SYMMETRIES OF 2-LATTICES AND SECOND ORDER ACCURACY OF THE CAUCHY–BORN MODEL

B. VAN KOTEN AND C. ORTNER

Abstract. We show that the Cauchy–Born model of a single-species 2-lattice is second order if the atomistic and continuum kinematics are connected in a novel way. Our proof uses a generalization to 2-lattices of the point symmetry of Bravais lattices.

Moreover, by identifying similar symmetries in multi-species pair interaction models, we construct a new stored energy density, using shift-gradients but not strain gradients, that is also second order accurate.

These results can be used to develop highly accurate continuum models and atomistic/continuum coupling methods for materials such as graphene, hcp metals, and shape memory alloys.

1. Introduction

The Cauchy–Born model is a widely used continuum model for crystal elasticity [4,5,20]. Moreover, it is a crucial ingredient in a new class of atomistic/continuum multi-scale methods [3, 12, 13, 19, 20]. Formal considerations and rigorous analyses have shown that the Cauchy–Born model for Bravais lattices (simple lattices) is second order accurate [4, 8, 10, 16]. By contrast, one expects that its generalization to multi-lattices should be only first order accurate [8], due to the absence of point symmetry in general multi-lattices.

In the present work, we identify two non-trivial generalizations of the Bravais lattice point symmetry. We show that this leads to second order accuracy of the classical Cauchy–Born model for a single-species 2-lattice, *provided* the atomistic and continuum kinematics are connected in a novel way. Moreover, we identify a new stored energy density for general multi-lattices under pair interaction model, and we show that this energy is also second order accurate.

While these are interesting observations on their own, they have important consequences for computational materials modeling. For example, our results provide higher-order continuum approximations *without* requiring the use of C^1-conforming numerical methods. (Higher order

BVK was supported in part by DMS-0757355, DMS-0811039, the PIRE Grant OISE-0967140, the University of Minnesota Supercomputing Institute, and the Department of Energy under Award Number DE-SC0002085. CO was supported by EPSRC grant EP/H003096 "Analysis of atomistic-to-continuum coupling methods".

continuum models can always be constructed provided they are discretized using higher-order conforming numerical methods [1].) Our own interest in this issue is the application of the Cauchy–Born model in atomistic/continuum coupling methods. At the atomistic/continuum interface, the order of accuracy is typically lower than in the continuum bulk, due to the loss of interaction symmetry [7,15,18,22]. By employing a second order continuum approximation, the loss can be made less severe. For example, in the blended quasicontinuum method [22], the interfacial error is controlled in terms of an approximation parameter k called the blending width. In 1D, it is shown in [22] that the leading order term in the error decreases as $k^{-\frac{3}{2}}$ when the site energy has point symmetry (see Definition (15) below). By contrast, we show in [17] that if the site energy does not have point symmetry, then the error decreases as $k^{-\frac{1}{2}}$. In higher dimensions, the loss in accuracy can be so severe that the method may cease to be consistent [17]. In addition, the symmetries that we identify allow us to investigate ghost-force removal techniques as discussed in [18, 19], which cannot be employed when site energies do not possess point symmetry.

Our framework encompasses all single-species materials with 2-lattice structure and general multi-lattices modeled by pure pair interactions. Physical systems of interest that can be described within this framework are hcp metals (e.g., Mg, Ti, Zn), the honeycomb lattice (graphene) or the diamond cubic structures (e.g., diamond or silicon). Common multi-species materials with multi-lattice structure are shape memory alloys such as Ni-Ti, Fe-Ni, Ni-Al, which are often modelled using only pair interactions [9, 11].

Outline. In Section 2, we introduce the atomistic energies that we consider, and the associated notation for atomistic kinematics. In Section 3, we derive the classical Cauchy–Born energy for simple and multi-lattices and prove first order accuracy of the energy in the multi-lattice case and second order accuracy in the simple lattice case. The second order result is based on the point symmetry of Bravais lattices, which motivates the search for similar symmetries in multi-lattices in Section 4. We identify two non-trivial types of point symmetries in this section. In Section 5, we exploit the symmetry in single-species 2-lattices to prove second order accuracy of the classical Cauchy–Born energy. This result does not extend immediately to the case of multi-lattice pair interactions. Instead, in Section 6, we construct a novel stored energy density for which we are again able to exploit the symmetries discovered in Section 4 to prove second order accuracy.

For the sake of simplicity, we formulate all our results for 2-lattices. However, it is straightforward to see that the results for pair interactions (and only these) extend to general multi-lattices.

2. Atomistic models for 2-lattices

2.1. **Atomistic kinematics.** For $d \in \{1, 2, 3\}$, a d-dimensional *Bravais lattice* (simple lattice or 1-lattice) is a set of the form $B\mathbb{Z}^d$ for some strain $B \in \mathrm{GL}(d)$. A *d-dimensional 2-lattice* is a set of the form

$$\big(B\mathbb{Z}^d + p_0\big) \bigcup \big(B\mathbb{Z}^d + p_1\big), \tag{1}$$

for some *shifts* $p = \{p_0, p_1\} \in \mathbb{R}^d \times \mathbb{R}^d$.

We call $\mathbb{Z}^d$ the *reference lattice* and a point $\xi \in \mathbb{Z}^d$ a *site*. A convenient index set for a 2-lattice is

$$\Lambda := \mathbb{Z}^d \times \{0, 1\},$$

which we call the *reference list*. The reference list serves a purpose similar to the reference domain in elasticity. We think of the elements of the reference list as atoms or nuclei, and we call (ξ, α) the *atom of index α at site ξ*.

An *atomistic deformation* is a map $y : \Lambda \to \mathbb{R}^d$. We will use the notation $y_\alpha(\xi) := y(\xi, \alpha)$ for evaluations of functions defined on Λ, and we call $y_\alpha(\xi)$ the *deformed position of atom* (ξ, α). To make our analysis as simple as possible, we impose *periodic boundary conditions* on the set of deformations. Fix $N \in \mathbb{N}$. We call a map $u : \mathbb{Z}^d \to \mathbb{R}^d$ an *N-periodic displacement* if

$$u_\alpha(\xi) = u_\alpha(\xi + N\eta) \text{ for all } \xi, \eta \in \mathbb{Z}^d,\ \alpha \in \{0, 1\},$$

and we call y an *N-periodic deformation* if for some N-periodic displacement u and some strain $B \in \mathrm{GL}(d)$ we have

$$y_\alpha(\xi) = B\xi + u_\alpha(\xi).$$

Throughout the remainder of the paper, we will assume that all deformations y are N-periodic.

Remark 2.1 (Index versus species). It is important for our purposes to distinguish between lattices that are composed of identical atoms and lattices that are composed of atoms of two or more species. Thus, we will draw a careful distinction between the species of an atom and its index. The *species* is the type of atom, e.g. Cu, Zn, C. The *index* belongs to the set $\{0, 1\}$, and it tells us which of the component Bravais lattices making up the 2-lattice should be associated with the atom. We assume that atoms of the same index must be of the same species.

2.2. **Atomistic energies.** Let y be an N-periodic deformation, and let $\Omega_N := \{0, 1, \ldots, N-1\}^d$ be a periodic cell. For a pair interaction model, the atomistic energy takes the form

$$\mathscr{E}^{\mathrm{a}}(y) := \sum_{\xi \in \Omega_N} \left\{ \sum_{\alpha \in \{0,1\}} \sum_{\substack{(\eta,\beta) \in \Lambda \\ (\eta,\beta) \neq (\xi,\alpha)}} \tfrac{1}{2}\phi_{\alpha\beta}(|y_\beta(\eta) - y_\alpha(\xi)|) \right\},$$

where the functions $\phi_{\alpha\beta} : (0,\infty) \to \mathbb{R}$ are *pair potentials* that may depend on the species of interacting atoms. If the material is composed of atoms of a single species, then there should be no dependence of the potentials on α and β. Examples of multi-lattice pair interaction models describing interesting mechanics such as the shape-memory effect are described in [9, 11]

We call the inner sum

$$\sum_{\alpha\in\{0,1\}} \sum_{\substack{(\eta,\beta)\in\Lambda \\ (\eta,\beta)\neq(\xi,\alpha)}} \tfrac{1}{2}\phi_{\alpha\beta}(|y_\beta(\eta) - y_\alpha(\xi)|) \tag{2}$$

the *site-energy at* ξ. To simplify our analysis, we will assume that $\phi_{\alpha\beta} \in C^3([0,\infty);\mathbb{R})$, even though physically realistic potentials (such as the Lennard-Jones potential) may have singularities at 0. We also assume that for some *cut-off radius* $r_c \in (0,\infty)$,

$$\phi_{\alpha\beta}(r) = 0 \text{ whenever } r > r_c.$$

Thus, the sum defining the site-energy is finite as long as $y(\Lambda)$ does not have an accumulation point. To avoid discussing this purely technical point, we assume in the following that the interaction range is finite in the reference configuration.

