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ON THE DERIVATION OF LINEAR ELASTICITY FROM ATOMISTIC MODELS

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Abstract. We derive linear elastic energy functionals from atomistic models as a Γ-limit when the number of atoms tends to infinity, respectively, when the interatomic distances tend to zero. Our approach generalizes a recent result of Braides, Solci and Vitali [2]. In particular, we study mass spring models with full nearest and next-to-nearest pair interactions. We also consider boundary value problems where a part of the boundary is free.

1. **Introduction.** The passage from discrete atomic models to continuum theories is an active area of current research in continuum mechanics. For elastic systems one usually refers to the Cauchy-Born rule to obtain macroscopic energy densities from atomistic interaction functionals. The Cauchy-Born rule states that – roughly speaking – each individual atom follows the macroscopic deformation gradient and in particular does not take into account fine scale oscillations on the microscopic scale.

For a two-dimensional mass spring model, the validity of the Cauchy-Born rule for deformations close to a rigid motion has been proved by Friesecke and Theil in [8]. Their result has been generalized to arbitrary dimensions by Conti, Dolzmann, Kirchheim and Müller in [3].

If the deformation gradients are very close to $SO(d)$, the set of orientation preserving rigid motions, then we expect linear elasticity theory to apply. This relation has been made rigorous by Dal Maso, Negri and Percivale who derive the energy functional of linear elasticity as a Γ-limit of nonlinear elasticity for small displacements in [5]. (See also the author's article [10] for a strong convergence result for the associated minimum problems.)

Recently it has been noted that one can derive linear elasticity functionals directly from certain atomistic pair potentials: For a special class of pair interaction models Braides, Solci and Vitali prove Γ-convergence of the discrete energy functionals to the energy functional of an associated continuum linear elasticity energy functional (see [2]). In this set-up one has to deal with two small parameters ε and δ measuring the typical interatomic distance and the local distance of the deformations from the set of rigid motions, respectively.

The aim of the present article is to extend these results in three directions. Firstly, we will drop the assumption that atoms are allowed to interact only along

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special edges of a simplicial decomposition of the lattice unit cell (thus answering positively an open problem posed in [2]). In particular, our approach will allow us to deal with full next-to-nearest neighbor interactions in mass spring models. (In a 2D square lattice, e.g., the contributions of both diagonal springs can be considered.)

Secondly, by considering more general 'cell energies', it will be possible to also deal with mass spring systems for which individual pair interactions might not be equilibrated in the reference lattice. In this regime it turns out that one has to carefully choose the two small parameters in the Γ-limit process to obtain the desired result: We will assume that $\varepsilon \ll \delta^2$. This seems to be a reasonable assumption from a physical point of view as ε refers to the ratio of microscopic to macroscopic length scales, while δ is a small macroscopic parameter describing the range of applicability of linear elasticity theory. Note that this would always be satisfied if one first applies the Cauchy-Born rule, i.e., sends $\varepsilon \to 0$ and then derives the linear limit $\delta \to 0$. Technically this condition ensures that even for mismatching equilibria of surface and bulk energy contributions, the surface terms cannot dominate the bulk terms.

Finally we will also consider more general non-affine boundary conditions and in particular also investigate the case when a part of the boundary is free. For the sequence of minimizers of the associated boundary value problem we also prove a strong convergence result to the minimizer of the limiting continuum functional. (If Dirichlet boundary conditions are imposed on every surface atom, by a suitable renormalization of the elastic energy, one can in fact drop the assumption $\varepsilon \ll \delta^2$ even for incompatible surface and bulk energy expressions.)

To be more specific, we consider the portion $\varepsilon\mathcal{L} \cap \Omega$ of some scaled Bravais lattice $\mathcal{L}$ that lies in some fixed domain $\Omega \subset \mathbb{R}^d$. If $E_\varepsilon(y)$ denotes the elastic energy of a deformation $y : \varepsilon\mathcal{L} \cap \Omega \to \mathbb{R}^d$, our main modeling assumption is that, roughly speaking, E_ε be decomposable as a sum of the form

$$E_\varepsilon(y) = \sum_Q W_{\mathrm{cell}}(\bar{\nabla} y_{|Q}) + \text{ surface terms},$$

where the sum runs over scaled unit cells $Q \subset \Omega$ induced by $\varepsilon\mathcal{L}$ and the discrete gradient $\bar{\nabla} y_{|Q}$ consists of all the relative displacements of the corners of Q. Here W_{cell} is of order one (in atomic units) and so we have to consider the scaled quantity $\varepsilon^d E_\varepsilon(y)$ so as to arrive at macroscopic energy expressions for small interatomic distances ε.

For mass spring systems for which not every individual spring is minimal in the reference configuration, W_{cell} typically assumes a positive mininmum value μ; and one has to renormalize by subtracting a term $\mu|\Omega|$ in the energy functional in order to ensure $W_{\mathrm{cell}} = 0$ at the identity. Note, however, that the surface terms, which are also decomposable into unit cell contributions, will in general not be equilibrated at the identity. As the number of surface atoms scales with $\sim \varepsilon^{1-d}$, our energy functional becomes

$$\varepsilon^d E_\varepsilon(y) = \varepsilon^d \sum_Q W_{\mathrm{cell}}(\bar{\nabla} y_{|Q}) + O(\varepsilon).$$

In order to derive the functional of linear elasticity theory, we consider deformations $y = \mathrm{Id} + \delta u$ in terms of the small displacement δu and multiply the energy by δ^{-2}. This way, we finally are led to investigate the functional

$$\delta^{-2}\varepsilon^d E_\varepsilon(\mathrm{Id} + \delta u) = \delta^{-2}\varepsilon^d \sum_Q W_{\mathrm{cell}}(\bar{\nabla}(\mathrm{Id} + \delta u)_{|Q}) + O(\delta^{-2}\varepsilon).$$

This formula also illustrates why the assumption $\varepsilon \ll \delta^2$ will be of importance.

Rigidity estimates will now guarantee that in the limit $\varepsilon, \delta \to 0$:

1. Manifestation of the Cauchy-Born rule: The discrete gradient of the atomic displacements reduce to classical gradients, i.e., the microscopic deformation gradient follows the macroscopic deformation gradient.
2. Linearization of the energy functional: W_{cell} reduces to its Hessian Q_{cell} at the identity.
3. Passage from discrete to continuum theory: The discrete energy functional converges to an integral functional.

As a consequence, the discrete energy functionals will be seen to Γ-converge to the common energy functional of linear elasticity, which is derived from W_{cell} by the Cauchy-Bern rule.

The paper is organized as follows. In Section 2 we introduce the atomistic models and state the main results on their discrete-to-continuum convergence properties: Theorem 2.6 states compactness of finite energy sequences and the Γ-convergence to a corresponding continuum limit as an integral functional over a suitable quadratic form of the limiting linear strain. In Theorem 2.7 we prove strong convergence of minimizers of the discrete problems to the minimizer of the continuum theory.

