 2, 3, 4$, *and let* $C_{\rm init} > 0$ *be a fixed constant.*

Then there exists $T^{\rm a} = \varepsilon^{-1}t^{\rm a} \in (0, T^{\rm c}]$ *and* $\varepsilon_0 > 0$ *such that, for all* $\varepsilon \leq \varepsilon_0$, *and for any initial data* $u^{\rm a}_0, u^{\rm a}_1$ *with*

$$\varepsilon^{d/2}\big\|\nabla I u^{\rm a}_0 - \nabla u^{\rm c}(0)\big\|_{L^2} + \varepsilon^{d/2}\big\|\nabla I u^{\rm a}_1 - \nabla \dot{u}^{\rm c}(0)\big\|_{L^2} \leq C_{\rm init}\varepsilon^2, \tag{6.8}$$

there exists $u^{\rm a} \in C^2([0, t^{\rm a}]; \ell^2)$ *satisfying* (6.1), *and*

$$\max_{0\leq t\leq t^{\rm a}} \varepsilon^{d/2}\big(\|\nabla I u^{\rm a}(t) - \nabla u^{\rm c}(t)\|_{L^2} + \|I\dot{u}^{\rm a}(t) - \dot{u}^{\rm c}(t)\|_{L^2}\big) \leq C\varepsilon^2, \tag{6.9}$$

where $C = C(\gamma, (M^{(j,2)}_{\rm d})^4_{j=2}, U^{\rm c}, C_{\rm init})$.

If $d \leq 2$ *or* $k \geq 5$, *then we may choose* $t^{\rm a} = t^{\rm c}$.

Proof. We give here an outline of the proof, but will establish the key technical results in the following subsections. All constants in this proof may depend on any property of $U^{\rm c}$.

1. Setup: From Lemma 6.3 we obtain local existence for the atomistic problem: there exists $t_1 > 0$ and $u \in C^2([0, t_1]; \ell^2)$ satisfying (6.1). Let $z(t) := \tilde{u}^{\rm c}(t)|_\Lambda = (\zeta * u^{\rm c}(t))|_\Lambda$ and let

$$e(\xi, t) := u^{\rm a}(\xi, t) - z(\xi, t),$$

whenever the left-hand side is well-defined. Moreover, let $w \in \ell^2$ such that $\tilde{w}(\xi, t) = e(\xi, t)$.

It follows from (6.7), Lemma A.2, and Lemma A.3, that the initial error satisfies

$$\|\dot{e}(0)\|^2_{\ell^2} + \tfrac{\gamma}{2}\|\nabla e(0)\|^2_{L^2} \leq C_0\varepsilon^{4-d}, \tag{6.10}$$

where C_0 depends on $U^{\rm c}_0, U^{\rm c}_1$, $C_{\rm init}$ but is independent of ε. We fix a constant $C_* > C_0$, which will be specified later on. Since $u^{\rm a} \in C^2([0, t_1], \ell^2)$ (and hence $e \in C^2([0, t_1], \ell^2)$) upon choosing t_1 sufficiently small, we obtain

$$\|\dot{e}(t)\|^2_{\ell^2} + \tfrac{\gamma}{2}\|\nabla e(t)\|^2_{L^2} \leq C_*\varepsilon^{4-d} \qquad \forall t \in [0, t_1]. \tag{6.11}$$

Thus the task is to prove that we may choose $t_1 \gtrsim \varepsilon^{-1}$.

From the definition of z and the assumption that $\|\nabla u^{\rm c}(t)\|_{L^\infty} \le \kappa' < \kappa$ for all $t \in [0, t^{\rm c}]$, we deduce that $|D_\rho z(t,\xi)| \le \kappa'$ for all t, ξ, ρ (cf. the proof of Lemma 4.5). Choosing ε_0 sufficiently small, then for $\varepsilon \le \varepsilon_0$ we obtain from (6.11) that

$$z(t) + \theta e(t) \in \mathscr{K} \qquad \forall t \in [0, t_1], \quad \theta \in [0,1]. \tag{6.12}$$

Since we assumed that κ was chosen sufficiently small, Proposition 5.1 implies that

$$\big\langle \delta^2 E^{\rm a}(z(t) + \theta e(t)) v, v\big\rangle \ge \tfrac{\gamma}{2}\|\nabla v\|_{L^2}^2 \qquad \forall v \in \ell^2, \quad t \in [0,t_1], \quad \theta \in [0,1]. \tag{6.13}$$

2. Error equation: Testing (6.1) with $\dot e$ and (6.5) with $\dot w$, yields

$$(\ddot e, \dot e)_\Lambda + \langle \delta E^{\rm a}(u^{\rm a}) - \delta E^{\rm a}(z), \dot e\rangle = \Big\{ (\ddot u^{\rm c}, \dot w)_{\mathbb{R}^d} - (\ddot z, \dot e)_\Lambda \Big\} + \Big\{ \langle \delta E^{\rm c}(u^{\rm c}), \dot w\rangle - \langle \delta E^{\rm a}(z), \dot e\rangle \Big\}. \tag{6.14}$$

Since $\tilde w = e$, the first group on the right-hand side can be rewritten as (cf. (A.3))

$$\Big\{ (\ddot u^{\rm c}, \dot w)_{\mathbb{R}^d} - (\ddot z, \dot e)_\Lambda \Big\} = (\ddot u^{\rm c} - \ddot z, \dot w)_{\mathbb{R}^d} =: (\alpha, \dot w)_{\mathbb{R}^d},$$

where z and w are identified with their first-order interpolants. Similarly, using Proposition 4.1, we can write

$$\Big\{ \langle \delta E^{\rm c}(u^{\rm c}), \dot w\rangle - \langle \delta E^{\rm a}(z), \dot e\rangle \Big\} = (\mathsf{S}^{\rm c}(u^{\rm c}) - \mathsf{S}^{\rm a}(z), \nabla \dot w)_{\mathbb{R}^d} =: (\beta, \nabla \dot w)_{\mathbb{R}^d},$$

Moreover, according to (6.12) we can expand

$$\big\langle \delta E^{\rm a}(u^{\rm a}) - \delta E^{\rm a}(z), \dot e\big\rangle =: \int_0^1 \langle \delta^2 E^{\rm a}(z + \theta e) e, \dot e\rangle {\rm d}\theta =: \langle H e, \dot e\rangle,$$

to rewrite (6.14) as

$$\frac{\rm d}{{\rm d}t}\Big\{ \|\dot e\|_\Lambda^2 + \langle He, e\rangle \Big\} = \langle \dot H e, e\rangle + 2(\alpha, \dot e)_{\mathbb{R}^d} + 2(\beta, \nabla \dot w)_{\mathbb{R}^d}. \tag{6.15}$$

We define $E^2(t) := \|\dot e\|_{\ell^2}^2 + \langle He, e\rangle$, and note that (6.13) immediately implies that

$$\|\dot e\|_{\ell^2}^2 + \tfrac{\gamma}{2}\|\nabla e\|_{L^2}^2 \le E^2(t) \le C_H\big(\|\dot e\|_{\ell^2}^2 + \tfrac{\gamma}{2}\|\nabla e\|_{L^2}^2\big) \qquad \forall t \in [0,t_1], \tag{6.16}$$

where C_H depends only on $M^{(2)}$. We integrate (6.15) over $(0,s)$, $s \le t_1$, to obtain

$$E^2(s) = E^2(0) + \int_0^s \Big\{ \langle \dot H e, e\rangle + 2(\alpha, \dot w)_{\mathbb{R}^d} + 2(\beta, \dot w)_{\mathbb{R}^d} \Big\}\, {\rm d}t, \tag{6.17}$$

and proceed to estimate the three terms on the right-hand side separately.

3. Consistency estimates and nonlinearity: The second and third term on the right-hand side of (6.17) measure the consistency between the atomistic and Cauchy–Born model. Standard interpolation error results (cf. §6.3 for the details) yield the estimate $\|\alpha\|_{L^2} \lesssim \|\nabla^2 \ddot u^{\rm c}\|_{L^2} \lesssim \varepsilon^{3-d/2}$, and hence, applying Cauchy's inequality and (2.5), we obtain

$$\int_0^s 2(\alpha, \dot w)_{\mathbb{R}^d}\, {\rm d}t \le C_\alpha\bigg(t_1 \varepsilon^{5-d} + \varepsilon \int_0^s E^2\, {\rm d}t\bigg), \tag{6.18}$$

where C_α depends only on the trajectory $U^{\rm c}$ through the bounds (6.7), but it is independent of ε.

The third term on the right-hand side of (6.17) requires an estimate that it similar to Lemma 4.5. We establish the required variant in §6.3:

$$(\beta, \nabla \dot w)_{L^2} \le C\varepsilon^{3-d/2}\|\dot w\|_{L^2}, \tag{6.19}$$

where $C = C(U^{\rm c}, (M_{\rm d}^{(j,2)})_{j=2}^4)$. Integrating over $(0, s)$, $s \le t_1$, and applying Cauchy's inequality, we again obtain

$$\int_0^s 2(\beta, \nabla \dot{w})_{L^2} \,{\rm d}t \le C_\beta \bigg(t_1 \varepsilon^{5-d} + \varepsilon \int_0^s E^2 \,{\rm d}t \bigg), \tag{6.20}$$

where C_β depends on $(M_{\rm s}^{(j,2)})_{j=2}^4$ and on $U^{\rm c}$, but not on ε (provided $\varepsilon \le \varepsilon_0$, which we chose above so that $u^{\rm a} = z + e \in \mathscr{K}$).