In our analysis, we will also allow a more general class of potentials than pair interactions. We only require that the total energy can be decomposed into a sum of localised site-energies. To that end, let

$$\mathcal{R} \subset \mathbb{Z}^d \times \{0,1\} \times \{0,1\} \setminus \big\{(0;0,0),(0;1,1)\big\}$$

be a finite *interaction range*. Throughout the remainder of the paper, $\boldsymbol{\rho} = (\rho;\alpha,\beta)$ will denote an element of $\mathcal{R}$. Given $\boldsymbol{\rho} \in \mathcal{R}$ and a deformation $y \in \mathscr{Y}$, we define the 2-*lattice finite difference*

$$D_{\boldsymbol{\rho}} y(\xi) := y_\beta(\xi+\rho) - y_\alpha(\xi),$$

and the $\mathcal{R}$-tuple $D_{\mathcal{R}} y(\xi) := (D_{\boldsymbol{\rho}} y(\xi))_{\boldsymbol{\rho}\in\mathcal{R}}$.

We assume that the total atomistic energy takes the form

$$\mathscr{E}^{\mathrm{a}}(y) = \sum_{\xi\in\Omega_N} V(D_{\mathcal{R}} y(\xi)), \tag{3}$$

where $V : (\mathbb{R}^d)^{\mathcal{R}} \to \mathbb{R}$ is a *site potential*. In our analysis, we will assume that $V \in C^3((\mathbb{R}^d)^{\mathcal{R}};\mathbb{R})$. Clearly, the pair interaction site-energy (2) is of this form.

Moreover, typical EAM potentials for hcp metals [2] or bond-angle and bond-order potentials for carbon structures (graphene) [6, 21] can be written in this form. However, it may be impossible to express potentials arising directly from quantum mechanics or electronic structure models as in (3).

Remark 2.2. Fixing the interaction range $\mathcal{R}$ in the *reference domain*, is justified by the fact that we consider only elastic effects in this paper.

3. The Cauchy–Born energy

The Cauchy–Born energy is an elastic energy which provides a good approximation of (3) for deformations which are close to homogeneous (i.e., smooth) [4, 8, 16].

3.1. **Continuum kinematics.** In continuum models for 2-lattices, the kinematic variables are a *deformation field* $Y \in C^1(\mathbb{R}^d;\mathbb{R}^d)$ and a *shift field* $P \in C^0(\mathbb{R}^d;\mathbb{R}^d)$. We say that a pair of fields (Y,P) is N-periodic if, for some macroscopic strain $B \in \mathrm{GL}(d)$,

$$P(x+N\eta) = P(x) \quad \text{and} \quad y(x+N\eta) = NB\eta + y(x) \quad \text{for all } \eta \in \mathbb{Z}^d.$$

3.2. **The Cauchy–Born energy for Bravais lattices.** We first review the Cauchy–Born approximation for Bravais lattices. In this case, we may ignore the shifts, and hence atomistic deformations are now maps from $\mathbb{Z}^d$ to $\mathbb{R}^d$, and the interaction range $\mathcal{R}$ is a subset of $\mathbb{Z}^d$. The continuum kinematic variable is just a single N-periodic deformation field $Y \in C^1(\mathbb{R}^d;\mathbb{R}^d)$.

Set $\Omega := [0,1)^d$. We observe that $N\Omega$ is a periodic cell for an N-periodic continuum deformation. The *Cauchy–Born energy* (for Bravais lattices) takes the form

$$\mathscr{E}^{\mathrm{cb}}(Y) = \int_{N\Omega} W(\nabla Y)\,dx, \tag{4}$$

where $W : \mathbb{R}^{d\times d} \to \mathbb{R}\cup\{+\infty\}$ is the *Cauchy–Born strain energy density*. For $F \in \mathrm{GL}(d)$, $W(F)$ is defined to be the atomistic energy per unit volume in the lattice $F\mathbb{Z}^d$. That is, for the atomistic deformation $y^F(\xi) := F\xi$,

$$W(F) := \lim_{N\to\infty} N^{-d} \sum_{\xi\in\Omega_N} V\big(D_{\mathcal{R}} y^F(\xi)\big) = V\big(D_{\mathcal{R}} y^F(0)\big), \tag{5}$$

since $D_{\mathcal{R}} y^F(\xi) = D_{\mathcal{R}} y^F(0) = \big\{F\rho\big\}_{\rho\in\mathcal{R}}$ for all $\xi \in \mathbb{Z}^d$.

Let Y be a continuum deformation. We observe that

$$W(\nabla Y(x)) = V(\nabla_{\mathcal{R}} Y(x)), \quad \text{and} \quad \mathscr{E}^{\mathrm{cb}}(Y) = \int_{N\Omega} V(\nabla_{\mathcal{R}} Y)\,\mathrm{d}x, \tag{6}$$

where $\nabla_{\mathcal{R}} Y(x) := \big\{\nabla_\rho Y(x)\big\}_{\rho\in\mathcal{R}}$.

3.3. **The Cauchy–Born energy for 2-lattices.** We now explain how the Cauchy–Born model is traditionally generalized to 2-lattices. Let Y and P be N-periodic deformation and shift fields. The *Cauchy–Born energy* (for 2-lattices) takes the form

$$\mathscr{E}^{\mathrm{cb}}(Y,P) := \int_{N\Omega} W(\nabla Y, P)\,\mathrm{d}x,$$

where $W : \mathbb{R}^{d\times d}\times(\mathbb{R}^d)^n \to \mathbb{R}\cup\{+\infty\}$ is the *Cauchy–Born strain energy density for 2-lattices.*

As in the case of Bravais lattices, $W(F,P)$ is the energy per unit volume in a lattice subjected to a homogeneous deformation with strain F and shift P. That is, for the deformation $y^{F,P}$ defined by $y^{F,P}_\alpha(\xi) := F\xi + \alpha P$, we have

$$W(F,P) := \lim_{N\to\infty} N^{-d} \sum_{\xi\in\Omega_N} V\big(D_{\mathcal{R}} y^{F,P}(\xi)\big) = V\big(D_{\mathcal{R}} y^{F,P}(0)\big), \qquad (7)$$

since $D_{\mathcal{R}} y^{F,P}(\xi) = D_{\mathcal{R}} y^{F,P}(0) = \big\{F\rho + (\beta-\alpha)P\big\}_{\boldsymbol{\rho}\in\mathcal{R}}$ for all $\xi \in \mathbb{Z}^d$. (Recall the convention $\boldsymbol{\rho} = (\rho;\alpha,\beta)$.)

We now generalize (6). For $\boldsymbol{\rho} \in \mathcal{R}$, we define the 2-*lattice directional derivative* $\nabla_{\boldsymbol{\rho}}$ by

$$\nabla_{\boldsymbol{\rho}}(Y,P)(x) := \nabla_\rho Y(x) + (\beta-\alpha)P(x), \qquad (8)$$

and we set $\nabla_{\mathcal{R}}(Y,P)(x) := \big\{\nabla_{\boldsymbol{\rho}}(Y,P)(x)\big\}_{\boldsymbol{\rho}\in\mathcal{R}}$. Thus, by (7),

$$\begin{aligned} W(\nabla Y, P) =& V(\nabla_{\mathcal{R}}(Y,P)(x)), \quad \text{and} \\ \mathscr{E}^{\mathrm{c}}(Y,P) =& \int_{N\Omega} V\big(\nabla_{\mathcal{R}}(Y,P)(x)\big)\,\mathrm{d}x. \end{aligned} \qquad (9)$$

3.4. **Error estimates for the Cauchy–Born energy.** In order to compare the atomistic and Cauchy–Born energies, we must specify how to generate an atomistic deformation y from a continuum deformation field Y and shift field P. In this section, we adopt the classical approach, however, we will see in Section 5 that for a different identification of the atomistic and continuum variables, the Cauchy–Born energy can be a better approximation.