The following Section 3 is devoted to technical preliminaries for the proofs of these results. The main tool is a careful interpolation in between the atomic positions, which will enable us to make use of the corresponding continuum results. By our general interaction assumptions, however, there is no associated triangulation of the body where the energy can be recovered from an energy density defined on the $d \times d$ gradients of some linear interpolation. Instead, we will have to consider discrete gradients, i.e., $d \times 2^d$ matrices that will account for all relative displacements in a typical lattice cell. The ideas in this section are inspired by [9]. As in this paper (also compare [11] for the 2D case), an important ingredient for our compactness results is (a discrete version of) the geometric rigidity result of Friesecke James and Müller, cf. [6]. However, near the free part of the boundary, discrete rigidity may fail. Our main focus in Section 3 will be on how to overcome this difficulty. As a by-product, we state a slightly generalized version of the discrete geometric rigidity result of [9], which allows for a more general shape of the macroscopic region occupied by the atoms.

In Section 4 we will then give the proofs of Theorems 2.6 and 2.7. The scheme to arrive at a linearized limiting functional follows [5, 10] and also draws ideas from [6]. In fact, the strategy of our proofs is to reduce the problem to the continuum setting investigated in [5, 10], and we refer the reader to these papers rather than re-deriving the results that are needed here. However, as mentioned above and also noticed in [2], the discrete nature of the atomistic interaction raises additional difficulties for the simultaneous linearization/discrete-to-continuum limiting process. We exploit techniques developed in [3, 9, 11] to overcome these problems.

In the last Section 5 we will give some examples of mass spring models as admissible atomistic interaction functionals and their limiting continuum linear energy functionals. In particular, we will discuss the nearest neighbor interaction in a triangular lattice (recovering the functional derived in [2]) and the nearest and next-to-nearest neighbor interaction in a square lattice in 2D. In 3D we will first discuss a general nearest and next-to-nearest neighbor model. By way of example of

an equilibrated bcc crystal, we will then also show how our technique can yield continuum theories rigorously even if the basic assumption on the interactions, namely, to be decomposable into individual lattice cell contributions, fails.

2. **The model and main results.** Let $\Omega \subset \mathbb{R}^d$ be a bounded Lipschitz domain and $\mathcal{L}$ some Bravais-lattice in $\mathbb{R}^d$, i.e.,

$$\mathcal{L} = \{\lambda_1 v_1 + \ldots + \lambda_d v_d : \lambda_1, \ldots, \lambda_d \in \mathbb{Z}\} = A\mathbb{Z}^d$$

for linearly independent vectors $v_1, \ldots, v_d \in \mathbb{R}^d$, where A is the matrix $(v_1, \ldots, v_d)$. For notational convenience we will suppose that the v_i are labeled such that $\det A > 0$. We assume that the atomic positions in the reference configuration are given by the points of the scaled lattice $\mathcal{L}_\varepsilon = \varepsilon\mathcal{L}$ that lie within Ω. Here ε is a small parameter measuring the interatomic distance and eventually tending to 0. Note that $\mathcal{L}_\varepsilon$ partitions $\mathbb{R}^d$ into 'unit cells' $\varepsilon A(\lambda + [0,1)^d)$, $\lambda \in \mathbb{Z}^d$.

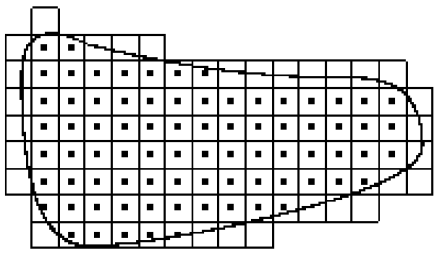

FIGURE 1. Reference configuration of an atomic system.

We denote the shifted lattice $\varepsilon A((\frac{1}{2}, \ldots, \frac{1}{2})^T + \mathbb{Z}^d)$ consisting of the midpoints of the unit cells by $\mathcal{L}'_\varepsilon$. Accordingly, if $x \in \mathbb{R}^d$ we denote by $\bar{x} = \bar{x}(x, \varepsilon)$ the element of $\mathcal{L}'_\varepsilon$ lying in the same unit cell as x. The ε-cell corresponding to x is defined by $Q_\varepsilon(x) = \bar{x} + A[-\frac{\varepsilon}{2}, \frac{\varepsilon}{2})^d$. A corner of $Q_\varepsilon(x)$ is an element of $\bar{x} + A\{-\frac{\varepsilon}{2}, \frac{\varepsilon}{2}\}^d$.

The deformations of our system are mappings $y : \Omega \cap \mathcal{L}_\varepsilon \to \mathbb{R}^d$. In order to keep track of the images of atoms under such deformations we choose a numbering $z_1, \ldots, z_{2^d}$ of the corners $A\{-\frac{1}{2}, \frac{1}{2}\}^d$ of the reference cell $A[-\frac{1}{2}, \frac{1}{2})^d$ and view

$$\begin{aligned} Y(x) &= (y_1, \ldots, y_{2^d}) = (y(\bar{x} + \varepsilon z_1), \ldots, y(\bar{x} + \varepsilon z_{2^d})) \quad \text{and} \\ Z &= (z_1, \ldots, z_{2^d}) \end{aligned} \tag{1}$$

as elements of $\mathbb{R}^{d \times 2^d}$. Let

$$\mathcal{L}'_\varepsilon(\Omega) = \{\bar{x} \in \mathcal{L}'_\varepsilon : Q_\varepsilon(\bar{x}) \cap \Omega \neq \emptyset\}, \qquad \mathcal{L}_\varepsilon(\Omega) = \mathcal{L}'_\varepsilon(\Omega) + \varepsilon\{z_1, \ldots, z_{2^d}\}.$$

Whenever convenient we will extend the deformations $y : \mathcal{L}_\varepsilon \cap \Omega \to \mathbb{R}^d$ to a function on $\mathcal{L}_\varepsilon(\Omega)$. (The energy functional will of course not be affected by this extension. For the precise definition of the values on the additional sites we refer to the next section.)

Our basic assumption is that the energy of a deformation y can be expressed by cell energies $W_\varepsilon : \mathcal{L}'_\varepsilon(\Omega) \times \mathbb{R}^{d \times 2^d} \to [0, \infty]$ in the form

$$E_\varepsilon(y) = \sum_{\bar{x} \in \mathcal{L}'_\varepsilon(\Omega)} W_\varepsilon(\bar{x}, Y(\bar{x})), \tag{2}$$

where $W_\varepsilon(\bar{x}, \cdot)$ splits into a bulk and a surface part

$$W_\varepsilon(\bar{x}, F) = \begin{cases} W_{\text{cell}}(\varepsilon^{-1}F), & \text{if } \mathcal{I}_\varepsilon(\bar{x}) = \{1, \dots, 2^d\}, \\ W_{\text{surface}}(\mathcal{I}_\varepsilon(\bar{x}), \varepsilon^{-1}F), & \text{if } \mathcal{I}_\varepsilon(\bar{x}) \neq \{1, \dots, 2^d\}, \end{cases} \tag{3}$$

where $\mathcal{I}_\varepsilon(\bar{x}) = \{i : \bar{x} + \varepsilon z_i \in \Omega\} \subset \{1, \dots, 2^d\}$. We also assume that the surface terms only depend on the atomic positions of those atoms that lie in $\mathcal{L}_\varepsilon \cap \Omega$ in the reference configuration, i.e., $W_{\text{surface}}(\mathcal{I}, \varepsilon^{-1}Y)$ depends on the second variable only through $(y_i)_{i\in I}$. Note in particular that there are no more than 2^{2^d} different surface functions $W_{\text{surface}}(\mathcal{I}, \cdot)$. The rescaling by ε^{-1} is due to our choice of measuring the energy contributions of cell deformations in atomic units.