Finally, the first term on the right-hand of (6.17) side is not a consistency term, but must be otherwise controlled. Our argument is a refinement of a method due to Makridakis [22] for the numerical analysis of nonlinear wave equations. In §6.4 we show that an integrating by parts argument leads to

$$\int_0^s \langle \dot{H} e, e \rangle \,{\rm d}t \le C_{\rm nl} \bigg(E^3(s) + E^3(0) + \int_0^s \Big(\varepsilon E^2 + \varepsilon E^3 + E^4 \Big) \,{\rm d}t \bigg), \tag{6.21}$$

where $C_{\rm nl} = C_{\rm nl}(M^{(3)}, M^{(4)}, U^{\rm c})$.

4. Gronwall lemma: Combining (6.18), (6.20), (6.21) with (6.17) yields

$$\begin{aligned} E^2(s) \le{}& E^2(0) + (C_\alpha + C_\beta) \bigg(t_1 \varepsilon^{5-d} + \varepsilon \int_0^s E^2 \,{\rm d}t \bigg) \\ &+ C_{\rm nl} \bigg(E^3(0) + E^3(s) + \int_0^s \Big(\varepsilon E^2 + \varepsilon E^3 + E^4 \Big) \,{\rm d}t \bigg). \end{aligned}$$

We employ (6.10), (6.11), (6.16) and $T_1 := t_1 \varepsilon$, to obtain

$$\begin{aligned} E^2(s) \le{}& \big[C_H C_0 + (C_\alpha + C_\beta) T_1 \big] \varepsilon^{4-d} + \varepsilon (C_\alpha + C_\beta + C_{\rm nl}) \int_0^s E^2 \,{\rm d}t \\ &+ C_{\rm nl} \bigg(C_H^{3/2} C_0^{3/2} \varepsilon^{6-3d/2} + C_H^{3/2} C_*^{3/2} \varepsilon^{6-3d/2} + \int_0^s C_H C_* \varepsilon^{4-d} E^2 \,{\rm d}t \bigg). \end{aligned}$$

Since $\varepsilon^{6-2d/2} \le \varepsilon^{4-d} \cdot \varepsilon_0^{2-d/2}$ and since $d \le 3$, choosing ε_0 sufficiently small ensures that

$$C_H^{3/2} C_0^{3/2} \varepsilon^{6-3d/2} + C_H^{3/2} C_*^{3/2} \varepsilon^{6-3d/2} \le C_H C_0 \varepsilon^{4-d}.$$

(However, if $d = 3$ then $\varepsilon^{4-d} = \varepsilon$, hence the integral term cannot be made arbitrarily small for $s = O(1/\varepsilon)$.) Upon defining $C_1 = C_1(T_1) = 2C_H C_0 + (C_\alpha + C_\beta) T_1$ and $C_2 = C_2(C_*, \varepsilon_0) = C_\alpha + C_\beta + C_{\rm nl}(1 + C_H C_* \varepsilon_0^{3-d})$, yields

$$E^2(s) \le C_1 \varepsilon^{4-d} + C_2 \int_0^s E^2 \,{\rm d}t, \qquad \text{for } 0 \le s \le t_1. \tag{6.22}$$

Applying Gronwall's inequality, we obtain

$$\max_{0 \le t \le t_1} E^2(t) \le C_1 \exp(C_2 T_1) \varepsilon^{4-d}. \tag{6.23}$$

We observe that $C_1 \exp(C_2 T_1) \to 2 C_H C_0$ as $T_1 \to 0$.

We now choose $C_*, \varepsilon_0, T^{\rm a}$ in the following order: 1. $C_* := 4 C_H C_0$ (or any constant larger than $2 C_H C_0$); 2. $\varepsilon_0 \le 1$ and sufficiently small as required in the estimates up to this point (dependent in particular on C_*); and 3. $T^{\rm a} > 0$ sufficiently small so that

$$C_1(T^{\rm a}) \exp(C_2(C_*, 1) T^{\rm a}) =: C_3(T^{\rm a}) \le C_* \qquad \text{and} \qquad T^{\rm a} \le T^{\rm c}.$$

This is possible due to the fact that $C_3(T^{\rm a}) \to \frac{1}{2} C_*$ as $T^{\rm a} \to 0$. We set $t^{\rm a} := T^{\rm a}/\varepsilon$.

Using these definitions, we can estimate (6.23) above by

$$\max_{0 \le t \le t_1} E^2(t) \le C_3(T_1) \varepsilon^{4-d} \le C_* \varepsilon^{4-d}. \tag{6.24}$$

5. Continuation argument: Suppose that $t_1 \leq t^{\mathrm{a}}$ is chosen maximally, such that the trajectory u^{a} exists in $[0, t_1]$ and (6.11) holds with the choice of C_* we made above. If $t_1 < t^{\mathrm{a}}$, then we end up with the stronger error estimate (6.24). We apply Lemma 6.3 again to extend u^{a} to an interval $[t_1, t_2]$ where $t_1 < t_2 \leq t^{\mathrm{a}}$. Since (6.24) holds in $[0, t_1]$, and since $C_3(T_1) < C_*$ when $T_1 < T^{\mathrm{a}}$, choosing t_2 sufficiently close to t_1 implies that (6.11) holds in $[0, t_2]$. This contradicts the maximality of t_1 and hence we must have $t_1 = t^{\mathrm{a}}$. Thus, we conclude that (6.11) holds in $[0, t^{\mathrm{a}}]$, where $t^{\mathrm{a}} = \varepsilon^{-1} T^{\mathrm{a}}$ and $T^{\mathrm{a}} > 0$.

6. Maximal time interval for $d < 3$: If $d < 3$ then one varies the argument following (6.23), exploiting the fact that $\varepsilon_0^{3-d} \to 0$ as $\varepsilon_0 \to 0$, as follows. 1. Choose $C_* := C_1(T^{\mathrm{c}}) \exp(C_2(1,1) T^{\mathrm{c}})$. 2. Choose ε_0 sufficiently small as required by the previous estimates, and in addition sufficiently small so that $C_* \varepsilon_0 \leq 1$. 3. Choose $T^{\mathrm{a}} = T^{\mathrm{c}}$. The rest of the argument is analogous.

7. Maximal time interval for $k \geq 5$: Now suppose that $d = 3$ and $k \geq 5$, then we need to vary the proof starting from (6.21). The assumption that $k \geq 5$ allows us to integrate the term $\langle \dot{H} e, e \rangle$ by parts twice, to prove in §6.4 that

$$\int_0^s \langle \dot{H} e, e \rangle \,\mathrm{d}t \leq C_{\mathrm{nl}} \bigg(E^3(s) + E^3(0) + E^4(s) + E^4(0) + \int_0^s \Big(\varepsilon E^2 + \varepsilon E^3 + \varepsilon E^4 + E^5(t) \Big) \,\mathrm{d}t \bigg), \tag{6.25}$$

where C_{nl} depends only on $(M^{(j)})_{j=3}^5$. Exploiting the higher powers of E and arguing similarly as in *4*, upon choosing ε_0 sufficiently small, we obtain

$$\int_0^s \langle \dot{H} e, e \rangle \,\mathrm{d}t \leq C_H C_0 \varepsilon^{4-d} + C_{\mathrm{nl}} \varepsilon \int_0^s E^2 \,\mathrm{d}t,$$

and eventually

$$\max_{0 \leq t \leq t_1} E^2(t) \leq C_1 \exp(C_2 T_1) \varepsilon^{4-d},$$

where $C_1 = 2 C_H C_0 + (C_\alpha + C_\beta) T_1$ and $C_2 = C_\alpha + C_\beta + C_{\mathrm{nl}}$. Since C_1 and C_2 are independent of C_* we can now argue as in step *6* to deduce that we may choose $T^{\mathrm{a}} = T^{\mathrm{c}}$. □

Lemma 6.3. *Let $u_0, u_1 \in \ell^2$, $\|\nabla u_0\|_{L^\infty} < \kappa$, then there exists $t_1 > 0$ and a unique trajectory $u \in C^2([0, t_1]; \ell^2)$ satisfying (6.1) with $u(0) = u_0, \dot{u}(0) = u_1$.*

Proof. The estimate (2.15) with $j = 2$ implies the existence of $\delta > 0$ such that, for all $v_1, v_2 \in B_{\ell^2}(u_0, \delta)$,

$$\big| \langle \delta E^{\mathrm{a}}(v_1) - \delta E^{\mathrm{a}}(v_2), w \rangle \big| \leq M^{(2)} \|\nabla v_1 - \nabla v_2\|_{L^2} \|\nabla w\|_{L^2} \lesssim M^{(2)} \|v_1 - v_2\|_{\ell^2} \|w\|_{\ell^2}.$$

that is, $\delta E^{\mathrm{a}} : \ell^2 \to \ell^2$ is Lipschitz. Hence the result follows from Picard's theorem. □

6.3. **Consistency estimates.** In this section, we prove the two consistency estimates (6.18) and (6.20). We begin by considering (6.18), which follows from standard interpolation error estimates.