The Cauchy–Born energy accurately approximates the atomistic energy when the deformation and shift fields are "smooth" or "nearly homogenous." To make this precise, we define a family of increasingly smooth deformations Y^N and shifts P^N. Let Y and P be fixed, 1-periodic deformation and shift fields. Define the *scaled* deformation and shift fields Y^N and P^N by

$$Y^N(x) := NY\left(\frac{x}{N}\right) \quad \text{and} \quad P^N(x) := P\left(\frac{x}{N}\right), \qquad (10)$$

and define a corresponding atomistic deformation y^N by

$$y^N_0(\xi) := Y^N(\xi) \quad \text{and} \quad y^N_1(\xi) := Y^N(\xi) + P^N(\xi). \qquad (11)$$

Observe that Y^N, P^N, and y^N are all N-periodic. We adopt the convention that the atomistic energy of an N-periodic deformation is always the energy of the periodic cell Ω_N, and that the Cauchy–Born energy is the energy of $N\Omega$; that is,

$$\begin{aligned} \mathscr{E}^{\mathrm{a}}\big(y^N\big) :=& \sum_{\xi\in\Omega_N} V\big(D_{\mathcal{R}} y^N(\xi)\big), \quad \text{and} \\ \mathscr{E}^{\mathrm{c}}\big(Y^N, P^N\big) :=& \int_{N\Omega} W\big(\nabla Y^N, P^N\big)\,\mathrm{d}x. \end{aligned}$$

Since we have $\nabla Y^N(x) = \nabla Y\left(\frac{x}{N}\right)$, the strain energy density satisfies

$$W\big(\nabla Y^N(x), P^N(x)\big) = W\left(\nabla Y\left(\frac{x}{N}\right), P\left(\frac{x}{N}\right)\right),$$

and so the Cauchy–Born energy has the scaling invariance

$$N^{-d}\mathscr{E}^{\mathrm{c}}\big(Y^N, P^N\big) = \mathscr{E}^{\mathrm{c}}(Y, P).$$

This suggests that we should treat $\mathscr{E}^{\mathrm{c}}(Y, P)$ as an approximation of the atomistic energy per atom $N^{-d}\mathscr{E}^{\mathrm{a}}\big(y^N\big)$. Indeed we show in Proposition 3.1 that

$$\lim_{N\to\infty} N^{-d}\mathscr{E}^{\mathrm{a}}\big(y^N\big) = \mathscr{E}^{\mathrm{c}}(Y, P).$$

That is, $\mathscr{E}^{\mathrm{c}}(Y, P)$ may be understood as the *continuum limit* of $N^{-d}\mathscr{E}^{\mathrm{a}}\big(y^N\big)$ as $N \to \infty$; see [4]. The proof is elementary, but we provide it nevertheless for comparison with our subsequent analysis.

Proposition 3.1 (Convergence of Cauchy–Born energy for 2-lattices)**.** *Let (Y, P) be a 1-periodic deformation and shift field. Let y^N be the scaled atomistic deformation defined by* (11)*. Then we have*

$$\big|N^{-d}\mathscr{E}^{\mathrm{a}}\big(y^N\big) - \mathscr{E}^{\mathrm{c}}(Y, P)\big| \leq CN^{-1}\left\{\|\nabla^2 Y\|_\infty + \|\nabla P\|_\infty\right\},$$

where the constant C is a function of $\mathcal{R}$ and $\|V\|_{C^1}$.

Proof. Since the midpoint rule is exact for constant functions, a standard quadrature estimate gives

$$\begin{aligned} N^{-d}\mathscr{E}^{\mathrm{c}}\big(Y^N, P^N\big) &= N^{-d}\int_{N\Omega} V\big(\nabla_{\mathcal{R}}\big(Y^N, P^N\big)\big)\,\mathrm{d}x \\ &= N^{-d}\sum_{\xi\in\Omega_N} V\big(\nabla_{\mathcal{R}}\big(Y^N, P^N\big)\big)(\xi) \\ &\quad + O\left(\|V\|_{C^1}\left\{\left\|\nabla^2 Y^N\right\|_\infty + \left\|\nabla P^N\right\|_\infty\right\}\right). \end{aligned}$$

Thus,

$$\begin{aligned} Err(N) :=& N^{-d}\left\{\mathscr{E}^{\mathrm{a}}\big(y^N\big) - \mathscr{E}^{\mathrm{c}}\big(Y^N, P^N\big)\right\} \\ =& N^{-d}\sum_{\xi\in\Omega_N} V\big(D_{\mathcal{R}}y^N(\xi)\big) - V\big(\nabla_{\mathcal{R}}\big(Y^N, P^N\big)\big)(\xi), \\ &+ O\left(\|V\|_{C^1}\left\{\left\|\nabla^2 Y^N\right\|_\infty + \left\|\nabla P^N\right\|_\infty\right\}\right). \end{aligned} \tag{12}$$

By the mean value theorem,

$$\begin{aligned} &\big|V\big(D_{\mathcal{R}}y^N(\xi)\big) - V\big(\nabla_{\mathcal{R}}\big(Y^N, P^N\big)(\xi)\big)\big| \\ &\qquad \leq \sum_{\boldsymbol{\rho}\in\mathcal{R}} \|V\|_{C^1}\big|D_{\boldsymbol{\rho}}y^N(\xi) - \nabla_{\boldsymbol{\rho}}\big(Y^N, P^N\big)(\xi)\big|, \end{aligned} \tag{13}$$

and using Taylor's theorem,

$$\begin{aligned} D_{\boldsymbol{\rho}} y^N(\xi) - \nabla_{\boldsymbol{\rho}}\big(Y^N, P^N\big)(\xi) &= y^N_\beta(\xi+\rho) - y^N_\alpha(\xi) \\ &\quad - \nabla_\rho Y^N(\xi) + (\alpha-\beta)P^N(\xi) \\ &= Y(\xi+\rho) - Y(\xi) - \nabla_\rho Y^N(\xi) \\ &\quad + \beta\big\{P^N(\xi+\rho) - P^N(\xi)\big\} \\ &= O\left(\left\|\nabla^2 Y^N\right\|_\infty + \left\|\nabla P^N\right\|_\infty\right). \end{aligned} \tag{14}$$

Combining (12), (13), and (14) shows

$$N^{-d}|\mathscr{E}^{\mathrm{a}}(y^N) - \mathscr{E}^{\mathrm{c}}(Y^N, P^N)| \le C\big\{\left\|\nabla^2 Y^N\right\|_\infty + \left\|\nabla P^N\right\|_\infty\big\}$$

where the constant C is a function of $\|V\|_{C^1}$ and $\mathcal{R}$. We now observe

$$\left\|\nabla^2 Y^N\right\|_\infty = N^{-1}\|\nabla^2 Y\|_\infty \quad \text{and} \quad \left\|\nabla P^N\right\|_\infty = N^{-1}\|\nabla P\|_\infty,$$

and the result follows. □

For Bravais lattices, the estimate given in Proposition 3.1 can be improved if we assume that the site potential V has *point symmetry* [10]:

$$V(\boldsymbol{g}) = V(-\{g_{-\rho}\}_{\rho\in\mathcal{R}}) \text{ for all } \boldsymbol{g} \in (\mathbb{R}^d)^{\mathcal{R}}. \tag{15}$$

We show in Lemma 3.1 that under physically reasonable assumptions, one can always take V to be point symmetric. Let $R : \mathbb{R}^d \to \mathbb{R}^d$ defined by $Rx = -x$ be *point reflection in the origin.* The first assumption is that

$$\mathscr{E}^{\mathrm{a}}(y) = \mathscr{E}^{\mathrm{a}}(y \circ R) \text{ for all } y \in \mathscr{Y}.$$

Physically, this assumption is motivated by the observation that permutation or relabelling of the atoms does not change the energy, and that Bravais lattices are invariant under the point inversion R, which means that R provides such a relabelling.

The second assumption is that

$$\mathscr{E}^{\mathrm{a}}(y) = \mathscr{E}^{\mathrm{a}}(-y) \text{ for all } y \in \mathscr{Y},$$

which is motivated by the principle that the energy should be unchanged if the configuration of the atoms is reflected.

Remark 3.1. Permutation invariance can be expected to hold whenever there is only one species of atoms. If there is more than one species, then we can only assume that the energy is invariant under those permutations which preserve the species of the atoms. Hence, Lemma 3.1 cannot be immediately applied to general multi-lattices.

Lemma 3.1. *Assume that for all deformations y,*

$$\mathscr{E}^{\mathrm{a}}(y) = \mathscr{E}^{\mathrm{a}}(-y \circ R), \tag{16}$$

where $Rx = -x$; then

$$\mathscr{E}^{\mathrm{a}}(y) = \sum_{\xi\in\Omega_N} \bar{V}\big(D_{\bar{\mathcal{R}}} y(\xi)\big),$$

where $\bar{\mathcal{R}} = \mathcal{R} \cup -\mathcal{R}$, *and* $\bar{V} : (\mathbb{R}^d)^{\bar{\mathcal{R}}} \to \mathbb{R}$ *defined by*

$$\bar{V}\big(\{g_{\boldsymbol{\rho}}\}_{\boldsymbol{\rho}\in\bar{\mathcal{R}}}\big) := \tfrac{1}{2}V\big(\{g_{\boldsymbol{\rho}}\}_{\boldsymbol{\rho}\in\mathcal{R}}\big) + \tfrac{1}{2}V\big(\{-g_{-\boldsymbol{\rho}}\}_{\boldsymbol{\rho}\in-\mathcal{R}}\big),$$

is point symmetric (15).