Remark. Note that such a decomposition of the energy is possible for suitable mass spring models; e.g., in a two-dimensional square lattice with nearest and next-to-nearest neighbor interaction one would assign half of the interaction energy of the nearest neighbor bonds to each of the two adjacent cells. Note also that even in this simple example W_{surface} and W_{cell} could have mismatching equilibria if the ratio of the preferred distance between next-to-nearest neighbors and nearest neighbors is not $\sqrt{2}$. See Section 5 for more general examples, also in 3D.

Before we describe the properties of these cell energies in more detail, we introduce the discrete gradient of a lattice deformation $y : \mathcal{L}_\varepsilon(\Omega) \to \mathbb{R}^d$: If $x \in Q_\varepsilon(\bar{x})$ with $\bar{x} \in \mathcal{L}'_\varepsilon(\Omega)$, set

$$\bar{\nabla} y(x) := \varepsilon^{-1}(y_1 - \bar{y}, \dots, y_{2^d} - \bar{y}), \qquad \bar{y} := \frac{1}{2^d}\sum_{i=1}^{2^d} y_i,$$

$y_i = y(\bar{x} + \varepsilon z_i)$, $i = 1, \dots, 2^d$. (So in particular $\bar{\nabla} y$ is a piecewise constant function on Ω with values in $\mathbb{R}^{d\times 2^d}$.) Also let

$$\bar{SO}(d) := \{\bar{R} := RZ : R \in SO(d)\} \subset \mathbb{R}^{d\times 2^d},$$

where Z is the $d \times 2^d$ matrix $(z_1, \dots, z_{2^d})$ introduced in (1).

Our general assumption on the cell energies is the following

Assumption 2.1. (i) Each of the energies $W_{\text{cell}}, W_{\text{surface}}(\mathcal{I}, \cdot) : \mathbb{R}^{d\times 2^d} \to [0, \infty]$, $\mathcal{I} \subset \{1, \dots, 2^d\}$, is invariant under translations and rotations, i.e. for $F \in \mathbb{R}^{d\times 2^d}$,

$$W_{\text{cell}}(RF + (c, \dots, c)) = W_{\text{cell}}(F),$$
$$W_{\text{surface}}(\mathcal{I}, RF + (c, \dots, c)) = W_{\text{surface}}(\mathcal{I}, F) \quad \forall \mathcal{I} \subset \{1, \dots, 2^d\}$$

for all $R \in SO(d)$, $c \in \mathbb{R}^d$.

(ii) $W_{\text{cell}}(Y)$ is minimal ($= 0$) if and only if there exists $R \in SO(d)$ and $c \in \mathbb{R}^d$ such that

$$y_i = Rz_i + c, \quad i = 1, \dots, 2^d.$$

W_{surface} is bounded in a neighborhood of $\bar{SO}(d)$.

(iii) W_{cell} is C^2 in a neighborhood of $\bar{SO}(d)$ and the Hessian $Q_{\text{cell}} = D^2 W_{\text{cell}}(Z)$ at the identity is positive definite on the orthogonal complement of the subspace spanned by infinitesimal translations $(x_1, \dots, x_{2^d}) \mapsto (c, \dots, c)$ and rotations $(x_1, \dots, x_{2^d}) \mapsto (Ax_1, \dots, Ax_{2^d})$, $A^T = -A$.

(iv) $W_{\rm cell}$ grows at infinity at least quadratically on the orthogonal complement of the subspace spanned by infinitesimal translations, i.e.

$$\liminf_{\substack{|F|\to\infty\\ F\in V}} \frac{W_{\rm cell}(F)}{|F|^2} > 0.$$

Here $V = \{F \in \mathbb{R}^{d\times 2^d} : F_1 + \ldots + F_{2^d} = 0\}$.

Note that for the quadratic form $Q_{\rm cell}$ these assumptions imply that

$$Q_{\rm cell}(v,\ldots,v) = 0 \quad \text{and} \quad Q_{\rm cell}(Az_1,\ldots,Az_{2_d}) = 0 \tag{4}$$

for all $v \in \mathbb{R}^d$ and $A \in \mathbb{R}^{d\times d}$ with $A^T = -A$.

Definition 2.2. We say that $W_{\rm surface}$ is compatible with $W_{\rm cell}$ if $W_{\rm surface}(\mathcal{I},\cdot) \le CW_{\rm cell}$ in a neighborhood of $S\bar{O}(d)$.

In order to study boundary value problems, we consider the Dirichlet boundary $\partial\Omega_*$, which is a closed subset of $\partial\Omega$ of positive $\mathcal{H}^{d-1}$-measure, and boundary data given by $g \in W^{1,\infty}(\Omega)$. The space of continuum displacements is $H^1(g,\partial\Omega_*,\Omega)$, the H^1-closure of $\{u \in W^{1,\infty}(\Omega,\mathbb{R}^d) : u(x) = g(x)\ \forall\, x \in \partial\Omega_*\}$.

The definition of the appropriate function space in the discrete setting is subtle, in particular since we do not assume that $\partial\Omega$ is smooth or that $\partial\Omega = \partial\Omega_*$. In order to avoid pathologies due to the loss of rigidity near the free boundary, one has to prescribe boundary values in a suitable ε-neighborhood of $\partial\Omega_*$ for the discrete displacements. We introduce the following notation.

Definition 2.3. (i) Fix a point $x_0 \in \Omega$ (independent of ε). Then by Ω_ε we denote the connected component of $\left(\bigcup_{\overline{Q}(\bar{x})\subset\Omega} Q_\varepsilon(\bar{x})\right)^\circ$ containing x_0.

(ii) We write $\bar{x} \in \mathcal{L}'_\varepsilon(\Omega)^\circ$ and call $Q_\varepsilon(\bar{x})$ an inner cell if $\bar{x} \in \mathcal{L}'_\varepsilon \cap \Omega_\varepsilon$. If $\bar{x} \in \partial\mathcal{L}'_\varepsilon(\Omega) := \mathcal{L}'_\varepsilon(\Omega) \setminus \mathcal{L}'_\varepsilon(\Omega)^\circ$, then $Q_\varepsilon(\bar{x})$ is called a boundary cell. The set of the corners of all boundary cells, respectively inner cells, is denoted $\partial\mathcal{L}_\varepsilon(\Omega)$, respectively $\mathcal{L}_\varepsilon(\Omega)^\circ$.

Note that as $\varepsilon \to 0$, Ω_ε does not depend on the particular choice of x_0. For sufficiently small ε, Ω_ε is the connected component of $\left(\bigcup_{\overline{Q}(\bar{x})\subset\Omega} Q_\varepsilon(\bar{x})\right)^\circ$ which contains the bulk part of the inner cells. Also note that since Ω is a Lipschitz domain, there exists a constant $C = C(\Omega)$ such that $\sup\{\operatorname{dist}(x,\Omega_\varepsilon) : x \in \Omega\} < C\varepsilon$.

For two points $\bar{x},\bar{x}' \in \mathcal{L}'_\varepsilon(\Omega)$ we denote their lattice geodesic distance, i.e., the length of the shortest polygonal path $(\bar{x} = \bar{x}_0, \bar{x}_1, \ldots, \bar{x}_n = \bar{x}')$ with $\bar{x}_i \in \mathcal{L}'_\varepsilon(\Omega)$ and $\bar{x}_{i+1} - \bar{x}_i \in \{\pm v_1,\ldots,\pm v_d\}$ connecting $\bar{x}$ and $\bar{x}'$ by $\operatorname{dist}_{\mathcal{L}'_\varepsilon(\Omega)}(\bar{x},\bar{x}')$. (Also because Ω is a Lipschitz domain, $\operatorname{dist}_{\mathcal{L}'_\varepsilon(\Omega)}(\bar{x},\bar{x}') \le C|\bar{x}-\bar{x}'|$.)