Lemma 6.4. *Let $v \in W^{2,2}$, and let $\overline{\zeta * v}$ be the first-order interpolant of $\zeta * v|_\Lambda$, then*

$$\big\| v - \overline{\zeta * v} \big\|_{L^2} \lesssim \|\nabla^2 v\|_{L^2}.$$

Proof. We first apply a triangle inequality,

$$\big\|v - \overline{\zeta * v}\big\|_{L^2} \le \big\|v - \zeta * v\big\|_{L^2} + \big\|\zeta * v - \overline{\zeta * v}\big\|_{L^2}.$$

The first term on the right-hand side is estimated using Lemma A.2,

$$\big\|v - \zeta * v\big\|_{L^2} \lesssim \|\nabla^2 v\|_{L^2}.$$

The second term on the right-hand side is a standard Q1-interpolation error, which can be estimated by [5]

$$\big\|\zeta * v - \overline{\zeta * v}\big\|_{L^2} \lesssim \|\nabla^2(\zeta * v)\|_{L^2} = \|\zeta * \nabla^2 v\|_{L^2} \le \|\nabla^2 v\|_{L^2}. \qquad \square$$

Proof of (6.18). Applying Lemma 6.4, the regularity bound (6.7), and the norm-equivalence $\|\dot w\|_{L^2} \approx \|\dot e\|_{\ell^2} \le E$ (see § 2.1), we can estimate

$$\int_0^s (\alpha, \dot w)_{L^2}\,\mathrm{d}t \lesssim \int_0^s \|\nabla^2 \ddot u^{\mathrm{c}}\|_{L^2}\|\dot w\|_{L^2}\,\mathrm{d}t \lesssim \int_0^s \varepsilon^{3-d/2} E\,\mathrm{d}t.$$

Applying Cauchy's inequality to $\varepsilon^{3-d/2}E = \varepsilon^{(5-d)/2}\cdot(\varepsilon^{1/2}E)$, we obtain

$$\int_0^s (\alpha, \dot w)_{L^2}\,\mathrm{d}t \lesssim \int_0^s \Big(\varepsilon^{5-d} + \varepsilon E^2\Big)\,\mathrm{d}t \le t_1 \varepsilon^{5-d} + \varepsilon \int_0^s E^2\,\mathrm{d}t \qquad \square$$

We now turn towards (6.20), which is the crucial ingredient in the dynamic analysis. Our strategy will be to integrate by parts, and estimate $\nabla\beta$, which is the error in the divergence of the stresses. To that end, we first need to prove that $x \mapsto \mathsf{S}^{\mathrm{a}}(u; x)$ is differentiable. For S^{c}, the analogous result follows from Lemma 3.1.

Lemma 6.5. *Let $u \in \mathscr{K}$, then $x \mapsto \mathsf{S}^{\mathrm{a}}(u; x) \in W^{1,\infty}$, with*

$$\operatorname{div} \mathsf{S}^{\mathrm{a}}(u; x) = \sum_{\rho \in \Lambda_*} \sum_{\xi \in \Lambda} \Phi_{\xi,\rho}(u) \nabla_\rho \chi_{\xi,\rho}(x), \tag{6.26}$$

where $\nabla_\rho \chi_{\xi,\rho}(x) = \nabla \chi_{\xi,\rho}(x) \cdot \rho$.

Proof. Since $\chi_{\xi,\rho} \ge 0$ and $(\chi_{\xi,\rho})_{\xi\in\Lambda}$ is a partition of unity, it is straightforward to show that $|\mathsf{S}^{\mathrm{a}}(u; x)| \le M^{(1)}$ for all $x \in \mathbb{R}^d$.

The rest of the proof is devoted to the assertion that S^{a} is Lipschitz continuous. First, we compute the Lipschitz constant of $\chi_{\xi,\rho}$. Let L be the global Lipschitz constant of ζ, let $S_x := \mathrm{supp}(\zeta(\,\cdot\, - x))$, and let $J_{x,y} := \{s \in (0, |\rho|) \,|\, \xi + s\frac{\rho}{|\rho|} \in S_x \cap S_y\}$; then

$$\begin{aligned}
\big|\chi_{\xi,\rho}(x) - \chi_{\xi,\rho}(y)\big| &\le \frac{1}{|\rho|}\int_{I_{x,y}} \big|\zeta\big(\xi + s\tfrac{\rho}{|\rho|} - x\big) - \zeta\big(\xi + s\tfrac{\rho}{|\rho|} - y\big)\big|\,\mathrm{d}s \\
&\le \frac{1}{|\rho|}\int_{I_{x,y}} L|x-y|\,\mathrm{d}s \le \frac{2L\mathrm{diam}(S_x)}{|\rho|}\,|x-y| \lesssim |\rho|\,|x-y|.
\end{aligned}$$

Next, we note that $\sum_{\xi\in\Lambda}(\chi_{\xi,\rho}(x) - \chi_{\xi,\rho}(y)) = 0$, and hence we can rewrite

$$\begin{aligned}
\mathsf{S}^{\mathrm{a}}(u; x) - \mathsf{S}^{\mathrm{a}}(u; y) &= \sum_{\rho\in\Lambda_*}\sum_{\xi\in\Lambda} [\Phi_{\xi,\rho}(u) \otimes \rho]\big(\chi_{\xi,\rho}(x) - \chi_{\xi,\rho}(y)\big) \\
&= \sum_{\rho\in\Lambda_*}\sum_{\xi\in\Lambda} \big[(\Phi_{\xi,\rho}(u) - \Phi_{\xi,\rho}(0)) \otimes \rho\big]\big(\chi_{\xi,\rho}(x) - \chi_{\xi,\rho}(y)\big).
\end{aligned}$$

Expanding $\Phi_{\xi,\rho}$, using that fact that

$$\#\{\xi \in \Lambda \,|\, \chi_{\xi,\rho}(x) \ne 0 \text{ and } \chi_{\xi,\rho}(y) \ne 0\} \lesssim |\rho|,$$

and the Lipschitz estimate for $\chi_{\xi,\rho}$, we obtain

$$\big|\mathsf{S}^{\rm a}(u;x) - \mathsf{S}^{\rm a}(u;y)\big| \lesssim M^{(2)} \|\nabla u\|_{L^\infty} |x-y|.$$

The formula for the divergence (6.26) is easy to establish. □

We see from the formula for $\mathrm{div}\mathsf{S}^{\rm a}$ that we will require symmetries of the weighting functions $\nabla_\rho \chi_{\xi,\rho}$, which we establish next.

Lemma 6.6. *Let $x \in \mathbb{R}^d$ and $\rho \in \Lambda_*$, then*

$$\sum_{\xi\in\Lambda} \nabla_\rho \chi_{\xi,\rho}(x) = 0, \tag{6.27}$$

$$\sum_{\xi\in\Lambda} \nabla_\rho \chi_{\xi,\rho}(x)\,(\xi - x) = \rho, \quad \textit{and} \tag{6.28}$$

$$\sum_{\xi\in\Lambda} \nabla_\rho \chi_{\xi,\rho}(x)\,(\xi - x)\otimes(\xi - x) = -\,\rho\otimes\rho. \tag{6.29}$$

Proof. First, we compute $\nabla_\rho \chi_{\xi,\rho}(x)$:

$$\begin{aligned}\nabla_\rho \chi_{\xi,\rho}(x) &= -\int_0^1 \nabla\zeta(\xi + t\rho - x)\rho\,\mathrm{d}t \\ &= -\int_0^1 \tfrac{\mathrm{d}}{\mathrm{d}t}\zeta(\xi + t\rho - x)\,\mathrm{d}t = \zeta(\xi - x) - \zeta(\xi + \rho - x).\end{aligned} \tag{6.30}$$

Using this identity and the fact that the nodal interpolant reproduces affine functions, we immediately obtain (6.27) and (6.28)

To prove (6.29), consider

$$\begin{aligned}&\sum_{\xi\in\mathbb{Z}^d} \nabla_\rho \chi_{\xi,\rho}(x)\,(\xi - x)\otimes(\xi - x) \\ &= \sum_{\xi\in\mathbb{Z}^d} \big[\zeta(\xi - x) - \zeta(\xi + \rho - x)\big]\,(\xi - x)\otimes(\xi - x) \\ &= \sum_{\xi\in\mathbb{Z}^d} \zeta(\xi - x)\big[(\xi - x)\otimes(\xi - x) - (\xi - \rho - x)\otimes(\xi - \rho - x)\big] \\ &= \sum_{\xi\in\mathbb{Z}^d} \zeta(\xi - x)\big[\rho\otimes(\xi - x) + (\xi - x)\otimes\rho - \rho\otimes\rho\big].\end{aligned}$$

Using again the fact that the nodal interpolant reproduces affine functions, we obtain

$$\sum_{\xi\in\mathbb{Z}^d} \nabla_\rho \chi_{\xi,\rho}(x)\,(\xi - x)\otimes(\xi - x) = \rho\otimes(x - x) + (x - x)\otimes\rho - \rho\otimes\rho = -\rho\otimes\rho.$$ □

The key step towards proving (6.20) is the next result, which is analogous to Lemma 4.3.