Proof. First, we note that, if y is an N-periodic deformation then so is $-y \circ R$, since for all $\eta \in \mathbb{Z}^d$

$$-y \circ R(\xi + N\eta) = -y(-\xi - N\eta) = -y(-\xi) = -y \circ R(\xi).$$

By (16), we have

$$\begin{aligned}
\mathscr{E}^{\mathrm{a}}(y) &= \tfrac{1}{2}\mathscr{E}^{\mathrm{a}}(y) + \tfrac{1}{2}\mathscr{E}^{\mathrm{a}}(-y \circ R) \\
&= \frac{1}{2}\sum_{\xi\in\Omega_N} V\big(D_{\mathcal{R}}y(\xi)\big) + \frac{1}{2}\sum_{\xi\in\Omega_N} V\big(-D_{\mathcal{R}}(y\circ R)(\xi)\big) \\
&= \frac{1}{2}\sum_{\xi\in\Omega_N} V(D_{\mathcal{R}}y(\xi)) + \frac{1}{2}\sum_{\xi\in\Omega_N} V(-D_{-\mathcal{R}}y(-\xi)).
\end{aligned}$$

The last equality follows since for $\rho \in \mathcal{R}$ we have

$$\begin{aligned}
D_\rho y \circ R(\xi) &= y \circ R(\xi + \rho) - y \circ R(\xi) \\
&= y(-\xi - \rho) - y(-\xi) \\
&= D_{-\rho}y(-\xi).
\end{aligned}$$

Employing periodicity of y, we can shift the second summation over $-\Omega_N$ back to Ω_N and upon relabelling, obtain

$$\begin{aligned}
\mathscr{E}^{\mathrm{a}}(y) &= \frac{1}{2}\sum_{\xi\in\Omega_N} V(Dy(\xi)) + \frac{1}{2}\sum_{\xi\in\Omega_N} V(-D_{-\mathcal{R}}y(\xi)) \\
&= \sum_{\xi\in\Omega_N} \bar{V}(\bar{D}_{\bar{\mathcal{R}}}y(\xi)).
\end{aligned}$$

Finally, point symmetry of $\bar{\mathcal{R}}$ and of $\bar{V}$ are obvious. □

Point symmetry of V implies a symmetry of the partial derivatives of V in homogeneous states. For $\rho \in \mathcal{R}$ and $\boldsymbol{g} \in (\mathbb{R}^d)^{\mathcal{R}}$, we define $V_\rho(\boldsymbol{g}) := \frac{\partial V}{\partial g_\rho}(\boldsymbol{g})$. If V is point symmetric, then we have

$$V_\rho(F \cdot \mathcal{R}) = -V_{-\rho}(F \cdot \mathcal{R}) \quad \text{for all } F \in \mathrm{GL}(d). \tag{17}$$

To see this, one differentiates the identity (15) with respect to g_ρ and then evaluates it at $\boldsymbol{g} = F \cdot \mathcal{R}$.

We can now prove the that the Cauchy–Born approximation for Bravais lattices is second order accurate, which was previously observed in [4, 10, 14]. We nevertheless give a complete proof of the result, since it motivates our subsequent analysis for 2-lattices. For Bravais lattices, there is no reason to make a distinction between the atomistic and continuum variables since we will not consider multiple ways of relating

the two. Thus, given a fixed 1-periodic deformation $Y : \mathbb{R}^d \to \mathbb{R}^d$, we let

$$Y^N(x) := NY\left(\frac{x}{N}\right), \tag{18}$$

and we interpret Y^N as both an atomistic and a continuum deformation.

Proposition 3.2 (Convergence for Bravais lattices.)**.** *Let $Y \in C^3(\mathbb{R}^d;\mathbb{R}^d)$ be a 1-periodic deformation, and let Y^N be defined by* (18)*; then,*

$$\left|N^{-d}\mathscr{E}^{\mathrm{a}}\big(Y^N\big) - \mathscr{E}^{\mathrm{c}}(Y)\right| \leq CN^{-2}\big\{\|\nabla^2 Y\|_\infty^2 + \|\nabla^3 Y\|_\infty\big\},$$

where the constant C is a function of $\mathcal{R}$ and $\|V\|_{C^2}$.

Proof. Since the midpoint rule is exact for affine functions, a standard quadrature estimate gives

$$\begin{aligned} N^{-d}\mathscr{E}^{\mathrm{c}}\big(Y^N\big) &= N^{-d}\int_{N\Omega} V\big(\nabla_{\mathcal{R}} Y^N\big)\,\mathrm{d}x \\ &= N^{-d}\sum_{\xi\in\Omega_N} V\big(\nabla_{\mathcal{R}} Y^N(\xi)\big) \\ &\quad + O\left(\left\|\nabla^2 V\big(\nabla_{\mathcal{R}} Y^N\big)\right\|_\infty\right). \end{aligned} \tag{19}$$

Set $V_\rho(\boldsymbol{g}) := \frac{\partial}{\partial g_\rho} V(\boldsymbol{g})$, and let $V_\rho(\xi) := V_\rho\big(\nabla_{\mathcal{R}} Y^N(\xi)\big)$. By Taylor's theorem,

$$\begin{aligned} V\big(D_{\mathcal{R}} Y^N(\xi)\big) - V\big(\nabla_{\mathcal{R}} Y^N(\xi)\big) &= \sum_{\rho\in\mathcal{R}} V_\rho(\xi)\cdot\big\{D_\rho Y^N(\xi) - \nabla_\rho Y^N(\xi)\big\} \\ &\quad + O(\|V\|_{C^2}\big|D_\rho Y^N(\xi) - \nabla_\rho Y^N(\xi)\big|^2), \end{aligned} \tag{20}$$

and

$$\begin{aligned} D_\rho Y^N(\xi) - \nabla_\rho Y^N(\xi) &= Y^N(\xi+\rho) - Y^N(\xi) - \nabla_\rho Y^N(\xi) \\ &= \frac{1}{2}\nabla_\rho^2 Y^N(\xi) + O\big(\big\|\nabla^3 Y^N\big\|_\infty\big). \end{aligned} \tag{21}$$

Combining (20) and (21), we have

$$\begin{aligned} V\big(D_{\mathcal{R}} Y^N(\xi)\big) - V\big(\nabla_{\mathcal{R}} Y^N\big) &= \frac{1}{2}\sum_{\rho\in\mathcal{R}} V_\rho(\xi)\cdot\nabla_\rho^2 Y^N(\xi) \\ &\quad + O\left(\big\{\big\|\nabla^2 Y^N\big\|_\infty^2 + \big\|\nabla^3 Y^N\big\|_\infty\big\}\right) \end{aligned} \tag{22}$$

By symmetry of the partial derivatives of V (17), the first term on the right hand side of (22) vanishes. We have

$$\begin{aligned} \sum_{\rho\in\mathcal{R}} V_\rho\cdot\nabla_\rho^2 Y^N &= \frac{1}{2}\sum_{\rho\in\mathcal{R}}\Big(V_\rho\cdot\nabla_\rho^2 y^N + V_{-\rho}\cdot\nabla_{-\rho}^2 Y^N\Big) \\ &= \frac{1}{2}\sum_{\rho\in\mathcal{R}}\Big(V_\rho\cdot\nabla_\rho^2 Y^N - V_\rho\cdot\nabla_\rho^2 Y^N\Big) = 0, \end{aligned}$$

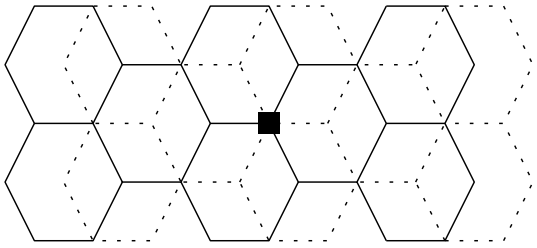

FIGURE 1. Point reflection of the honeycomb lattice about a lattice site yields a shifted honeycomb lattice.

where all functions above are evaluated at $\xi \in \Omega_N$. Therefore, combining (19),(20), and (22) gives

$$N^{-d}\big|\mathscr{E}^{\mathrm{a}}\big(Y^N\big) - \mathscr{E}^{\mathrm{c}}\big(Y^N\big)\big| \leq C\big\{\big\|\nabla^2 Y^N\big\|_\infty^2 + \big\|\nabla^3 Y^N\big\|_\infty\big\},$$

where the constant C depends on $\mathcal{R}$ and $\|V\|_{C^2}$. Finally, we observe that

$$\big\|\nabla^2 Y^N\big\|_\infty^2 = N^{-2}\big\|\nabla^2 Y\big\|_\infty^2 \quad \text{and} \quad \big\|\nabla^3 Y^N\big\|_\infty = N^{-2}\big\|\nabla^3 Y\big\|_\infty,$$

and the result follows. □

4. Symmetries of the 2-lattice site energy

We showed in the previous section how the point symmetry (15) of Bravais lattices implies second order accuracy of the Cauchy–Born energy in the continuum limit. At first glance, 2-lattices do not possess a point symmetry: e.g., inversion of the honeycomb lattice about a lattice point yields a shifted honeycomb lattice; see Figure 1. Note, however, that inverting the lattice about the center of an edge leaves it invariant.