By extension we may furthermore assume that $g \in W^{1,\infty}(\mathbb{R}^d,\mathbb{R}^d)$.

Definition 2.4. (i) A boundary cell $Q = Q_\varepsilon(\bar{x})$, $\bar{x} \in \partial\mathcal{L}'_\varepsilon(\Omega)$, is called a Dirichlet boundary cell ($\bar{x} \in \partial\mathcal{L}'_\varepsilon(\Omega)_*$) if there exists a cell $Q' = Q_\varepsilon(\bar{x}')$, $\bar{x}' \in \partial\mathcal{L}'_\varepsilon(\Omega)$ such that $\overline{Q'} \cap \partial\Omega_* \neq \emptyset$ and $\operatorname{dist}_{\mathcal{L}'_\varepsilon(\Omega)}(Q,Q') \le \operatorname{dist}_{\mathcal{L}'_\varepsilon(\Omega)}(Q',\Omega_\varepsilon)$. The set of corners of these cells is denoted $\partial\mathcal{L}_\varepsilon(\Omega)_*$.

(ii) Now suppose $u : \mathcal{L}_\varepsilon(\Omega) \to \mathbb{R}^d$ is a lattice mapping. We say that $u \in \mathcal{A}_\varepsilon(g,\partial\Omega_*,\Omega)$, if $u(x) = g(x)$ for every $x \in \partial\mathcal{L}_\varepsilon(\Omega)_*$.

Remark. This definition of $\mathcal{A}_\varepsilon$ guarantees that even under very weak assumptions on the surface energy $W_{\rm surface}$, the bulk part of the body 'feels' the boundary condition g. Under additional assumptions either on the geometry of Ω (asking, e.g., $\partial\Omega$

to be C^1) or on the rigidity properties of W_{surface} (e.g., imposing suitable growth conditions), the notion $u \in \mathcal{A}_\varepsilon$ can be relaxed in the sense that only those boundary cells that actually contain a piece of $\partial\Omega_*$ are defined to be Dirichlet boundary cells.

Finally we have to make precise in which sense discrete lattice mappings are understood to converge to continuum deformations. To this end, for $f \in L^2(\mathbb{R}^d, \mathbb{R}^m)$ define $P_\varepsilon f \in L^2$ by

$$P_\varepsilon f(x) := \fint_{Q_\varepsilon(x)} f(\xi)\, d\xi, \tag{5}$$

where $Q_\varepsilon(x)$ is the lattice cell containing x. It is not hard to see that $P_\varepsilon f \to f$ in L^2 as $\varepsilon \to 0$. Now if $f \in L^2(\Omega, \mathbb{R}^m)$, then we first extend f to a function in $L^2(\mathbb{R}^d, \mathbb{R}^m)$, again denoted f, and define $P_\varepsilon f$ as before.

Definition 2.5. Let $\varepsilon_k \to 0$ and suppose $y_k : \Omega \cap \mathcal{L}_{\varepsilon_k} \to \mathbb{R}^d$, $y \in L^2(\Omega, \mathbb{R}^d)$. We say that y_k converges to y, i.e., $y_k \to y$, if

$$\varepsilon_k^d \sum_{x \in \Omega \cap \mathcal{L}_{\varepsilon_k}} |y_k(x) - P_{\varepsilon_k} y(x)|^2 \to 0.$$

Note that this definition does not depend on the particular extension that has been chosen for y. We also remark that our notion of convergence is equivalent to asking that suitable interpolations (e.g., piecewise constant or piecewise affine on a triangulation subordinate to the lattice) of y_k converge to y in $L^2(\Omega, \mathbb{R}^d)$.

We will derive linear elasticity functionals by studying the functionals

$$\begin{aligned} I_{\varepsilon,\delta} &: \mathcal{A}_\varepsilon(g, \partial\Omega_*, \Omega) \to \mathbb{R}, \\ &u \mapsto \delta^{-2}\varepsilon^d E_\varepsilon(\mathrm{Id} + \delta u) = \delta^{-2}\varepsilon^d \sum_{\bar{x} \in \mathcal{L}'_\varepsilon(\Omega)} W_\varepsilon(\bar{x}, \varepsilon(Z + \delta \bar{\nabla} u(\bar{x}))) \end{aligned}$$

for lattice displacements $u : \mathcal{L}_\varepsilon(\Omega) \to \mathbb{R}^d$. The main results of this paper are the following:

Theorem 2.6. *Suppose W_{cell} and W_{surface} satisfy Assumption 2.1 and ε_k, δ_k are sequences converging to 0 as $k \to \infty$. In case W_{cell} and W_{surface} are not compatible, assume that also $\lim_{k\to\infty} \varepsilon_k \delta_k^{-2} = 0$. Set $I_k = I_{\varepsilon_k, \delta_k}$.*

Compactness: If $I_k(u_k)$ is equibounded for a sequence (u_k) of lattice displacements, then there exist modifications $u'_k \in \mathcal{A}_{\varepsilon_k}(g, \partial\Omega_*, \Omega)$ with $u'_k = u_k$ on $\mathcal{L}_{\varepsilon_k}(\Omega)^\circ \cup \partial\mathcal{L}_{\varepsilon_k}(\Omega)_*$ such that for a subsequence (not relabeled) $u'_k \to u$ for some $u \in H^1(g, \partial\Omega_*, \Omega)$. Moreover, the (piecewise constant) discrete gradients $\bar{\nabla} u'_k$ converge to $\nabla u \cdot Z$ weakly in $L^2(\Omega)$ and thus $\bar{\nabla} u_k \rightharpoonup \nabla u \cdot Z$ in $L^2_{\text{loc}}(\overline{\Omega} \setminus \overline{\partial\Omega \setminus \partial\Omega_*})$.

Γ-convergence: The functionals I_k Γ-converge to the functional

$$I : H^1(g, \partial\Omega_*, \Omega) \to \mathbb{R}, \quad u \mapsto \frac{1}{2 \det A} \int_\Omega Q_{\text{cell}}(e(u) \cdot Z).$$

(Here $e(u)$ denotes the linear strain $e(u) = \frac{1}{2}((\nabla u)^T + \nabla u)$.) I.e.,

(i) Γ-lim inf inequality: All sequences (u_k), $u_k \in \mathcal{A}_{\varepsilon_k}(g, \partial\Omega_*, \Omega)$, converging to some $u \in H^1(g, \partial\Omega_*, \Omega)$ satisfy the estimate

$$\liminf_{k\to\infty} I_k(u_k) \geq I(u).$$

In fact, this is true under the weaker assumption

$$\varepsilon_k^d \sum_{x\in\mathcal{L}_{\varepsilon_k}(\Omega)^\circ\cup\partial\mathcal{L}_{\varepsilon_k}(\Omega)_*} |u_k(x)-P_{\varepsilon_k}u(x)|^2\to 0.$$