Lemma 6.7. *Let $u \in W^{4,\infty}_{\rm loc} \cap K$; then*

$$\big|{\rm div}\mathsf{S}^{\rm a}(u;x) - {\rm div}\mathsf{S}^{\rm c}(u;x)\big| \lesssim \sum_{\boldsymbol{\rho}\in\Lambda_*^4} m_{\rm d}^{(\infty)}(\boldsymbol{\rho}) \prod_{j=2}^4 \|\nabla^2 u\|_{L^\infty(x+\nu_{\rho_1\rho_j})} + \sum_{\boldsymbol{\rho}\in\Lambda_*^3} m_{\rm d}^{(\infty)}(\boldsymbol{\rho}) \|\nabla^3 u\|_{L^\infty(x+\nu_{\rho_1,\rho_2})}\|\nabla^2 u\|_{L^\infty(x+\nu_{\rho_1,\rho_3})} + \sum_{\boldsymbol{\rho}\in\Lambda_*^2} m_{\rm d}^{(\infty)}(\boldsymbol{\rho}) \|\nabla^4 u\|_{L^\infty(x+\nu_{\rho_1,\rho_2})}.$$

where $m_{\rm d}^{(\infty)}$ is defined in §2.3.4.

Proof. Recall from the proof of Lemma 4.3 the definition of the sets $\nu_{\xi,\varsigma}$ and $\nu_{\rho,\varsigma}$ and the quantities $\varepsilon_{\xi,\varsigma}$ and $\delta_{\xi,\varsigma}$. In addition, we define $\mu_{\xi,\varsigma} := \|\nabla^4 u\|_{L^\infty(\nu_{\xi,\varsigma})}$.

Recall from (6.26) the algebraic expression for ${\rm div}\mathsf{S}^{\rm a}$. Since $\mathsf{S}^{\rm c} = \sum_{\rho\in\Lambda_*} V_\rho \otimes \rho$, where $V_\rho := V_\rho(\nabla u(x)\cdot\Lambda_*)$, we also obtain

$$\text{div}\mathsf{S}^{\rm c}(x) = \sum_{\rho,\varsigma\in\Lambda_*} V_{\rho\varsigma}[\,\cdot\,, \nabla_\rho\nabla_\varsigma u(x)]. \tag{6.31}$$

To proceed, we expand $\Phi_{\xi,\rho}$ in (6.26) to third order:

$$\begin{aligned}\Phi_{\xi,\rho} &= V_\rho + \Big\{ \sum_{\varsigma\in\Lambda_*} V_{\rho\varsigma}[\,\cdot\,, D_\varsigma u(\xi) - \nabla_\varsigma u(x)]\Big\} \\ &\quad + \Big\{ \sum_{\varsigma,\tau\in\Lambda_*} V_{\rho\varsigma\tau}[\,\cdot\,, D_\varsigma u(\xi) - \nabla_\varsigma u(x), D_\tau u(\xi) - \nabla_\tau u(x)]\Big\} + E_2(\xi,\rho), \\ &=: V_\rho + T_1(\xi,\rho) + E_1(\xi,\rho) + E_2(\xi,\rho)\end{aligned} \tag{6.32}$$

$$\text{where}\quad |E_2(\xi,\rho)| \lesssim \sum_{\rho_2,\rho_3,\rho_4\in\Lambda_*} \tfrac{m(\rho,\rho_2,\rho_3,\rho_4)}{|\rho|} \prod_{i=2}^4 (|\rho|+|\rho_i|)\,\varepsilon_{\xi,\rho_i},$$

where the estimate for E_2 is fully analogous to the estimate of E_1 in (4.11) (taking into account the finite support of $\chi_{\xi,\rho}$). Summing over $\xi\in\Lambda, \rho\in\Lambda_*$, employing the fact that $\sum_{\xi\in\Lambda}|\nabla_\rho\chi_{\xi,\rho}| \le 2$ (this is an immediate consequence of (6.30)), and otherwise arguing as in the proof of Theorem 4.3, we obtain

$$\begin{aligned}|E_2'| &:= \sum_{\rho\in\Lambda_*}\sum_{\xi\in\Lambda} |\nabla_\rho\chi_{\xi,\rho}||E_2(\xi,\rho)| \lesssim \sum_{\boldsymbol{\rho}\in\Lambda_*^4} \frac{m(\boldsymbol{\rho})|\boldsymbol{\rho}|^3}{\prod_{i=1}^4|\rho_i|} \sum_{\xi\in\Lambda}|\nabla_{\rho_1}\chi_{\xi,\rho_1}| \prod_{i=2}^4 |\rho_i|\varepsilon_{\xi,\rho_i} \\ &\lesssim \sum_{\boldsymbol{\rho}\in\Lambda_*^4} \frac{m(\boldsymbol{\rho})|\boldsymbol{\rho}|^3}{|\rho_1|} \prod_{i=2}^4 \max_{\substack{\xi\in\Lambda\\ \chi_{\xi,\rho_1}(x)\neq 0}} \varepsilon_{\xi,\rho_i} \sum_{\xi\in\Lambda}|\nabla_{\rho_1}\chi_{\xi,\rho_1}| \\ &\lesssim \sum_{\boldsymbol{\rho}\in\Lambda_*^4} m_{\rm d}^{(\infty)}(\boldsymbol{\rho}) \prod_{i=2}^4 \|\nabla^2 u\|_{L^\infty(x+\nu_{\rho_1,\rho_i})}.\end{aligned} \tag{6.33}$$

Moreover, using (6.27), it is straightforward to treat the first term in (6.32):

$$\sum_{\rho\in\Lambda_*}\sum_{\xi\in\Lambda} \nabla_\rho\chi_{\xi,\rho}(x) V_\rho = 0. \tag{6.34}$$

We will now independently estimate the two remaining groups involving T_1 and E_1.

Estimating T_1: We expand

$$D_\varsigma u(\xi) - \nabla_\varsigma u(x) = \big(\nabla_{\xi-x}\nabla_\varsigma + \tfrac{1}{2}\nabla_\varsigma^2 + \tfrac{1}{2}\nabla_{\xi-x}^2\nabla_\varsigma + \tfrac{1}{2}\nabla_{\xi-x}\nabla_\varsigma^2 + \tfrac{1}{6}\nabla_\varsigma^3\big)u(x) + E_3(\xi,\varsigma),$$
$$\text{where} \quad |E_3(\xi,\varsigma)| \lesssim (|\rho| + |\varsigma|)^3|\varsigma|\mu_{\xi,\varsigma}.$$

Summing over ξ, ρ, applying (6.27)–(6.29), and applying the symmetry $V_{\rho\varsigma} = V_{\varsigma\rho}$, yields

$$\begin{aligned}
\sum_{\rho\in\Lambda_*}\sum_{\xi\in\Lambda} \nabla_\rho \chi_{\xi,\rho} T_1(\xi,\rho) &= \sum_{\rho,\varsigma\in\Lambda_*} V_{\rho\varsigma}\big[\,\cdot\,, (\nabla_\rho\nabla_\varsigma - \tfrac{1}{2}\nabla_\rho^2\nabla_\varsigma + \tfrac{1}{2}\nabla_\rho\nabla_\varsigma^2)u(x)\big] + E_3' \\
&= \sum_{\rho,\varsigma\in\Lambda_*} V_{\rho\varsigma}[\,\cdot\,, \nabla_\rho\nabla_\varsigma u] + E_3' = \mathrm{div}\mathsf{S}^{\mathrm{c}} + E_3', \qquad (6.35)
\end{aligned}$$
$$\text{where} \quad |E_3'| \lesssim \sum_{\boldsymbol{\rho}\in\Lambda_*^2} m_{\mathrm{d}}^{(\infty)}(\boldsymbol{\rho})\, \|\nabla^4 u\|_{L^\infty(x+\nu_{\rho_1,\rho_2})},$$

and where the estimate of $|E_3'|$ is analogous to the estimate of $|E_2'|$ in (6.33).

Estimating E_1: To estimate E_1 we use the simpler expansion (4.12), which can be written as

$$\begin{aligned}
&D_\varsigma u(\xi) - \nabla_\varsigma u = \nabla_{\xi-x}\nabla_\varsigma u + \tfrac{1}{2}\nabla_\varsigma^2 u + \delta_{\xi,\varsigma}', \\
&\text{where} \quad |\delta_{\xi,\varsigma}'| \lesssim (|\rho| + \varsigma|)^2|\varsigma|\delta_{\xi,\varsigma}.
\end{aligned} \qquad (6.36)$$