The purpose of this section is to explore how this and other symmetries may be exploited to extend (15). We will identify two such non-trivial extensions: for the case of a single species 2-lattice with a general site energy, and for the case of a multi-lattices with pair interaction energy (however, we will only formulate the result for 2-lattices). In Sections 5 and 6, we will then exploit these observations to derive "simple" second order continuum models.

4.1. **Symmetries for single-species 2-lattices.** Any single-species 2-lattice has a reflection symmetry about the "centroid" of a lattice site; see Figure 2. Algebraically, let $B \in \mathrm{GL}(d)$, $p \in \mathbb{R}^d \setminus B\mathbb{Z}^d$, and let $\mathscr{L} := B\mathbb{Z}^d \bigcup (B\mathbb{Z}^d + p)$ be a single-species 2-lattice. Equivalently, we may shift the lattice by $-p/2$ to redefine it as

$$\mathscr{L} := \big(B\mathbb{Z}^d - \tfrac{p}{2}\big) \bigcup \big(B\mathbb{Z}^d + \tfrac{p}{2}\big),$$

which immediately reveals the symmetry

$$-\mathscr{L} = \mathscr{L} \tag{23}$$

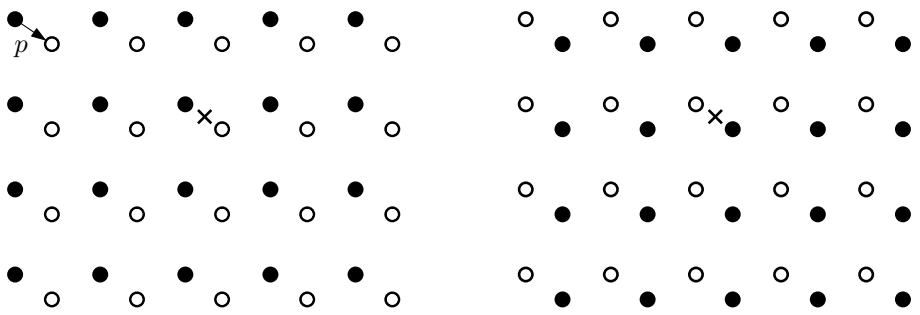

FIGURE 2. Point reflection of a 2-lattice about the "centroid" x of a lattice site, containing $\{\circ, \bullet\}$. The lattice remains invariant, however the atom indices are reversed. If the atoms are of the same species, then the physical configuration remains invariant.

Note, however, that if $\mathscr{L}$ has two species, then this operation reverses the species and is therefore *not* a symmetry of a 2-species 2-lattice.

The symmetry (15) can also be thought of as a permutation of the reference list: $R(\rho;\alpha) := (-\rho;\neg\alpha)$ where $\neg 0 := 1$ and $\neg 1 := 0$, then $R\Lambda = \Lambda$. We can also define an analogous operation on interactions $\neg : \mathbb{Z}^d \times \{0,1\} \times \{0,1\} \to \mathbb{Z}^d \times \{0,1\} \times \{0,1\}$,

$$\neg(\rho;\alpha,\beta) := (-\rho;\neg\alpha,\neg\beta). \tag{24}$$

The following Proposition provides a 2-lattice analogy to the observation that $D_\rho y^F = -D_{-\rho} y^F$ in Bravais lattices, which was a key step to obtain second order accuracy of the Bravais lattice Cauchy–Born energy.

Proposition 4.1. *Let $F \in \mathrm{GL}(d)$ and $p = (p_0, p_1) \in \mathbb{R}^{2d}$, then*

$$D_{\boldsymbol{\rho}} y^{F,p} = -D_{\neg\boldsymbol{\rho}} y^{F,p} \qquad \forall \boldsymbol{\rho} \in \mathcal{R}.$$

Proof. Let $y = y^{F,p}$ and $\boldsymbol{\rho} = (\rho;\alpha,\beta) \in \mathcal{R}$, then

$$\begin{aligned} -D_{\neg\boldsymbol{\rho}} y(0) &= -\big(y_{\neg\beta}(-\rho) - y_{\neg\alpha}(0)\big) \\ &= -\big(F(-\rho) + p_{\neg\beta}\big) + \big(p_{\neg\alpha}\big) \\ &= F\rho + p_{\neg\alpha} - p_{\neg\beta} \end{aligned}$$

One readily checks by case distinction that $p_{\neg\alpha} - p_{\neg\beta} = p_\beta - p_\alpha$, which concludes the proof. □

Definition 4.1 (Point symmetry for a single-species 2-lattice)**.** We say that the site potential V is *point symmetric (with respect to $\neg$)* if $\mathcal{R} = \neg\mathcal{R}$ and

$$V\big(\{g_{\boldsymbol{\rho}}\}_{\boldsymbol{\rho}\in\mathcal{R}}\big) = V\big(-\{g_{\neg\boldsymbol{\rho}}\}_{\boldsymbol{\rho}\in\mathcal{R}}\big) \qquad \forall \{g_{\boldsymbol{\rho}}\}_{\boldsymbol{\rho}\in\mathcal{R}} \in (\mathbb{R}^d)^{\mathcal{R}}. \tag{25}$$

We show next that, under physically realistic assumptions (invariance of the energy under permutations and isometries) it is always

possible to define a point symmetric site potential for a single-species 2-lattice.

Proposition 4.2. *Suppose that $\mathscr{E}^{\mathrm{a}}$ given by* (3) *is invariant under the permutation R of the index list, and under the isometry $x \mapsto -x$:*

$$\mathscr{E}^{\mathrm{a}}(y) = \mathscr{E}^{\mathrm{a}}(y \circ R) = \mathscr{E}^{\mathrm{a}}(-y \circ R); \tag{26}$$

then,

$$\mathscr{E}^{\mathrm{a}}(y) = \sum_{\xi \in \Omega_N} \bar{V}\big(D_{\bar{\mathcal{R}}} y(\xi)\big),$$

where $\bar{\mathcal{R}} = \mathcal{R} \cup \neg\mathcal{R}$, and $\bar{V} : (\mathbb{R}^d)^{\bar{\mathcal{R}}} \to \bar{\mathbb{R}}$,

$$\bar{V}\big(\{g_{\boldsymbol{\rho}}\}_{\boldsymbol{\rho} \in \bar{\mathcal{R}}}\big) := \tfrac{1}{2} V\big(\{g_{\boldsymbol{\rho}}\}_{\boldsymbol{\rho} \in \mathcal{R}}\big) + \tfrac{1}{2} V\big(\{-g_{\neg\boldsymbol{\rho}}\}_{\boldsymbol{\rho} \in \neg\mathcal{R}}\big),$$

is point symmetric (25).

Proof. Fix $y \in \mathscr{Y}_N$ and let $\bar{\mathcal{R}}, \bar{V}$ be defined as above. We first show that $y' := -y \circ R \in \mathscr{Y}_N$. To that end we must show that the associated displacement $u' := y' - y^{B,0}$ is N-periodic. To see this, let $u := y - y^{B,0}$, then u is N-periodic and we have

$$\begin{aligned} u'_\alpha(\xi) &= -(y \circ R)_\alpha(\xi) - B\xi = -y_{\neg\alpha}(-\xi) - B\xi \\ &= -u_{\neg\alpha}(-\xi) + B\xi - B\xi = -u_{\neg\alpha}(-\xi). \end{aligned}$$

Since $u_{\neg\alpha}$ is N-periodic it follows that u'_α is N-periodic.

The rest of the proof is analogous to the proof of Proposition 3.1. Employing (26), we have

$$\begin{aligned} \mathscr{E}^{\mathrm{a}}(y) &= \tfrac{1}{2}\mathscr{E}^{\mathrm{a}}(y) + \tfrac{1}{2}\mathscr{E}^{\mathrm{a}}(-y \circ R) \\ &= \frac{1}{2} \sum_{\xi \in \Omega_N} V\big(D_{\mathcal{R}} y(\xi)\big) + \frac{1}{2} \sum_{\xi \in \Omega_N} V\big(-D_{\mathcal{R}}(y \circ R)(\xi)\big) \\ &= \frac{1}{2} \sum_{\xi \in \Omega_N} V(D_{\mathcal{R}} y(\xi)) + \frac{1}{2} \sum_{\xi \in \Omega_N} V(-D_{\neg\mathcal{R}} y(-\xi)). \end{aligned}$$

The last equality follows since for $\boldsymbol{\rho} = (\rho; \alpha, \beta) \in \mathcal{R}$ we have

$$\begin{aligned} D_{\boldsymbol{\rho}} y \circ R(\xi) &= y \circ R(\xi + \rho, \beta) - y \circ R(\xi, \alpha) \\ &= y(-\xi - \rho, \neg\beta) - y(-\xi, \neg\alpha) \\ &= D_{\neg\boldsymbol{\rho}} y(-\xi). \end{aligned}$$

Since $y - y^{B,0}$ is periodic, we can shift the second summation over $-\Omega_N$ back to Ω_N and, upon relabelling the summation variable, obtain

$$\begin{aligned}\mathscr{E}^{\mathrm{a}}(y) &= \frac{1}{2}\sum_{\xi\in\Omega_N} V(Dy(\xi)) + \frac{1}{2}\sum_{\xi\in\Omega_N} V(-D_{\neg\mathcal{R}}y(Ne-\xi))\\ &= \frac{1}{2}\sum_{\xi\in\Omega_N} V(Dy(\xi)) + \frac{1}{2}\sum_{\xi\in\Omega_N} V(-D_{\neg\mathcal{R}}y(\xi))\\ &= \sum_{\xi\in\Omega_N} \bar{V}(\bar{D}y(\xi)),\end{aligned}$$

where $e = (1,\dots,1) \in \mathbb{R}^d$.