(ii) Existence of recovery sequences: For every $u\in H^1(g,\partial\Omega_*,\Omega)$ there is a sequence (u_k), $u_k\in\mathcal{A}_{\varepsilon_k}(g,\partial\Omega_*,\Omega)$, such that $u_k\to u$ and

$$\lim_{k\to\infty} I_k(u_k)=I(u).$$

By general arguments in the theory of Γ-convergence and the fact that the minimizer of the limiting problem is unique (by Korn's inequality), one can now deduce that, if w_k is a minimizer of I_k, then $w_k'\to w$ (and so '$w_k\to w$ away from the free boundary') and $\bar\nabla w_k\rightharpoonup\nabla w\cdot Z$ weakly in $L^2_{\mathrm{loc}}(\overline{\Omega\setminus\overline{\partial\Omega\setminus\partial\Omega_*}})$, where w is the minimizer of I. In fact, following the approach in [10] we can show that recovery sequences converge even strongly:

Theorem 2.7. *Suppose (u_k) is a recovery sequence for u. Then $\bar\nabla u_k\to\nabla u\cdot Z$ strongly in $L^2_{\mathrm{loc}}(\overline{\Omega\setminus\overline{\partial\Omega\setminus\partial\Omega_*}})$.*

We call (w_k), $w_k\in\mathcal{A}_{\varepsilon_k}(g,\partial\Omega_*,\Omega)$, a sequence of almost minimizers if

$$\lim_{k\to\infty}\left(I_k(w_k)-\inf\{I_k(v):v\in\mathcal{A}_{\varepsilon_k}(g,\partial\Omega_*,\Omega)\}\right)\to 0$$

for $k\to\infty$. The previous theorem immediately implies strong convergence of w_k:

Corollary 2.8. *If (w_k) is a sequence of almost minimizers, then $\bar\nabla w_k\to\nabla w\cdot Z$ strongly in $L^2_{\mathrm{loc}}(\overline{\Omega\setminus\overline{\partial\Omega\setminus\partial\Omega_*}})$, where w is the unique minimizer of I.*

Remarks. (i) As our definition of convergence can be reformulated in terms of the usual L^2-convergence of suitable interpolations as remarked before, we are indeed proving a Γ-limit result in the usual set-up of convergence in metric spaces (see, e.g., [1, 4] for general introductions to the theory of Γ-convergence).

In the next section we will associate carefully chosen modifications u_k' (on the free part of the boundary) and interpolations $\tilde u_k$ to lattice displacements u_k. Our proofs will in particular show that one has weak H^1-compactness for the interpolations: $I_k(u_k)\le C$ implies $\tilde u_k\rightharpoonup u$ in H^1 (up to subsequences). For recovery sequences $u_k\to u$ and sequences of almost minimizers (w_k) we will see that $\tilde u_k\to u$ and $\tilde w_k\to w$ strongly in H^1.

(ii) By standard arguments in the theory of Γ-convergence it is straightforward to include loading terms of the form

$$L_\varepsilon(u)=\sum_{x\in\Omega\cap\mathcal{L}_\varepsilon} l_\varepsilon(x)\cdot u(x),$$

where $l_\varepsilon\to l$ for some $l\in L^2(\Omega)$ in the sense of Definition 2.5, e.g., $l_\varepsilon(x)=P_\varepsilon l(x)$.

(iii) In case $\partial\Omega_*=\partial\Omega$ we can renormalize the energy by setting

$$E_\varepsilon^{\mathrm{ren}}(y):=E_\varepsilon(y)-\sum_{\bar x\in\partial\mathcal{L}_\varepsilon'(\Omega)} W_\varepsilon(\bar x,Y(\bar x))=\sum_{\bar x\in\mathcal{L}_\varepsilon'(\Omega)\setminus\partial\mathcal{L}_\varepsilon'(\Omega)} W_{\mathrm{cell}}(\bar\nabla y(\bar x)).$$

Then $I_{\varepsilon,\delta}^{\mathrm{ren}}$, defined accordingly, will satisfy all the assertions in Theorems 2.6, 2.7 and Corollary 2.8 with limiting functional I, even if W_{surface} is not admissible in the sense of Assumption 2.1.

(iv) Note that indeed $F \mapsto \frac{1}{2\det A} Q_{\mathrm{cell}}(F \cdot Z)$ is the quadratic form of the energy per unit volume of linear elasticity obtained from the atomistic model by applying the Cauchy-Born rule. Here, the Cauchy-Born rule does not enter as an assumption but rather is a consequence of our analysis: For a given linear macroscopic deformation gradient F, the discrete gradient of a typical unit cell is the discrete gradient $F \cdot Z$ induced by F.

3. **Discrete deformations.** In the following paragraphs we introduce the main technical tools for passing from discrete lattice deformations to continuum objects which are more amenable to the analytical limiting process in the proofs of Section 4. Recall Definitions 2.3 and 2.4. In the following we will call two cells Q and Q' neighbors if $\overline{Q} \cap \overline{Q'} \neq \emptyset$. The $d \times 2^d$ matrix assumed by the discrete gradient $\bar{\nabla} y$ on some cell Q will be denoted $\bar{\nabla} y_{|Q}$.

3.1. **Modification.** To every lattice displacement $u \in \mathcal{A}_\varepsilon$ (resp., deformation $y = \mathrm{Id} + \delta u$) we associate a modified displacement u' (resp. deformation y') in the following way. On Dirichlet boundary cells and inner cells in the bulk nothing changes, i.e.,

$$y'(x) = y(x) \text{ for } x \in (\mathcal{L}_\varepsilon(\Omega) \cap \overline{\Omega_\varepsilon}) \cup \partial\mathcal{L}_\varepsilon(\Omega)_*;$$

in particular, $u(x) = g(x)$ for $x \in \partial\mathcal{L}_\varepsilon(\Omega)_*$. On the remaining boundary cells we proceed as follows: Consider the 2^d sublattices $\mathcal{L}'_{\varepsilon,i}$ with $\mathcal{L}'_{\varepsilon,i} = z_i + 2\mathcal{L}_\varepsilon$ and extend successively in the following Steps 1.1+, 1.1-, 1.2+, 1.2-, ..., 1.d+, 1.d-, 2.1+, 2.1-, 2.2+, ..., 2.d-, 3.1+, ..., where

> Step i.j± : For every cell $Q = Q_\varepsilon(\bar{x})$ with $\bar{x} \in \mathcal{L}'_{\varepsilon,i}$ such that there exists a cell $Q' = Q_\varepsilon(\bar{x} \pm \varepsilon v_j)$, i.e. sharing a $(d-1)$-face with Q, on the corners of which y' has been defined already, we extend y' to all corners of Q by choosing an extension y' such that $\mathrm{dist}^2(\bar{\nabla} y'_{|Q}, \bar{SO}(d))$ is minimal.

Since Ω is assumed to have a Lipschitz boundary, the number of iterations needed to define y' on all boundary cells is bounded independently of ε.

If y' is being extended to the corners of Q in some step as described above, let $\mathcal{Q}_Q$ be the set of cells on every corner of which y' has already been defined in a previous step. Note that $\left(\bigcup_{Q' \in \mathcal{Q}_Q} Q'\right)^\circ$ is connected by Definition 2.4. Since Ω has a Lipschitz boundary, we can choose a subset $\mathcal{B}_Q$ of $\mathcal{Q}_Q$ containing all neighbors of Q that lie in $\mathcal{Q}_Q$ in such a way that $\left(\bigcup_{Q' \in \mathcal{B}_Q} Q'\right)^\circ$ is connected and such that $\#\mathcal{B}_Q$ is bounded independently of Q and ε (see Figure 2).