We apply again (6.27)–(6.29), followed by the symmetry $V_{\rho\varsigma\tau} = -V_{-\rho,-\varsigma,-\tau}$, to obtain

$$\begin{aligned}
\sum_{\rho\in\Lambda_*}\sum_{\xi\in\Lambda} \nabla_\rho\chi_{\xi,\rho} E_1(\xi,\rho) &= \sum_{\rho,\varsigma,\tau\in\Lambda_*}\sum_{\xi\in\Lambda} \nabla_\rho\chi_{\xi,\rho} V_{\rho\varsigma\tau}\big[\,\cdot\,, \nabla_{\xi-x}\nabla_\varsigma u + \tfrac{1}{2}\nabla_\varsigma^2 u, \nabla_{\xi-x}\nabla_\tau u + \tfrac{1}{2}\nabla_\tau^2 u\big] + E_1' \\
&= \sum_{\rho,\varsigma,\tau\in\Lambda_*} \Big(-\tfrac{1}{2}V_{\rho\varsigma\tau}[\,\cdot\,, \nabla_\rho\nabla_\varsigma u, \nabla_\rho\nabla_\tau u] + \tfrac{1}{2}V_{\rho\varsigma\tau}[\,\cdot\,, \nabla_\rho\nabla_\varsigma u, \nabla_\tau^2 u] \\
&\qquad + \tfrac{1}{2}V_{\rho\varsigma\tau}[\,\cdot\,, \nabla_\varsigma^2 u, \nabla_\rho\nabla_\tau u] + \tfrac{1}{4}V_{\rho\varsigma\tau}[\,\cdot\,, \nabla_\varsigma^2 u, \nabla_\tau^2 u]\Big) + E_1' \\
&= E_1', \qquad (6.37)
\end{aligned}$$

where

$$\begin{aligned}
E_1' &= \sum_{\rho,\varsigma,\tau\in\Lambda_*}\sum_{\xi\in\Lambda} \nabla_\rho\chi_{\xi,\rho} V_{\rho\varsigma\tau}\big[\,\cdot\,, \nabla_{\xi-x}\nabla_\varsigma u + \tfrac{1}{2}\nabla_\varsigma^2 u, \delta_{\xi,\tau}' u\big] \\
&\quad + \sum_{\rho,\varsigma,\tau\in\Lambda_*}\sum_{\xi\in\Lambda} \nabla_\rho\chi_{\xi,\rho} V_{\rho\varsigma\tau}\big[\,\cdot\,, \delta_{\xi,\varsigma}', \nabla_{\xi-x}\nabla_\tau u + \tfrac{1}{2}\nabla_\tau^2 u\big] \\
&\quad + \sum_{\rho,\varsigma,\tau\in\Lambda_*}\sum_{\xi\in\Lambda} \nabla_\rho\chi_{\xi,\rho} V_{\rho\varsigma\tau}\big[\,\cdot\,, \delta_{\xi,\varsigma}', \delta_{\xi,\tau}'\big] \\
&=: E_{1,1}' + E_{1,2}' + E_{1,3}'.
\end{aligned}$$

The first and second terms can be treated in a straightforward manner, employing (6.36):

$$|E_{1,1}'| \lesssim \sum_{\boldsymbol{\rho}\in\Lambda_*^3} m_{\mathrm{d}}^{(\infty)}(\boldsymbol{\rho}) |\nabla^2 u(x)| \|\nabla^3 u\|_{L^\infty(x+\nu_{\rho_1,\rho_3})}, \quad \text{and}$$
$$|E_{1,2}'| \lesssim \sum_{\boldsymbol{\rho}\in\Lambda_*^3} m_{\mathrm{d}}^{(\infty)}(\boldsymbol{\rho}) |\nabla^2 u(x)| \|\nabla^3 u\|_{L^\infty(x+\nu_{\rho_1,\rho_2})}.$$

However, the term $E_{1,3}'$ must be treated more carefully. Note that simply using (6.36) to estimate

$$|E_{1,3}'| \lesssim \sum_{\boldsymbol{\rho}\in\Lambda_*^3} \frac{m(\boldsymbol{\rho})|\boldsymbol{\rho}|^4}{|\rho_1|} \|\nabla^3 u\|_{L^\infty(x+\nu_{\rho_1,\rho_2})} \|\nabla^3 u\|_{L^\infty(x+\nu_{\rho_1,\rho_3})}$$

would impose a decay on the interaction potential that would rule out the Lennard-Jones potential. Instead, we use (6.36) only for the terms $\delta'_{\xi,\varsigma}$ and the weaker estimate

$$|\delta'_{\xi,\tau}| = \big|D_\tau u(\xi) - \nabla_\tau u - \nabla_{\xi-x}\nabla_\tau u - \tfrac{1}{2}\nabla_\tau^2 u\big| \lesssim (|\rho| + |\tau|)|\tau|\varepsilon_{\xi,\tau},$$

which leads to

$$|E'_{1,3}| \lesssim \sum_{\boldsymbol{\rho}\in\Lambda^3_*} \frac{m(\boldsymbol{\rho})|\boldsymbol{\rho}|^3}{|\rho_1|}\|\nabla^3 u\|_{L^\infty(x+\nu_{\rho_1,\rho_2})}\|\nabla^2 u\|_{L^\infty(x+\nu_{\rho_1,\rho_3})}.$$

Note that the coefficients in this last estimate are precisely $m_{\rm d}^{(\infty)}(\boldsymbol{\rho})$, which are controlled also for the Lennard-Jones case. Combining the estimates for $E'_{1,1}, E'_{1,2}$ and $E'_{1,3}$, we arrive at

$$|E'_1| \lesssim \sum_{\boldsymbol{\rho}\in\Lambda^3_*} m_{\rm d}^{(\infty)}(\boldsymbol{\rho})\|\nabla^3 u\|_{L^\infty(x+\nu_{\rho_1,\rho_2})}\|\nabla^2 u\|_{L^\infty(x+\nu_{\rho_1,\rho_3})}. \tag{6.38}$$

Note that we have seemingly ignored the term $E'_{1,1}$, however, due to the symmetry $m(\rho_1, \rho_2, \rho_3) = m(\rho_1, \rho_3, \rho_2)$, this term is in fact included.

Combining the estimates: Combining (6.33), (6.35) and (6.38) we obtain the desired upper bound on $|{\rm div}\mathsf{S}^{\rm a} - {\rm div}\mathsf{S}^{\rm c}|$. ☐

Repeating the arguments of the proof of Lemma 4.5 almost verbatim, we obtain the following global consistency error estimate.

Lemma 6.8. *Let $u \in \dot W^{4,p}$, $\tilde u := \zeta * u|_\Lambda$ and $v \in \ell^{p'}$; then*

$$\big|\langle \delta E^{\rm a}(\tilde u), \tilde v\rangle - \langle \delta E^{\rm c}(u), v\rangle\big| \lesssim \big(M_{\rm d}^{(2,p)}\|\nabla^4 u\|_{L^p} + M_{\rm d}^{(3,p)}\|\nabla^3 u\|_{L^{3p/2}}\|\nabla^2 u\|_{L^{3p}} + M_{\rm d}^{(4,p)}\|\nabla^2 u\|^3_{L^{3p}}\big)\|v\|_{L^{p'}}.$$

We are now in a position to prove (6.20).

Proof of (6.20). Recall that

$$(\beta, \nabla \dot w) = \langle \delta E^{\rm c}(u^{\rm c}), \dot w\rangle - \langle \delta E^{\rm a}(z), \dot e\rangle,$$

where $\tilde w = e$ and $z = (\zeta * u^{\rm c})|_\Lambda$. Hence, Lemma 6.8 and (6.7) yield

$$\big|(\beta, \nabla \dot w)\big| \le C\varepsilon^{3-d/2}\|\dot w\|_{L^2},$$

where C depends only on $M_{\rm d}^{(j,2)}$, $j = 2, 3, 4$, and is otherwise generic. This proves (6.19), from which (6.20) follows immediately after application of Cauchy's inequality. ☐

6.4. **Estimating the nonlinearity.** In this section, we prove two estimates on the term $\langle \dot H e, e\rangle$ occurring in the error equation (6.15).

Proof of (6.21). Recall (6.12), which states that $z(t) + \theta e(t) \in \mathscr{K}$ for all $t \in [0, s]$ and $\theta \in [0, 1]$.

We write out $\langle \dot H e, e\rangle$ explicitly and exchange the order of integration (this is justified since $M^{(3)}$ is finite, which implies that the integrand is uniformly bounded),

$$\begin{aligned}\int_0^s \langle \dot H e, e\rangle \,{\rm d}t &= \int_0^s\int_0^1 \delta^3 E^{\rm a}(z+\theta e)[\dot z + \theta \dot e, e, e]{\rm d}\theta\ {\rm d}t \\ &= \int_0^1\int_0^s \delta^3 E^{\rm a}(z+\theta e)[\dot z, e, e]\ {\rm d}t{\rm d}\theta + \int_0^1 \theta\int_0^s \delta^3 E^{\rm a}(z+\theta e)[\dot e, e, e]\,{\rm d}t\,{\rm d}\theta.\end{aligned}$$

The first group on the right-hand side is easily estimated, using (2.15) and (6.7),

$$\delta^3 E^{\rm a}(z+\theta e)[\dot z, e, e] \lesssim M^{(3)}\|\nabla \dot z\|_{L^\infty}\|\nabla e\|^2_{L^2} \lesssim \varepsilon M^{(3)}\|\nabla \dot U^{\rm c}\|_{L^\infty}E^2.$$

To estimate the second group, we focus on the inner integral only. Since $\delta^3 E^{\rm a}(\,\cdot\,)[v_1, v_2, v_3]$ is invariant under permutation of the arguments v_1, v_2, v_3 it follows that

$$\tfrac{\rm d}{{\rm d}t}\tfrac13 \delta^3 E^{\rm a}(z+\theta e)[e,e,e] = \delta^3 E^{\rm a}(z+\theta e)[\dot e, e, e] + \tfrac13 \delta^4 E^{\rm a}(z+\theta e)[\dot z + \theta \dot e, e, e, e],$$

which gives

$$\int_0^s \delta^3 E^{\rm a}(z+\theta e)[\dot e, e, e]\,{\rm d}t = \tfrac13 \big[\delta^3 E^{\rm a}(z+\theta e)[e,e,e]\big]_{t=0}^s - \tfrac13 \int_0^s \delta^4 E^{\rm a}(z+\theta e)[\dot z + \theta \dot e, e, e, e]\,{\rm d}t. \tag{6.39}$$