Finally, point symmetry of $\bar{\mathcal{R}}$ and of $\bar{V}$ are obvious. □

4.2. **Symmetry of pair interaction energies.** Suppose that $\mathscr{E}^{\mathrm{a}}$ is given by the pair interaction model (2) for a 2-lattice with two different species; that is, the site energy $V : (\mathbb{R}^d)^{\mathcal{R}} \to \mathbb{R}$ is defined by

$$V(\boldsymbol{g}) = \frac{1}{2}\sum_{\boldsymbol{\rho}\in\mathcal{R}} \phi_{\alpha\beta}\big(|D_{\boldsymbol{\rho}}y(\xi)|\big). \tag{27}$$

(Recall the convention that $\boldsymbol{\rho} = (\rho,\alpha,\beta)$.) We will now identify a symmetry in this model that will play a role analogous to the operation $\neg$ in the previous section.

The key observation in this case is that, physically, we should require $\phi_{\alpha\beta} = \phi_{\beta\alpha}$, which motivates the operation $\sim : \mathbb{Z}^d \times \{0,1\} \times \{0,1\} \to \mathbb{Z}^d \times \{0,1\} \times \{0,1\}$ by

$$\sim(\rho;\alpha,\beta) := (-\rho;\beta,\alpha). \tag{28}$$

We immediately obtain the following result.

Proposition 4.3 (Symmetry of pair interaction site potentials)**.** *Let the site energy V be defined by* (27) *and suppose that $\mathcal{R} = \sim\mathcal{R}$ and $\phi_{\alpha\beta} = \phi_{\beta\alpha}$ for all $\alpha,\beta \in \{0,1\}$; then V satisfies the point symmetry*

$$V\big(\{g_{\boldsymbol{\rho}}\}_{\boldsymbol{\rho}\in\mathcal{R}}\big) = V\big(\{-g_{\sim\boldsymbol{\rho}}\}_{\boldsymbol{\rho}\in\mathcal{R}}\big) \qquad \forall \{g_{\boldsymbol{\rho}}\}_{\boldsymbol{\rho}\in\mathbb{R}} \in (\mathbb{R}^d)^{\mathcal{R}}. \tag{29}$$

Proof. Under the stated assumptions,

$$\begin{aligned}V\big(\{-g_{\sim\boldsymbol{\rho}}\}_{\boldsymbol{\rho}\in\mathcal{R}}\big) &= \sum_{\boldsymbol{\rho}\in\mathcal{R}} \phi_{\alpha\beta}(|-g_{(-\rho;\beta,\alpha)}|)\\ &= \sum_{\boldsymbol{\rho}\in\sim\mathcal{R}} \phi_{\beta\alpha}(|g_{(-\rho;\beta,\alpha)}|).\end{aligned}$$

Relabelling $\rho' = -\rho, \alpha' = \beta, \beta' = \alpha$ we obtain (29). □

Remark 4.1. 1. Unlike the symmetry $\neg$ of a single-species 2-lattice, $\sim$ does not arise from any globally defined permutation of the atoms of the material. For this reason, one cannot expect that an arbitrary total energy will be symmetric under $\sim$, and therefore one cannot hope to symmetrize general site potentials.

2. The symmetry $\sim$ can be immediately applied to n-lattice pair interactions for $n > 2$. All our subsequent results generalize as well.

5. Second order accuracy of the Cauchy–Born Energy

In this section, we give a new rule relating the atomistic and continuum variables, and we show that under this rule, the Cauchy–Born energy for single-species 2-lattices is second order accurate. Given 1-periodic deformation and shift fields Y and P, we first rescale them to atomic units

$$Y^N(x) := NY\left(\frac{x}{N}\right) \quad \text{and} \quad P^N(x) := P\left(\frac{x}{N}\right).$$

We then define a corresponding atomistic deformation y^N by

$$y_0^N(\xi) := Y^N(\xi) - \frac{1}{2}P^N(\xi) \quad \text{and} \quad y_1^N(\xi) := Y^N(\xi) + \frac{1}{2}P^N(\xi). \quad (30)$$

When (30) is used to connect the atomistic and continuum fields, we interpret $Y^N(\xi)$ as the *deformation of the centroid* of the atoms at site ξ; indeed, the inverse transformation of (30) is

$$Y^N(\xi) := \frac{1}{2}\big\{y_0^N(\xi) + y_1^N(\xi)\big\} \quad \text{and} \quad P^N(\xi) := y_1^N(\xi) - y_0^N(\xi).$$

As in the Bravais lattice case, we need a symmetry of the partial derivatives of V (17) to show second order convergence. The following lemma establishes the appropriate generalization.

Lemma 5.1. *Suppose that V is point symmetric* (25) *with respect to the permutation operator $\neg$. Let $\nabla_{\boldsymbol{\rho}}$ be defined by* (8)*, and let $V_{\boldsymbol{\rho}}(\boldsymbol{g}) := \frac{\partial}{\partial g_{\boldsymbol{\rho}}} V(\boldsymbol{g})$. Then, for any deformation and shift fields Y and P, we have*

$$V_{\boldsymbol{\rho}}\big(\nabla_{\mathcal{R}}(Y,P)(x)\big) = -V_{\neg\boldsymbol{\rho}}\big(\nabla_{\mathcal{R}}(Y,P)(x)\big). \quad (31)$$

Proof. Differentiating (25) and (29) with respect to $g_{\boldsymbol{\rho}}$ yields

$$V_{\boldsymbol{\rho}}\big(\{g_{\boldsymbol{\rho}}\}_{\boldsymbol{\rho}\in\mathcal{R}}\big) = -V_{\neg\boldsymbol{\rho}}\big(\{-g_{\neg\boldsymbol{\rho}}\}_{\boldsymbol{\rho}\in\mathcal{R}}\big).$$

Evaluating at $g_{\boldsymbol{\rho}} = \nabla_{\boldsymbol{\rho}}(Y,P)$ and noting that

$$\begin{aligned} -\nabla_{\neg\boldsymbol{\rho}}(Y,P) &= -\nabla_{-\rho}Y - (\neg\beta - \neg\alpha)P \\ &= \nabla_{\rho}Y - \big((1-\beta) - (1-\alpha)\big)P \\ &= \nabla_{\rho}Y + (\beta - \alpha)P \\ &= \nabla_{\boldsymbol{\rho}}(Y,P), \end{aligned}$$

we obtain (31). □

We are now in a position to prove second order accuracy of the Cauchy–Born model.

Theorem 5.1 (Second order convergence for single species 2-lattices)**.** *Let $Y \in C^3(\mathbb{R}^d;\mathbb{R}^d)$ be a 1-periodic deformation field and $P \in C^2(\mathbb{R}^d;\mathbb{R}^d)$ a 1-periodic shift field. Let y^N be the scaled atomistic configuration defined by* (30)*. Then*

$$\big|N^{-d}\mathscr{E}^{\rm a}\big(y^N\big) - \mathscr{E}^{\rm c}\big(Y,P\big)\big| \le CN^{-2}\big\{\,\|\nabla^3 Y\|_\infty + \|\nabla^2 P\|_\infty + \|\nabla^2 Y\|_\infty^2 + \|\nabla P\|_\infty^2\big\}.$$

where the constant C is a function of $\mathcal{R}$ and $\|V\|_{C^2}$.