The advantage of this particular modification scheme is that the rigidity of the modified deformations on non-Dirichlet boundary cells is controlled by the behavior in the bulk and on the Dirichlet boundary cells.

Lemma 3.1. *Suppose y' is defined on a boundary cell $Q = Q_\varepsilon(\bar{x})$, $\bar{x} \in \partial\mathcal{L}'_\varepsilon(\Omega) \setminus \partial\mathcal{L}'_\varepsilon(\Omega)_*$ as described above. Then there is a constant C such that*

$$\mathrm{dist}^2(\bar{\nabla} y'_{|Q}, \bar{SO}(d)) \leq C \sum_{Q' \in \mathcal{B}_Q} \mathrm{dist}^2(\bar{\nabla} y'_{|Q'}, \bar{SO}(d)).$$

We defer the proof of this lemma, which is based on a discrete geometric rigidity estimate, to the end of this section. As a consequence we note the following estimate.

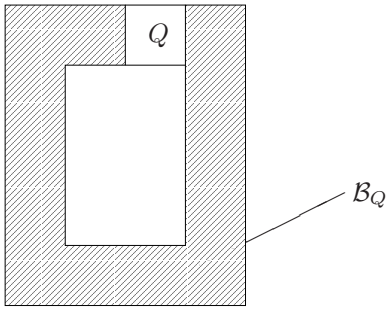

FIGURE 2. $\mathcal{B}_Q$ (shaded) and Q.

Lemma 3.2. *There exist constants $c, C > 0$ (independent of ε and y) such that, setting $V_\varepsilon := \{x \in \Omega : \operatorname{dist}(x, \partial\Omega) \geq c\varepsilon\}$, the estimate*

$$\sum_{\bar{x} \in \partial\mathcal{L}'_\varepsilon(\Omega) \setminus \partial\mathcal{L}'_\varepsilon(\Omega)_*} \operatorname{dist}^2(\bar{\nabla} y'(\bar{x}), S\bar{O}(d)) \leq C \sum_{\bar{x} \in \mathcal{B}_\varepsilon} \operatorname{dist}^2(\bar{\nabla} y'(\bar{x}, S\bar{O}(d)),$$

where $\mathcal{B}_\varepsilon = \{\bar{x} \in \mathcal{L}'_\varepsilon(\Omega)^\circ \cup \partial\mathcal{L}'_\varepsilon(\Omega) : \bar{x} \notin V_\varepsilon\}$, is satisfied.

Proof. This follows directly from Lemma 3.1 by induction on the extension steps. □

The versions of Lemma 3.1 and Lemma 3.2 for displacements $u(x) = \delta^{-1}(y(x) - x)$ read as follows. (Also the proof of Lemma 3.3 will be given at the end of this section.)

Lemma 3.3. *Suppose u is the extension on a non-Dirichlet boundary cell $Q = Q_\varepsilon(\bar{x})$ as described above. Then there is a constant C such that*

$$|\bar{\nabla} u'_{|Q}|^2 \leq C \sum_{Q' \in \mathcal{B}_Q} |\bar{\nabla} u'_{|Q'}|^2.$$

Lemma 3.4. *There exist constants $c, C > 0$ (independent of ε, δ and u) such that, setting $V_\varepsilon := \{x \in \Omega : \operatorname{dist}(x, \partial\Omega) \geq c\varepsilon\}$, the estimate*

$$\sum_{\bar{x} \in \partial\mathcal{L}'_\varepsilon(\Omega) \setminus \partial\mathcal{L}'_\varepsilon(\Omega)_*} |\bar{\nabla} u'(\bar{x})|^2 \leq C \sum_{\bar{x} \in \mathcal{B}_\varepsilon} |\bar{\nabla} u'(\bar{x})|^2,$$

where $\mathcal{B}_\varepsilon = \{\bar{x} \in \mathcal{L}'_\varepsilon(\Omega)^\circ \cup \partial\mathcal{L}'_\varepsilon(\Omega) : \bar{x} \notin V_\varepsilon\}$, is satisfied for all for $u \in \mathcal{A}_\varepsilon(g, \partial\Omega_*, \Omega)$.

Proof. This follows directly from Lemma 3.3 by induction on the extension steps. □

3.2. **Interpolation.** In the sequel it will be convenient to choose a particular interpolation $\tilde{y}$ for a lattice deformation y'. We first explain the procedure on a single cell with $\varepsilon = 1$ and $y' = y$. Let

$$y : A\left\{-\frac{1}{2}, \frac{1}{2}\right\}^d = \{z_i : i \in \{1, \dots, 2^d\}\} \to \mathbb{R}^d, \quad \overline{Q} = A\left[-\frac{1}{2}, \frac{1}{2}\right]^d.$$

First interpolate linearly on one-dimensional faces of $\overline{Q}$, i.e., on those segments $[z_i, z_j]$ with $z_i - z_j$ parallel to one of the vectors v_n spanning the lattice. Then

define a triangulation and interpolation on all two-dimensional faces of Q in the following way: If the face is

$$\operatorname{co}\{z_{i_1},\dots,z_{i_4}\},\quad z_{i_2}=z_{i_1}+v_n,\ z_{i_3}=z_{i_1}+v_n+v_m,\ z_{i_4}=z_{i_1}+v_m,$$

then set $\zeta=\frac{1}{4}(z_{i_1}+\ldots+z_{i_4})$, $y(\zeta)=\frac{1}{4}(y(z_{i_1})+\ldots+y(z_{i_4}))$ and interpolate linearly on each of the triangles

$$\operatorname{co}\{z_{i_j},z_{i_{j+1}},\zeta\},\quad j=1,2,3,4\ (\mathrm{mod}\,4).$$

In general, assuming that we have chosen a simplicial decomposition and corresponding linear interpolation on all $(n-1)$-dimensional faces, we decompose and interpolate an n-dimensional face $F=\operatorname{co}\{z_{i_1},\dots,z_{i_{2^n}}\}$ as follows. Set

$$\zeta=\frac{1}{2^n}\sum_{j=1}^{2^n}z_{i_j},\qquad y(\zeta)=\frac{1}{2^n}\sum_{j=1}^{2^n}y(z_{i_j}).$$

Now decompose F by the simplices $\operatorname{co}\{w_1,\dots,w_n,\zeta\}$, where $\operatorname{co}\{w_1,\dots,w_n\}$ is a simplex that belongs to the decomposition of an $(n-1)$-face already constructed. On these simplices interpolate linearly.

For later reference we note that each simplex constructed in this interpolation scheme contains at least one corner z_i of Q. One of the advantages of choosing this particular interpolation is that it is not hard to see that if $\tilde{y}$ is the interpolation of y on the unit cell Q, then

$$\fint_Q\tilde{y}(x)\,dx=\frac{1}{2^d}\sum_{i=1}^{2^d}y(z_i)=\tilde{y}(0).\tag{6}$$

(By induction, $\fint_F\tilde{y}(x)\,dx=\frac{1}{2^n}\sum_{j=1}^{2^n}y(z_{i_j})$ on each n-face $F=\operatorname{co}\{z_{i_1},\dots,z_{i_{2^n}}\}$ of Q.)