Applying (2.15) and the inverse estimate Lemma 2.3 with $j = 0, m = 1$ and $p = \infty$, $q = 2$ to bound $\|\nabla \dot e\|_{L^\infty} \lesssim \|\dot e\|_{L^2}$, we obtain

$$\begin{aligned}
\int_0^s \delta^3 E^{\rm a}(z+\theta e)[\dot e, e, e]\,{\rm d}t &\lesssim M^{(3)}\big(\|\nabla e(0)\|_{L^2}^3 + \|\nabla e(s)\|_{L^2}^3\big) + M^{(4)} \int_0^s \|\nabla \dot z\|_{L^\infty} \|\nabla e\|_{L^2}^3 \\
&\quad + M^{(4)} \int_0^s \|\nabla \dot e\|_{L^\infty} \|\nabla e\|_{L^2}^3\,{\rm d}t \\
&\lesssim M^{(3)}\big(E(0)^3 + E(s)^3\big) + M^{(4)} \int_0^s \Big(\varepsilon E^3 + E^4\Big)\,{\rm d}t.
\end{aligned}$$ □

Proof of (6.25)*.* To prove (6.25) we may now use the fact that $k \geq 5$, that is, $E^{\rm a}$ is five times differentiable in a neighborhood of $z(t) + \theta e(t)$, $\theta \in [0,1], t \in [0, t_1]$. Thus, starting from (6.39) we can repeat the integration by parts argument to obtain (6.25). □

7. Conclusion

In the small deformation or short time regimes we have developed an essentially complete approximation theory of the Cauchy–Born model for Bravais lattices for both static and dynamic problems. The main open questions are 1. the extension to large deformations and/or the charactisation of maximal time intervals for which the error estimates hold; and 2. the extension to multi-lattices.

Acknowledgements

We thank E. Süli for discussions to help clarify the properties of homogeneous Sobolev spaces; C. Makridakis and E. Süli for discussions on the error analysis for nonlinear wave equations during two visits of C. Ortner to the University of Crete funded by the Archimedes Center for Modeling, Analysis and Computation; and A. Shapeev for suggesting a variant of the "localisation trick" (1.2) during a research visit of C. Ortner to the EPFL funded by the Chair of A. Abdulle.

Appendix A. Auxiliary Approximation and Interpolation Results

In this appendix we collect several auxiliary results related to the smoothing properties of the convolution operator $f \mapsto \zeta * f$, and the accuracy of the approximation $\zeta * f$ to f.

Lemma A.1. *Let ζ be the basis function defined in §2.1, and $f(x) = a + b \cdot x$ where $a \in \mathbb{R}, b \in \mathbb{R}^d$ are constants, then $\zeta * f = f$.*

Proof. Since $\int \zeta(x)\,{\rm d}x = 1$, it follows that $\zeta * a = a$. Further,

$$\int_{\mathbb{R}^d} \zeta(x-y) y\,{\rm d}y = x - \int_{\mathbb{R}^d} \zeta(x-y)(x-y)\,{\rm d}y = x - \int_{\mathbb{R}^d} \zeta(-y)\cdot(-y)\,{\rm d}y = x,$$

where we used that fact that ζ is an even function. □

Lemma A.2. *Let $f \in W^{2,p}$, $p \in [1,\infty]$, then*
$$\|\zeta * f - f\|_{L^p} \lesssim \|\nabla^j f\|_{L^p}, \qquad \text{for } j = 0,1,2.$$

Proof. This result follows immediately from Lemma A.1 and Poincaré inequalities. □

Corollary A.3. *Let $u \in \dot W^{3,p}$ with $p > d/3$ and let $\tilde u := \zeta * u$, then*
$$\|\nabla u - \nabla I\tilde u\|_{L^p} \lesssim \|\nabla^3 u\|_{L^p}.$$

Proof. Under the assumption that $p > d/3$ (which guarantees the embedding $\dot W^{3,p} \subset C$) we know from [25] that
$$\|\nabla \tilde u - \nabla I\tilde u\|_{L^p} \lesssim \|\nabla^3 \tilde u\|_{L^p} \lesssim \|\nabla^3 u\|_{L^p}.$$
Applying also Lemma A.2 with $f = \nabla u$, we obtain
$$\|\nabla u - \nabla I\tilde u\|_{L^p} \le \|\nabla u - \nabla \tilde u\|_{L^p} + \|\nabla \tilde u - \nabla I\tilde u\|_{L^p} \lesssim \|\nabla^3 u\|_{L^p}.$$ □

Lemma A.4. *Let $\nu \subset \mathbb{R}^d$ be measurable, $-\nu = \nu$, and $f \in L^p(\mathbb{R}^d)^j$, then*
$$\int_{\mathbb{R}^d} \|\zeta * f\|^p_{L^\infty(x+\nu)} \,\mathrm{d}x \le \mathrm{vol}(\nu')\, \|f\|^p_{L^p},$$
where $\nu' := \bigcup_{x\in\nu} \mathrm{supp}(\zeta(x - \,\cdot\,))$.

Proof. Let $\zeta'(x,z) := \max_{y\in x+\nu} \zeta(y-z)$. Since $\zeta \ge 0$ and $\int_{\mathbb{R}^d} \zeta \,\mathrm{d}x = 1$, Jensen's inequality yields
$$\begin{aligned}\|\zeta * f\|^p_{L^\infty(\nu(x))} &= \max_{y\in x+\nu} \left| \int_{\mathbb{R}^d} \zeta(y-z) f(z)\,\mathrm{d}z \right|^p \le \max_{y\in x+\nu} \int_{\mathbb{R}^d} \zeta(y-z)|f(z)|^p \,\mathrm{d}z \\ &\le \int_{\mathbb{R}^d} \max_{y\in x+\nu} \zeta(y-z)|f(z)|^p\,\mathrm{d}z = \int_{\mathbb{R}^d} \zeta'(x,z)|f(z)|^p\,\mathrm{d}z.\end{aligned}$$
Integrating with respect to x, we obtain
$$\begin{aligned}\int_{\mathbb{R}^d} \|\zeta * f\|^p_{L^\infty(x+\nu)}\,\mathrm{d}x &\le \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \zeta'(x,z)|f(z)|^p\,\mathrm{d}z\,\mathrm{d}x \\ &= \int_{\mathbb{R}^d} |f(z)|^p \int_{\mathbb{R}^d} \zeta'(x,z)\,\mathrm{d}x\,\mathrm{d}z.\end{aligned}$$
From its definition it is clear that $0 \le \zeta' \le 1$. Moreover, if $\zeta'(x,z) \ne 0$, then $\zeta(y-z) \ne 0$ for some $y \in x+\nu$, that is,
$$y - x \in \nu \quad \text{and} \quad z - y \in \mathrm{supp}\zeta.$$
Since both ν and $\mathrm{supp}\zeta$ are symmetric about the origin, this implies that $x - z \in \bigcup_{y\in\nu} \mathrm{supp}(y - \cdot\,) =: \nu'$. Thus, we obtain $\int_{\mathbb{R}^d} \zeta'(x,z)\,\mathrm{d}x \le \mathrm{vol}(\nu')$, which concludes the proof. □

Lemma A.5. *Let $f^{\mathrm{c}} \in L^1_{\mathrm{loc}} \cap \dot W^{-1,2}$ and let $f^{\mathrm{a}} \in \mathscr{W}$ be defined by*
$$f^{\mathrm{a}}(\xi) := \int_{\mathbb{R}^d} \zeta(\xi - x) f^{\mathrm{c}}(x)\,\mathrm{d}x, \tag{A.1}$$
then $f^{\mathrm{a}} \in \dot{\mathscr{W}}^{-1,2}$. Moreover, if $\nabla f^{\mathrm{c}} \in L^2$, then
$$\big|(f^{\mathrm{a}}, \tilde v)_\Lambda - (f^{\mathrm{c}}, v)_{\mathbb{R}^d}\big| \le \|\nabla f^{\mathrm{c}}\|_{L^2} \|\nabla v\|_{L^2} \qquad \forall v \in \mathscr{W}_0. \tag{A.2}$$

Proof. Let $v \in \mathscr{W}_0$, then

$$(f^{\rm a}, v)_\Lambda = \sum_{\xi\in\Lambda} f^{\rm a}(\xi)\cdot v(\xi) = \int_{\mathbb{R}^d} f^{\rm c}(x) \sum_{\xi\in\Lambda} \zeta(x-\xi) v(\xi)\,{\rm d}x = (f^{\rm c}, v)_{\mathbb{R}^d},$$

which implies that $f^{\rm a} \in \dot{\mathscr{W}}^{-1,2}$ with $\|f^{\rm a}\|_{\dot{\mathscr{W}}^{-1,2}} \le \|f^{\rm c}\|_{\dot{W}^{-1,2}}$.