Proof. Since the midpoint rule is exact for affine functions, a standard quadrature estimate gives

$$\begin{aligned} N^{-d}\mathscr{E}^{\rm c}\big(Y^N,P^N\big) &= N^{-d}\int_{N\Omega} V\big(\nabla_{\mathcal{R}}\big(Y^N,P^N\big)\big) \\ &= N^{-d}\sum_{\xi\in\Omega_N} V\big(\nabla_{\mathcal{R}}\big(Y^N,P^N\big)\big) \\ &\quad + O\big(\big\|\nabla^2 V\big(\nabla_{\mathcal{R}}\big(Y^N,P^N\big)\big)\big\|_\infty\big). \end{aligned} \tag{32}$$

It is easy to see that

$$\begin{aligned} &\big\|\nabla^2 V\big(\nabla_{\mathcal{R}}\big(Y^N,P^N\big)\big)\big\|_\infty \\ &\qquad \le C\big(\big\|\nabla^3 Y^N\big\|_\infty + \big\|\nabla^2 P^N\big\|_\infty + \big\|\nabla^2 Y^N\big\|_\infty^2 + \big\|\nabla P^N\big\|_\infty^2\big). \end{aligned}$$

We now estimate the error in $V\big(\nabla_{\mathcal{R}}\big(Y^N,P^N\big)(\xi)\big)$. By Taylor's theorem,

$$\begin{aligned} V\big(D_{\mathcal{R}}y^N\big) - V\big(\nabla_{\mathcal{R}}\big(Y^N,P^N\big)\big) &= \sum_{\boldsymbol{\rho}\in\mathcal{R}} V_{\boldsymbol{\rho}}\cdot\big\{D_{\boldsymbol{\rho}}y - \nabla_{\boldsymbol{\rho}}y\big\} \\ &\quad + O\Big(\|V\|_{C^2}\big|D_{\boldsymbol{\rho}}y^N - \nabla_{\boldsymbol{\rho}}\big(Y^N,P^N\big)\big|^2\Big), \end{aligned} \tag{33}$$

where all functions above are evaluated $\xi\in\Omega_N$, and $V_{\boldsymbol{\rho}} := V_{\boldsymbol{\rho}}\big(\nabla_{\mathcal{R}}\big(Y^N,P^N\big)(\xi)\big)$. By a second application of Taylor's theorem,

$$\begin{aligned} D_{\boldsymbol{\rho}}y^N(\xi) - \nabla_{\boldsymbol{\rho}}\big(Y^N,P^N\big)(\xi) &= y^N_\beta(\xi+\rho) - y^N_\alpha(\xi) \\ &\quad - \nabla_\rho Y^N(\xi) - (\beta-\alpha)P^N(\xi) \\ &= Y^N(\xi+\rho) + \big(\beta-\tfrac12\big)P^N(\xi+\rho) \\ &\quad - Y^N(\xi) - \big(\alpha-\tfrac12\big)P^N(\xi) \\ &\quad - \nabla_\rho Y^N(\xi) - (\beta-\alpha)P^N(\xi) \\ &= \tfrac12\nabla_\rho^2 Y^N(\xi) + \big(\beta-\tfrac12\big)\nabla_\rho P^N(\xi) \\ &\quad + O\big(\big\|\nabla^3 Y^N\big\|_\infty + \big\|\nabla^2 P^N\big\|_\infty\big). \end{aligned} \tag{34}$$

Substituting (34) into (33), and assuming again that all functions are evaluated at $\xi \in \Omega_N$, we obtain

$$V\big(D_{\mathcal{R}} y^N\big) - V\big(\nabla_{\mathcal{R}}\big(Y^N, P^N\big)\big) = \sum_{\boldsymbol{\rho}\in\mathcal{R}} V_{\boldsymbol{\rho}} \cdot e(\boldsymbol{\rho}) + O\big(\big\|\nabla^3 Y^N\big\|_\infty + \big\|\nabla^2 P^N\big\|_\infty\big), \quad (35)$$

where

$$e(\boldsymbol{\rho}) := \tfrac{1}{2}\nabla_\rho^2 Y^N(\xi) + \big(\beta - \tfrac{1}{2}\big)\nabla_\rho P^N(\xi).$$

We now observe that

$$\begin{aligned} e(\neg\boldsymbol{\rho}) &= \tfrac{1}{2}\nabla_{-\rho}^2 Y^N(\xi) + \big(\neg\beta - \tfrac{1}{2}\big)\nabla_{-\rho} P^N(\xi) \\ &= \tfrac{1}{2}\nabla_{-\rho}^2 Y^N(\xi) + \big((1-\beta) - \tfrac{1}{2}\big)\nabla_{-\rho} P^N(\xi) \\ &= \tfrac{1}{2}\nabla_{\rho}^2 Y^N(\xi) + (\beta - \tfrac{1}{2})\nabla_{\rho} P^N(\xi) \\ &= e(\boldsymbol{\rho}), \end{aligned} \quad (36)$$

from which we deduce that the the first term on the right-hand side of (35) vanishes: using (37) and point symmetry of the derivatives (31), we obtain

$$\begin{aligned} \sum_{\boldsymbol{\rho}\in\mathcal{R}} V_{\boldsymbol{\rho}} \cdot e(\boldsymbol{\rho}) &= \frac{1}{2}\sum_{\boldsymbol{\rho}\in\mathcal{R}} V_{\boldsymbol{\rho}} \cdot e(\boldsymbol{\rho}) + V_{*\boldsymbol{\rho}} \cdot e(*\boldsymbol{\rho}) \\ &= \frac{1}{2}\sum_{\boldsymbol{\rho}\in\mathcal{R}} V_{\boldsymbol{\rho}} \cdot \big\{e(\boldsymbol{\rho}) - e(*\boldsymbol{\rho})\big\} \\ &= 0. \end{aligned} \quad (37)$$

Finally, combining (32), (33), (34), (35), and (37) gives

$$\begin{aligned} &\big|N^{-d}\mathscr{E}^{\mathrm{a}}\big(y^N\big) - \mathscr{E}^{\mathrm{c}}\big(Y, P\big)\big| \\ &\qquad \le C\big(\big\|\nabla^3 Y^N\big\|_\infty + \big\|\nabla^2 P^N\big\|_\infty + \big\|\nabla^2 Y^N\big\|_\infty^2 + \big\|\nabla P^N\big\|_\infty^2\big). \end{aligned}$$

The result follows by rescaling

$$\begin{aligned} \big\|\nabla^3 Y^N\big\|_\infty &= N^{-2}\big\|\nabla^3 Y\big\|_\infty, & \big\|\nabla^2 Y^N\big\|_\infty^2 &= N^{-2}\big\|\nabla^2 Y\big\|_\infty^2, \\ \big\|\nabla^2 P^N\big\|_\infty &= N^{-2}\big\|\nabla^2 P\big\|_\infty, \quad \text{and} & \big\|\nabla P^N\big\|_\infty^2 &= N^{-2}\big\|\nabla P\big\|_\infty^2. \end{aligned}$$

□

Remark 5.1. Suppose that we are in the multi-species 2-lattice case, and must use the symmetry $\sim$ instead of $\neg$. In this case, we have

$$\begin{aligned} e(\sim\boldsymbol{\rho}) &= \tfrac{1}{2}\nabla_{-\rho}^2 Y^N(\xi) + \big(\alpha - \tfrac{1}{2}\big)\nabla_{-\rho} P^N(\xi) \\ &= \tfrac{1}{2}\nabla_{\rho}^2 Y^N(\xi) + \big(\tfrac{1}{2} - \alpha\big)\nabla_{\rho} P^N(\xi) \neq e(\boldsymbol{\rho}), \end{aligned}$$

whenever $\alpha = \beta$. Thus, in our above proof the first order terms do not cancel and the Cauchy–Born model is only first order accurate in this case. We will show in the next section how a new strain energy density can be constructed that is second order accurate in this case.

6. A second order accurate stored energy density for pair interactions

In this section, we show how the symmetry $\sim$ for multi-lattice pair interactions can be exploited to derive a "simple" second order accurate stored energy density, which does *not* coincide with the Cauchy–Born strain energy density. To maintain a notation consistent with the rest of the paper, we state all results only for 2-lattices, but stress that they can be immediately extended to general multi-lattices composed of more than two Bravais lattices.

Suppose we are again given 1-periodic deformation and shift fields (Y, P). Let $\big(Y^N, P^N\big)$ and $y^N = \big(y_0^N, y_1^N\big)$ be defined as in the classical Cauchy–Born setting in (11).

To exploit the symmetry $\sim$ defined in (28), we define a different multi-lattice directional derivative. If, for the moment, we interpret y^N as a continuum field, then we may define

$$\nabla_{\boldsymbol{\rho}} y^N := \tfrac{1}{2}\nabla_\rho y_\alpha^N + \tfrac{1}{2}\nabla_\rho y_\beta^N + (y_\beta^N - y_\alpha^N).$$

We observe that $\nabla_{\sim\boldsymbol{\rho}} = -\nabla_{\boldsymbol{\rho}}$ for this definition. Written in terms of (Y^N, P^N), $\nabla_{\boldsymbol{\rho}}$ becomes

$$\nabla_{\boldsymbol{\rho}}(Y^N, P^N) := \nabla_\rho Y^N + (\beta - \alpha)P^N + \tfrac{\alpha+\beta}{2}\nabla_\rho P^N. \tag{38}$$

Note that, in contrast to the previous multi-lattice directional derivative (8), this is not a scale-invariant field. Indeed, defining, $\varepsilon := 1/N$ and rewriting the directional derivative in terms of (Y, P), we arrive at

$$\nabla^\varepsilon_{\boldsymbol{\rho}}(Y, P) := \nabla_{\boldsymbol{\rho}}\big(Y^N, P^N\big) = \nabla_\rho Y + (\beta - \alpha)P + \tfrac{\alpha+\beta}{2}\varepsilon\nabla_\rho P,$$

which gives rise to the new stored energy density

$$W_\varepsilon(\nabla Y, P) := V\big(\nabla^\varepsilon_{\mathcal{R}}(Y, P)\big).$$

Remark 6.1. The fact that W_ε employs shift gradients but not strain gradients makes the resulting model straightforward to implement using C^0-conforming discretizations. By contrast, the higher-order models derived, e.g., in [1] require also higher-order conforming discretizations.