Now let $u\in\mathcal{A}_\varepsilon(g,\partial\Omega_*,\Omega)$ and let u' its modification constructed in Paragraph 3.1. We interpolate u' on $\bigcup_{\bar{x}\in\mathcal{L}'_\varepsilon(\Omega)}\overline{Q_\varepsilon}(\bar{x})$ such that $\tilde{u}_{|\Omega}\in H^1(g,\partial\Omega_*,\Omega)$:

On Dirichlet boundary cells we set $\tilde{u}(x)=g(x)$. If, on the other hand, $Q_\varepsilon(x)$ is neither a neighbor of a Dirichlet boundary cell nor a Dirichlet boundary cell itself, we define $\tilde{u}(x)=\delta^{-1}(\tilde{y}(x)-x)$ on $Q_\varepsilon(x)$ by interpolating as described above (with v_n, z_i replaced by εv_n, $\bar{x}+\varepsilon z_i$, respectively).

Finally, if $Q=Q_\varepsilon(\bar{x})$ is a cell having neighbors Q'_j that are Dirichlet boundary cells, we also follow the interpolation scheme described above, but without linearly interpolating on faces of Q that are shared by some Q'_j: If $F=\bar{x}+\varepsilon\operatorname{co}\{z_{i_1},\dots,z_{i_{2^n}}\}\subset Q'_j$ for some Q'_j, let $\tilde{u}(x)=g(x)$ for $x\in F$. If $F\not\subset Q'_j$ for all Q'_j, then also $\zeta=\bar{x}+\frac{\varepsilon}{2^n}\sum_{j=1}^{2^n}z_{i_j}\notin\bigcup_j Q'_j$. In this case we define $\tilde{u}(\zeta)=\frac{1}{2^n}\sum_{j=1}^{2^n}\tilde{u}(\bar{x}+\varepsilon z_{i_j})$ as before and interpolate on the simplices $\operatorname{co}\{w_1,\dots,w_n,\zeta\}$ linearly on each segment $[\zeta,w]$, $w\in\operatorname{co}\{w_1,\dots,w_n\}$, where $\operatorname{co}\{w_1,\dots,w_n\}$ is a simplex that belongs to the decomposition of an $(n-1)$-face already constructed.

The following lemma is an easy consequence of our interpolation procedure.

Lemma 3.5. *Suppose $u'\in\mathcal{A}_\varepsilon(g,\partial\Omega_*,\Omega)$ is (the modification of) a lattice displacement interpolated as described above. There exist constants $c,C>0$ such that the following conditions are satisfied.*

(i) *If Q is not a Dirichlet boundary cell itself, nor the neighbor of any Dirichlet boundary cell, then*

$$c\left|\bar{\nabla} u'_{|Q}\right|^2 \leq \fint_Q |\nabla \tilde{u}|^2 \leq C\left|\bar{\nabla} u'_{|Q}\right|^2.$$

(ii) *If Q is not a Dirichlet boundary cell, but Q is neighboring a Dirichlet boundary cell, then*

$$c\left|\bar{\nabla} u'_{|Q}\right|^2 - C \leq \fint_Q |\nabla \tilde{u}|^2 \leq C\left|\bar{\nabla} u'_{|Q}\right|^2 + C.$$

(iii) *If Q is a Dirichlet boundary cell, then*

$$\left|\bar{\nabla} u'_{|Q}\right|^2, \fint_Q |\nabla \tilde{u}|^2 \leq C.$$

Proof. These estimates can be seen along the same lines as the estimates in the following lemma. We refer to the proof of Lemma 3.6. □

Lemma 3.6. *Suppose $u \in \mathcal{A}_\varepsilon(g, \partial\Omega_*, \Omega)$ and $y'(x) = x + \delta u'(x)$ are lattice mappings modified and interpolated as described above. There exist constants $c, C > 0$ such that the following conditions are satisfied.*

(i) *If Q is not a Dirichlet boundary cell itself, nor the neighbor of any Dirichlet boundary cell, then*

$$\begin{aligned} c\,\mathrm{dist}^2(\bar{\nabla} y'_{|Q}, \bar{SO}(d)) &\leq \fint_Q \mathrm{dist}^2(\nabla \tilde{y}, SO(d)) \\ &\leq C\,\mathrm{dist}^2(\bar{\nabla} y'_{|Q}, \bar{SO}(d)). \end{aligned}$$

(ii) *If Q is not a Dirichlet boundary cell, but Q is neighboring a Dirichlet boundary cell, then*

$$\begin{aligned} c\,\mathrm{dist}^2(\bar{\nabla} y'_{|Q}, \bar{SO}(d)) - C\delta^2 &\leq \fint_Q \mathrm{dist}^2(\nabla \tilde{y}, SO(d)) \\ &\leq C\,\mathrm{dist}^2(\bar{\nabla} y'_{|Q}, \bar{SO}(d)) + C\delta^2. \end{aligned}$$

(iii) *If Q is a Dirichlet boundary cell, then*

$$\fint_Q \mathrm{dist}^2(\nabla \tilde{y}, SO(d)) \leq C\delta^2 \quad \text{and} \quad \mathrm{dist}^2(\bar{\nabla} y'_{|Q}, \bar{SO}(d)) \leq C\delta^2.$$

Proof. (i) The first inequality is straightforward: Note that, since $\tilde{y}$ is linear on simplices whose volume is comparable to $|Q|$, we have $\|\mathrm{dist}^2(\nabla \tilde{y}, SO(d))\|_{L^\infty(Q)} \leq C \fint_Q \mathrm{dist}^2(\nabla \tilde{y}, SO(d))$.

For the proof of the second inequality assume without loss of generality $\varepsilon = 1$, $\overline{Q} = A[-\frac{1}{2}, \frac{1}{2}]^d$. Let $R \in SO(d)$ such that $\mathrm{dist}(\bar{\nabla} y', \bar{SO}(d)) = |\bar{\nabla} y' - \bar{R}|$. By induction we prove that on each n-dimensional simplex $S = \mathrm{co}\{w_1, \dots, w_n, \zeta\}$ of Q constructed in the interpolation procedure we have

$$|(\nabla \tilde{y} - R)P_S| \leq C|\bar{\nabla} y' - \bar{R}|,$$

where P_S is the projection onto the space $\mathrm{span}\{w_2 - w_1, \dots, w_n - w_1, \zeta - w_1\}$:

Note first that by the remark above equation (6), we may without loss of generality assume that $w_1 = z_i$ for some i. Let e be a unit vector in $P_S(\mathbb{R}^d)$. If $e \in \mathrm{span}\{w_2 - w_1, \dots, w_n - w_1\}$, then

$$|(\nabla \tilde{y} - R)e| \leq C|\bar{\nabla} y' - \bar{R}|$$

by assumption. Now if $e = \frac{\zeta - z_i}{|\zeta - z_i|}$, then

$$|(\nabla \tilde{y} - R)e| = \frac{|y(\zeta) - y'(z_i) - R(\zeta - z_i)|}{|\zeta - z_i|} \leq C \sup_j |y'(z_j) - Rz_j - (y'(z_i) - Rz_i)| \leq C|\bar{\nabla} y' - \bar{R}|,$$

and the induction step is proved. The claim now follows by letting $n = d$.

(ii) Suppose y^* is the function obtained by interpolating y' in Q as for cells described in (i). Since $g \in W^{1,\infty}$, it follows that $\|\nabla y^* - \nabla \tilde{y}\|_{L^\infty(Q)} \leq C\delta$. The estimates now follow from (i).