To prove (A.2), we first note that

$$\begin{aligned}(f^{\rm a}, \tilde v)_\Lambda &= \sum_{\xi\in\Lambda} f^{\rm a}(\xi) \int_{\mathbb{R}^d} \zeta(x-\xi) v(x)\,{\rm d}x \\ &= \int_{\mathbb{R}^d} v(x)\cdot \sum_{\xi\in\Lambda} \zeta(x-\xi) f^{\rm a}(\xi)\,{\rm d}x = (f^{\rm a}, v)_{\mathbb{R}^d}. \end{aligned} \tag{A.3}$$

This allows us to write

$$(f^{\rm a}, \tilde v)_\Lambda - (f^{\rm c}, v)_{\mathbb{R}^d} = \sum_{\xi\in\Lambda} \int_{\mathbb{R}^d} \zeta(\xi - x)(f^{\rm a}(\xi) - f^{\rm c}(x)) v(x)\,{\rm d}x.$$

From the definition of $f^{\rm a}$ (A.1) it follows that

$$\int \zeta(\xi - x)(f^{\rm a}(\xi) - f^{\rm c}(x)) = 0,$$

and hence we obtain, for some arbitrary constants $c_\xi \in \mathbb{R}$,

$$\begin{aligned}\big|(f^{\rm a}, \tilde v)_\Lambda - (f^{\rm c}, v)_{\mathbb{R}^d}\big| &= \bigg|\sum_{\xi\in\Lambda} \int_{\mathbb{R}^d} \zeta(\xi - x)\big(f^{\rm a}(\xi) - f^{\rm c}(x)\big)\big(u(x) - c_\xi\big)\,{\rm d}s\bigg| \\ &\le \sum_{\xi\in\Lambda} \bigg(\int_{\mathbb{R}^d} \zeta(\xi - x)^2 \big|f^{\rm a}(\xi) - f^{\rm c}(x)\big|^2\,{\rm d}x\bigg)^{1/2} \big\|v - c_\xi\big\|_{L^2(Q_\xi)}.\end{aligned}$$

Choosing $c_\xi = (v)_{Q_\xi}$ and applying Poincaré's Inequality, we can estimate

$$\big\|v - c_\xi\big\|_{L^2(Q_\xi)} \le \big(\tfrac{2}{\pi}\big)^d \big\|\nabla v\big\|_{L^2(Q_\xi)}.$$

Moreover, estimating $\zeta \le 1$, and using the fact that $f^{\rm a}(\xi)$ is the orthogonal projection of $f^{\rm c}$ with respect to the kernel $\zeta(\xi - \,\cdot\,)$, we obtain

$$\begin{aligned}\bigg(\int \zeta(\xi - x)^2 \big|f^{\rm a}(\xi) - f^{\rm c}(x)\big|^2\,{\rm d}x\bigg)^{1/2} &\le \bigg(\int \zeta(\xi - x) \big|f^{\rm a}(\xi) - f^{\rm c}(x)\big|^2\,{\rm d}x\bigg)^{1/2} \\ &\le \bigg(\int \zeta(\xi - x) \big|(f^{\rm c})_{Q_\xi} - f^{\rm c}(x)\big|^2\,{\rm d}x\bigg)^{1/2} \\ &\le \big\|(f^{\rm c})_{Q_\xi} - f^{\rm c}\big\|_{L^2(Q_\xi)} \le \big(\tfrac{2}{\pi}\big)^d \big\|\nabla f^{\rm c}\big\|_{L^2(Q_\xi)}.\end{aligned}$$

Combining the foregoing estimates and estimating the overlaps we arrive at

$$\big|(f^{\rm a}, \tilde v)_\Lambda - (f^{\rm c}, v)_{\mathbb{R}^d}\big| \le C \|\nabla f^{\rm c}\|_{L^2} \|\nabla v\|_{L^2}.$$

with $C = 2^{3d}/\pi^{2d} \le 1$ for $d \in \{1, 2, 3\}$. This establishes (A.2). □

Appendix B. Examples of admissible potentials

We discuss the most common interatomic potentials and show that they can be accommodated within our framework. We remark from the outset that our smoothness requirement (at least four times continuously differentiable for the error analysis) is reasonable for physical interaction potentials, but is not satisfied by typical potentials constructed for molecular dynamics simulations, which employ cut-off functions that are often only once differentiable.

B.1. **Lennard-Jones type potentials.** For a pure pair interaction model, we define

$$V(\boldsymbol{g}) := \frac{1}{2} \sum_{\rho \in \Lambda_*} \big[\varphi\big(|g_\rho|\big) - \varphi\big(|\mathsf{A}\rho|\big)\big]. \tag{B.1}$$

With this definition, V clearly satisfies the symmetry (2.11).

The prototypical example is of course the Lennard–Jones potential [17],

$$\varphi(r) = r^{-12} - 2r^{-6}.$$

In this case, one readily sees that $\varphi^{(j)}(r) \lesssim r^{-6-j}$, for $r \geq 1$ and $j \in \mathbb{N}$. More generally, suppose that V is of the form (B.1) with

$$|\varphi^{(j)}(r)| \lesssim r^{-\alpha-j}, \quad \text{for } r \geq 1, \quad j \in \mathbb{N}, \tag{B.2}$$

then one may readily deduce that

$$m(\boldsymbol{\rho}) \lesssim \begin{cases} |\rho|^{-\alpha}, & \boldsymbol{\rho} = (\rho, \dots, \rho) \in \Lambda_*^j, \\ 0, & \text{otherwise,} \end{cases}$$

and consequently,

$$M^{(j)} \lesssim \sum_{\rho \in \Lambda_*} |\rho|^{-\alpha} \qquad \text{and} \qquad M_{\rm s}^{(j,2)} + M_{\rm d}^{(j,2)} \lesssim \sum_{\rho \in \Lambda_*} |\rho|^{-\alpha+5/2}.$$

Thus, $M^{(j)}$ is finite (and hence $E^{\rm a}$ well-defined and k times differentiable) if and only if $\alpha > d$; and $M_{\rm d}^{(j,2)}, M_{\rm s}^{(j,2)}$ are finite (and hence our error analysis applies) if and only if $\alpha > d + 5/2$.

In particular, it follows that the Lennard-Jones potential is included in our analysis. Another commonly employed potential is the Morse potential [23], which decays exponentially and is hence trivially included our analysis. The Coulomb potential, $\varphi(r) = r^{-1}$, is excluded.

B.2. **Embedded atom method.** In the embedded atom method [7] one postulates site energies of the form

$$V(\boldsymbol{g}) = \sum_{\rho \in \Lambda_*} \varphi(|g_\rho|) + G\big(\textstyle\sum_{\rho \in \Lambda_*} \psi(|g_\rho|)\big), \tag{B.3}$$

where φ is a Lennard-Jones or Morse type pair potential, $\psi(|g_\rho|)$ is a model of the electron density at 0 generated by a nucleus at distance $|g_\rho|$, and G is the energy to embed a nucleus into a see of electrons. Again, it is clear from the functional form of V, that it satisfies the symmetry (2.11).

The computation of the partial derivatives is now more involved. Suppose, for simplicity, that $\varphi \equiv 0$, define $\bar\psi := \sum_{\rho \in \Lambda_*} \psi(|g_\rho|)$, and $\Psi(g) := \psi(|g|)$, then

$$\begin{aligned}
V_\rho(\boldsymbol{g}) &= G'(\bar\psi)\nabla\Psi(g_\rho), \\
V_{\rho\varsigma}(\boldsymbol{g}) &= G''(\bar\psi)\nabla\Psi(g_\rho) \otimes \nabla\Psi(g_\varsigma) + G'(\bar\psi)\nabla^2\Psi(g_\rho)\delta_{\rho,\varsigma}, \\
V_{\rho\varsigma\tau}(\boldsymbol{g}) &= G'''(\bar\psi)\nabla\Psi(g_\rho) \otimes \nabla\Psi(g_\varsigma) \otimes \nabla\Psi(g_\tau) + G'(\bar\psi)\nabla^3\Psi(g_\rho)\delta_{\rho,\varsigma}\delta_{\rho,\tau} \\
&\quad + G''(\bar\psi)\Big(\nabla^2\Psi(g_\rho) \otimes \nabla\Psi(g_\varsigma)\delta_{\rho,\tau} + \nabla\Psi(g_\rho) \otimes \nabla^2\Psi(g_\varsigma)\delta_{\varsigma,\tau} + \nabla^2\Psi(g_\rho) \otimes \nabla\Psi(g_\tau)\delta_{\rho,\varsigma}\Big),
\end{aligned}$$

and so forth. G is typically chosen smooth and φ, ψ decay exponentially. In that case, one immediately sees that all constants $M^{(j)}, M_{\rm s}^{(j,p)}, M_{\rm d}^{(j,p)}$ are bounded. More generally, let $\varphi \equiv 0$ and suppose that

$$\psi^{(j)}(r) \lesssim r^{-\beta-j}. \tag{B.4}$$

In this case, also $|\nabla^j \Psi(g)| \lesssim |g|^{-\beta-j}$, and we conclude that

$$\begin{aligned} m(\rho) &\lesssim |\rho|^{-\beta}, \qquad \rho \in \Lambda_*, \\ m(\rho,\varsigma) &\lesssim |\rho|^{-\beta}|\varsigma|^{-\beta} + |\rho|^{-\beta}\delta_{\rho\varsigma}, \qquad \rho,\varsigma \in \Lambda_*, \\ m(\rho,\varsigma,\tau) &\lesssim |\rho|^{-\beta}|\varsigma|^{-\beta}|\tau|^{-\beta} + |\rho|^{-\beta}\delta_{\rho,\varsigma}\delta_{\rho,\tau} \\ &\quad + \Big(|\rho|^{-\beta}|\varsigma|^{-\beta}\delta_{\rho,\varsigma} + |\rho|^{-\beta}|\tau|^{-\beta}\delta_{\rho,\tau} + |\varsigma|^{-\beta}|\tau|^{-\beta}\delta_{\varsigma,\tau}\Big), \quad \rho,\varsigma,\tau \in \Lambda_*, \end{aligned}$$

and so forth. Due to the product structure, one can readily see that $M^{(j)}$ is finite provided that $\beta > d$.