The symmetry $\nabla_{\sim\boldsymbol{\rho}} = -\nabla_{\boldsymbol{\rho}}$ was the first key ingredient in the proof of of second order consistency of the single-species 2-lattice strain energy density. We now generalize the second key ingredient, the symmetry of partial derivatives of V.

Lemma 6.1. *Suppose that V is point symmetric* (29) *with respect to the permutation operator $\sim$. Let $\nabla_{\boldsymbol{\rho}}$ be defined by* (8)*, and let $V_{\boldsymbol{\rho}}(\boldsymbol{g}) := \frac{\partial}{\partial g_{\boldsymbol{\rho}}} V(\boldsymbol{g})$. Then, for any deformation and shift fields Y and P, we have*

$$V_{\boldsymbol{\rho}}\big(\nabla_{\mathcal{R}}(Y^N, P^N)(x)\big) = -V_{\sim\boldsymbol{\rho}}\big(\nabla_{\mathcal{R}}(Y^N, P^N)(x)\big). \tag{39}$$

Proof. The proof closely follows the proof of Lemma 5.1. □

Theorem 6.1 (Second order convergence for 2-lattices)**.** *Let $Y \in C^3(\mathbb{R}^d;\mathbb{R}^d)$ be a 1-periodic deformation field and $P \in C^2(\mathbb{R}^d;\mathbb{R}^d)$ a 1-periodic shift field. Let y^N be the scaled atomistic configuration defined by* (11)*; then*

$$N^{-d}\left|\mathscr{E}^{\mathrm{a}}\big(y^N\big) - \mathscr{E}^{\mathrm{c}}\big(Y^N,P^N\big)\right| \leq CN^{-2}\big\{\,\|\nabla^3 Y\|_\infty + \|\nabla^3 P\|_\infty + \|\nabla^2 P\|_\infty + \|\nabla^2 Y\|_\infty^2 + \|\nabla P\|_\infty^2\big\}.$$

where the constant C is a function of $\mathcal{R}$ and $\|V\|_{C^2}$.

Proof. The proof of the result is the same as the proof of Theorem 5.1 up to (33), except that we need $P \in C^3$ for the quadrature estimate, since ∇P now enters the definition of the multi-lattice directional derivative. A computation analogous to (34) yields

$$D_{\boldsymbol{\rho}} y^N - \nabla_{\boldsymbol{\rho}}(Y^N,P^N) = \tfrac{\beta-\alpha}{2}\nabla_\rho P^N + \tfrac{1}{2}\nabla_\rho^2 Y^N + O\big(\|\nabla^3 Y^N\|_\infty + \|\nabla^2 P^N\|_\infty\big).$$

Continuing as in the proof of Theorem 5.1, we obtain

$$V\big(D_{\mathcal{R}} y^N\big) - V\big(\nabla_{\mathcal{R}}\big(Y^N,P^N\big)\big) = \sum_{\boldsymbol{\rho}\in\mathcal{R}} V_{\boldsymbol{\rho}}\cdot e(\boldsymbol{\rho}) + O\big(\big\|\nabla^3 Y^N\big\|_\infty + \big\|\nabla^2 P^N\big\|_\infty\big), \quad (40)$$

where

$$e(\boldsymbol{\rho}) := \tfrac{\beta-\alpha}{2}\nabla_\rho P^N + \tfrac{1}{2}\nabla_\rho^2 Y^N.$$

It is straightforward to see that $e(\sim\boldsymbol{\rho}) = e(\boldsymbol{\rho})$, and hence the rest of the proof follows Theorem 5.1. □

7. Conclusion

We have identified two new second order continuum models for multi-lattices. Our approach is based on the identification of symmetries similar to the point symmetry of Bravais lattices. We then extend the standard proof of second order accuracy of the Cauchy–Born rule for Bravais lattices to derive second order models for multi-lattices.

For single-species 2-lattices, we show that the classical Cauchy–Born model is of second order in the continuum limit, *provided* that the atomistic and continuum kinematic variables are related in a new way. If the classical relationship between the variables is adopted, then the Cauchy–Born model is only first order. We also give a new stored energy density for a general multi-lattice modeled using pair interactions, and we show that this energy is second order accurate, as well.

These results are being used to develop accurate atomistic/continuum couplings. We show in [22] that the interfacial error of a coupling can be dramatically reduced when a point symmetric site energy is used, and we make similar applications of the results of this paper in [17]. We also remark that our methods achieve second order accuracy without

requiring the use of C^1-conforming elements, and so our models are easier to implement than the second order models of [1].

References

[1] M. Arndt and M. Griebel. Derivation of higher order gradient continuum models from atomistic models for crystalline solids. *Multiscale Model. Simul.*, 4(2):531–562 (electronic), 2005.

[2] M. Baskes and R. Johnson. Modified embedded atom potentials for hcp metals. *Modelling Simul. Mater. Sci. Eng.*, 2:147, 1994.

[3] T. Belytschko and S. P. Xiao. Coupling methods for continuum model with molecular model. *International Journal for Multiscale Computational Engineering*, 1:115–126, 2003.

[4] X. Blanc, C. Le Bris, and P.-L. Lions. From molecular models to continuum mechanics. *Arch. Ration. Mech. Anal.*, 164(4):341–381, 2002.

[5] M. Born and K. Huang. *Dynamical Theory of Crystal Lattices*. Oxford University Press, 1954.

[6] D. W. Brenner. Empirical potential for hydrocarbons for use in simulating the chemical vapor deposition of diamond films. *Phys. Rev. B*, 42:9458–9471, Nov 1990.

[7] M. Dobson and M. Luskin. An optimal order error analysis of the one-dimensional quasicontinuum approximation. *SIAM Journal on Numerical Analysis*, 47(4):2455–2475, 2009.

[8] W. E and P. Ming. Cauchy-Born rule and the stability of crystalline solids: static problems. *Arch. Ration. Mech. Anal.*, 183(2):241–297, 2007.

[9] V. Ghutikonda and R. Elliott. Stability and elastic properties of the stress-free B2 (CsCl-type) crystal for the morse pair potential model. *J. Elasticity*, 92:151–186, 2008.

[10] T. Hudson and C. Ortner. On the stability of bravais lattices and their cauchy–born approximations. *ESAIM:M2AN*, 46:81–110, 2012.

[11] O. Kastner and G. Ackland. Mesoscale kinetics produces martensitic microstructure. *J. Mech. Phys. Solids*, 57:109–121, 2009.

[12] P. A. Klein and J. A. Zimmerman. Coupled atomistic-continuum simulations using arbitrary overlapping domains. *J. Comput. Phys.*, 213(1):86–116, 2006.

[13] M. Luskin, C. Ortner, and B. Van Koten. Formulation and optimization of the energy-based blended quasicontinuum method. 2011. http://arxiv.org/abs/1112.2377, submitted.

[14] C. Makridakis and E. Süli. Finite element analysis of Cauchy–Born approximations to atomistic models. preprint.

[15] C. Ortner. A priori and a posteriori analysis of the quasinonlocal quasicontinuum method in 1D. *Math. Comp.*, 80(275):1265–1285, 2011.

[16] C. Ortner and F. Theil. Analysis of the Cauchy–Born approximation. *ArXiv e-prints*, arXiv:1202.3858, 2012.

[17] C. Ortner and B. Van Koten. Blended atomistic/continuum hybrid methods I: Formulation and consistency. manuscript.

[18] C. Ortner and L. Zhang. Construction and sharp consistency estimates for atomistic/continuum coupling methods with general interfaces: a 2D model problem. *ArXiv e-prints*, 1110.0168, 2011.

[19] T. Shimokawa, J. J. Mortensen, J. Schiotz, and K. W. Jacobsen. Matching conditions in the quasicontinuum method: Removal of the error introduced at the interface between the coarse-grained and fully atomistic region. *Phys. Rev. B*, 69(21):214104, 2004.

[20] E. B. Tadmor, M. Ortiz, and R. Phillips. Quasicontinuum analysis of defects in solids. *Philosophical Magazine A*, 73(6):1529–1563, 1996.
[21] J. Tersoff. New empirical approach for the structure and energy of covalent systems. *Phys. Rev. B*, 37:6991–7000, 1988.
[22] B. Van Koten and M. Luskin. Analysis of energy-based blended quasi-continuum approximations. *SIAM Journal on Numerical Analysis*, 49(5):2182–2209, 2011.

B. Van Koten, 127 Vincent Hall, 206 Church St. SE, Minneapolis, MN 55455, USA
E-mail address: vankoten@math.umn.edu

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