However, to ensure that $M_{\rm d}^{(j,2)}, M_{\rm s}^{(j,2)}$ are finite, we now require more stringent requirements. For example, considering only the first group in $m(\rho,\varsigma,\tau)$ and indicating the missing terms by "…", and using $|\rho \times \varsigma| \le |\rho||\varsigma|$, we can estimate

$$\begin{aligned} M_{\rm s}^{(3,2)} &\lesssim \sum_{\rho,\varsigma,\tau\in\Lambda_*} (|\rho| + |\varsigma| + |\tau|)^3 |\rho|^{-\beta}|\varsigma|^{-\beta}|\tau|^{-\beta} + \dots \\ &\lesssim \sum_{\rho,\varsigma,\tau\in\Lambda_*} \big[|\rho|^{3-\beta}|\varsigma|^{-\beta}|\tau|^{-\beta} + |\rho|^{2-\beta}|\varsigma|^{1-\beta}|\tau|^{-\beta} + \dots\big] + \dots, \end{aligned}$$

which is finite provided that $\beta > d+3$. The remaining terms can be treated analogously. For the dynamic case, the extra factor $|\rho_1|^{-1}$ does not help except in the case of pair interactions, and we require $\beta > d+4$ to ensure that the constants $M_{\rm d}^{(j,2)}$ are finite.

In summary, if V is of the form (B.3) with the pair interaction φ satisfying (B.2) and the electron density function ψ satisfying (B.4), then we require $\alpha, \beta > d$ to ensure that the constants $M^{(j)}$, $1 \le j \le k$ are finite; we require $\alpha > d + 5/2, \beta > d+3$ to ensure that $M_{\rm s}^{(j,2)}$, $j = 2,3$, are finite; and we require $\alpha > d+5/2, \beta > d+4$ to ensure that $M_{\rm d}^{(j,2)}$, $2 \le j \le 4$ are finite.

B.3. **Bond-angle potentials.** Lennard-Jones type pair interactions and embedded atom potentials are the prototypical long-ranged potentials with infinite interaction range. Most other potentials used in molecular simulations act only on a finite interaction neighborhood. For example, bond-angle potentials (3-body or 4-body) act only on angles between nearest neighbors. We only need to check whether they can be written in a way that preserves the inversion symmetry (2.11). 3-body bond-angle energies are typically written in the form

$$\sum_{\xi,\eta,\mu\in\Lambda} \varphi(|r_{\eta\xi}|)\varphi(|r_{\mu,\xi}|)\psi(\theta_{\eta\xi\mu}),$$

where $r_{\eta\xi} = \eta + u(\eta) - \xi - u(\xi)$, $\theta_{\eta\xi\mu}$ is the angle between the bond directions $r_{\eta\xi}, r_{\mu\xi}$, φ is a cut-off function to ensure that the potential acts only on nearest-neighbors, and ψ is an angle potential that drives towards preferred bond-angles. This term is symmetric about the center-atom, which suggests to write

$$V(\boldsymbol{g}) = \sum_{\substack{\rho,\varsigma\in\Lambda_* \\ \rho\ne\varsigma}} \varphi(|r_\rho|)\varphi(|r_\varsigma|)\psi(\theta_{\rho\varsigma}),$$

where $r_\rho := \rho + g_\rho$, and $\theta_{\rho\varsigma}$ is the angle between r_ρ, r_ς. This sum is fully permutation invariant, and hence the inversion symmetry (2.11) holds.

4-body (or, dihedral angle; or, torsion) potentials can be treated similarly. There are now two center atoms in bonds of this type, and hence one "splits" the bond between the two corresponding site energies (similarly as in the pair potential case). By summing over all quadruples involved with the given site, the resulting site potential will again be permutation invariant.

B.4. **Generic multi-body potentials.** A more recent development are potentials without physical interpretation, but simply postulating a general functional form for V, and fitting a large number of parameters to energy and forces obtained from electronic structure calculations; see, e.g., [2]. Such general potentials are normally constructed to satisfy the permutation invariance, and hence the inversion symmetry (2.11), and are therefore still included in our analysis.

Appendix C. Lattice Stability versus Ellipticity

We show that the lattice stability assumption (5.7) is not only sufficient but also *necessary* to obtain Theorems 5.4 and 6.2. This can already be seen for 1D second-neighbour harmonic pair interactions:

$$\Phi_\xi(u) = \tfrac{a_1}{4}\big(|u'_\xi|^2 + |u'_{\xi+1}|^2\big) + \tfrac{a_2}{4}\big(|u'_{\xi-1} + u'_\xi|^2 + |u'_{\xi+1} + u'_{\xi+2}|^2\big),$$

where $u'_\eta = u_\eta - u_{\eta-1}$. In this case, the atomistic and Cauchy–Born energies are more conveniently written in the form

$$E^{\rm a}(u) = \sum_{\xi\in\Lambda} \Big(\tfrac{a_1}{2}|u'_\xi|^2 + \tfrac{a_2}{2}|u'_\xi + u'_{\xi+1}|^2\Big) \quad \text{and} \quad E^{\rm c}(u) = \tfrac{(a_1+4a_2)}{2}\int_{\mathbb{R}} |u'|^2 \,{\rm d}x.$$

We consider two choices for the coefficients a_1, a_2:

$$\begin{aligned} a_1^{(1)} &= 2, \\ a_2^{(1)} &= -\tfrac{1}{4}, \end{aligned} \qquad \text{and} \qquad \begin{aligned} a_1^{(2)} &= -1, \\ a_2^{(2)} &= \tfrac{1}{2}, \end{aligned}$$

then in both of these cases we have

$$a_1^{(j)} + 4a_2^{(j)} = 1.$$

Thus, the continuum energy is positive definite and hence the continuum wave equation is well-posed.

In the atomistic case, we can use the parallelogram formula to rewrite

$$E^{\rm a}(u) = \sum_{\xi\in\Lambda} \Big(\tfrac{a_1+4a_2}{2}|u'_\xi|^2 - \tfrac{a_2}{2}|u''_\xi|^2\Big), \tag{C.1}$$

where $u''_\xi = u_{\xi+1} - 2u_\xi + u_{\xi-1}$. Hence, in the case $a_i = a_i^{(1)}$ we have that $E^{\rm a}(u) \geq E^{\rm c}(u)$, so that (5.7) is satisfied and the dynamic atomistic and continuum solutions will remain close for a macroscopic time interval (cf. Theorem 6.2).

By contrast, in the case $a_i = a_i^{(2)}$, where $a_2 > 0$ we can see from (C.1) that oscillations are energetically advantageous. Indeed we note that, formally, defining $\hat\varphi'(\xi) = (-1)^\xi$ gives infinite negative energy,

$$E^{\rm a}(\hat\varphi) = \sum_{\xi\in\Lambda} \Big(-\tfrac{1}{2}|1|^2 + \tfrac{1}{4}|0|^2\Big) = -\infty.$$

Formally (since $\hat\varphi \notin \dot{\mathscr{W}}^{1,2}$) one easily checks that $H\hat\varphi = -\hat\varphi$, where $H := \delta^2 E^{\rm a}(0)$. A straightforward approximation argument shows that -1 belongs to the spectrum of H.

For the static case, this means that even if atomistic solutions exist, they are not local minimizers.

For the dynamic case, it means that there exist exponentially growing solutions. Using the characterization of the spectrum in terms of approximate eigenfunctions, there exists for each $\delta > 0$ a function $\psi_\delta \in \ell^2$ with $\|\psi_\delta\|_{\ell^2} = 1$, such that $\|H\psi_\delta + \psi_\delta\| \le \delta$ (see Section VIII.3 in [30]). Suppose now that we solve the Cauchy–Born equation with $u(0) = \dot{u}(0) = 0$ and the atomistic equation with $u(0) = 0$ and $\dot{u}(0) = \varepsilon^2\psi_\delta$. The function $v(t) := \sinh(t)\varepsilon^2\psi_\delta$ then solves the atomistic evolution equation to order $O(\delta)$. By estimating the difference $u(t) - v(t)$ it is straightforward to prove that

$$\|\dot{u}(t)\|_{\ell^2} \ge \varepsilon^2 \tfrac{1}{2} e^t \qquad \text{for } t \le 3|\log\varepsilon|,$$

and in particular, $\|\dot{u}\|_{\ell^2}$ becomes of order one for $t \sim |\log\varepsilon|$.

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C. Ortner, Mathematics Institute, Zeeman Building, University of Warwick, Coventry CV4 7AL, UK
E-mail address: `christoph.ortner@warwick.ac.uk`

F. Theil, Mathematics Institute, Zeeman Building, University of Warwick, Coventry CV4 7AL, UK
E-mail address: `f.theil@warwick.ac.uk`