(iii) This is clear since $y'(x) = x + \delta g(x)$ on Q. □

3.3. **Discrete geometric rigidity.** An important ingredient for the derivation of linear elasticity from nonlinear energy functionals is a quantitative rigidity estimate for deformations near $SO(d)$ as given in [6], see [5]. The discrete version of this result proved in [9, Theorem 3.3] states that lattice deformations

$$y : \mathcal{L} \cap U \to \mathbb{R}^d,$$

where U is a union of closed lattice cells such that U° is connected, satisfy the following rigidity estimate (in unrescaled variables): For each y there exists $R \in SO(d)$ such that

$$\sum_{\bar{x} \in \mathcal{L}' \cap U} |\bar{\nabla} y(\bar{x}) - \bar{R}|^2 \leq C \sum_{\bar{x} \in \mathcal{L}' \cap U} \operatorname{dist}^2(\bar{\nabla} y(\bar{x}), \bar{SO}(d)), \tag{7}$$

$\bar{R} = R \cdot Z$.

For later use we record here that Assumption 2.1 implies the following estimate.

Lemma 3.7. *There is a constant C such that for all $F \in \mathbb{R}^{d \times 2^d}$*

$$\operatorname{dist}^2(F, \bar{SO}(d)) \leq C W_{\text{cell}}(F).$$

Proof. This is essentially contained in Lemma 3.2 of [9]. The arguments detailed there show that this estimate is a consequence of the growth assumptions on W_{cell} near $\bar{SO}(d)$ and ∞ imposed in Assumption 2.1. □

Proof of Lemma 3.1. By rescaling we may assume that $\varepsilon = 1$.

Let $\eta > 0$ and suppose

$$\sum_{Q' \in \mathcal{B}_Q} \operatorname{dist}^2(\bar{\nabla} y'_{|Q'}, \bar{SO}(d)) \leq \eta.$$

By the discrete geometric rigidity result (7) there is a rotation $R \in SO(d)$ such that

$$\sum_{Q' \in \mathcal{B}_Q} |\bar{\nabla} y'_{|Q'} - \bar{R}|^2 \leq C\eta.$$

But then y', restricted to $\mathcal{L}_\varepsilon \cap \overline{\mathcal{B}_Q}$, has an extension y'' to the corners of Q with $|\bar{\nabla} y''_{|Q} - \bar{R}|^2 \leq C\eta$. The claim now follows by construction of y'. □

Proof of Lemma 3.3. Let $y'(x) = x + \delta u'(x)$ and suppose $\sum_{Q' \in \mathcal{B}_Q} |\bar{\nabla} u'_{|Q'}|^2 \leq \eta\delta^{-2}$. Applying Lemma 3.1 and (7), we find a rotation R such that

$$|\bar{\nabla} y'_{|Q} - \bar{R}|^2 + \sum_{Q' \in \mathcal{B}_Q} |\bar{\nabla} y'_{|Q'} - \bar{R}|^2 \leq C\eta \tag{8}$$

holds. But by assumption we also have

$$\sum_{Q'\in\mathcal{B}_Q} |\bar\nabla y'_{|Q'} - Z|^2 = \sum_{Q'\in\mathcal{B}_Q} \delta^2 |\bar\nabla u'_{|Q'}|^2 \le C\eta,$$

whence $|R - \mathrm{Id}|^2 \le C\eta$. The claim now follows from (8). □

As a by-product we also mention the following discrete geometric rigidity result, which generalizes Theorem 3.3 in [9] in the sense that the constant C only depends on the domain Ω.

Theorem 3.8. *There exists a constant $C > 0$, independent of ε, such that for all lattice deformations $y : \mathcal{L}_\varepsilon(\Omega) \to \mathbb{R}^d$ there exists a rotation $\bar R \in \bar{SO}(d)$ such that*

$$\sum_{\bar x\in\mathcal{L}'_\varepsilon(\Omega)} |\bar\nabla y(\bar x) - \bar R|^2 \le C \sum_{\bar x\in\mathcal{L}'_\varepsilon(\Omega)} \operatorname{dist}^2(\bar\nabla y(\bar x), \bar{SO}(d)).$$

Proof. Apply the modification scheme of Paragraph 3.1 with $\partial\Omega_* = \emptyset$ and the interpolation procedure of Paragraph 3.2 to define y' and $\tilde y$. By Lemmas 3.1 and 3.6 we then have

$$\int_\Omega \operatorname{dist}^2(\nabla\tilde y(x), SO(d))\,dx \le C \sum_{\bar x\in\mathcal{L}'_\varepsilon(\Omega)^\circ} \operatorname{dist}^2(\bar\nabla y(\bar x), \bar{SO}(d)).$$

The continuum geometric rigidity result in [6] now provides a rotation $R \in SO(d)$ such that

$$\int_\Omega |\nabla\tilde y(x) - R|^2\,dx \le C \int_\Omega \operatorname{dist}^2(\nabla\tilde y(x), SO(d))\,dx$$

for a constant $C = C(\Omega)$ and from Lemma 3.5 we thus obtain

$$\sum_{\bar x\in\mathcal{L}'_\varepsilon(\Omega)^\circ} |\bar\nabla y'(\bar x) - \bar R|^2 \le C \sum_{\bar x\in\mathcal{L}'_\varepsilon(\Omega)} \operatorname{dist}^2(\bar\nabla y(\bar x), \bar{SO}(d)).$$

To extend this estimate to $\mathcal{L}'_\varepsilon(\Omega)$, cover the boundary cells by sets D_i such that $D_i = \bigcup_{\bar x\in\mathcal{L}'_\varepsilon\cap D_i} Q_\varepsilon(\bar x)$, is connected for all i, $\sup_i \operatorname{diam} D_i \le C\varepsilon$ and each D_i contains at least one inner cell Q_i. The number of possible shapes of the D_i is bounded independently of ε, so by applying the rigidity estimate (7) on each of these sets, we obtain rotations R_i such that

$$\sum_{\bar x\in\mathcal{L}'_\varepsilon\cap D_i} |\bar\nabla y(\bar x) - \bar R_i|^2 \le C \sum_{\bar x\in\mathcal{L}'_\varepsilon\cap D_i} \operatorname{dist}^2(\bar\nabla y(\bar x), \bar{SO}(d)).$$

Since in particular

$$\begin{aligned}\sum_i |\bar R_i - \bar R|^2 &\le 2\sum_i \left(|\bar\nabla y_{|Q_i} - \bar R_i|^2 + |\bar\nabla y_{|Q_i} - \bar R|^2\right)\\ &\le C \sum_{\bar x\in\mathcal{L}'_\varepsilon(\Omega)} \operatorname{dist}^2(\bar\nabla y(\bar x), \bar{SO}(d)),\end{aligned}$$

the claim now follows. □

4. **Proofs.** The proofs of Theorems 2.6 and 2.7 are split into the following three subsections. Throughout this section we will suppose that the assumptions of Theorems 2.6 and 2.7 are satisfied.

4.1. **Compactness.** We first prove the compactness statement in Theorem 2.6. Let

$$\Omega_k' = \left(\bigcup_{\bar{x} \in \mathcal{L}'_{\varepsilon_k}(\Omega)} \overline{Q}_{\varepsilon_k}(\bar{x}) \right)^\circ, \qquad \Omega_k'' = \left(\bigcup_{\bar{x} \in \mathcal{L}'_{\varepsilon_k}(\Omega)^\circ \cup \partial \mathcal{L}'_{\varepsilon_k}(\Omega)_*} \overline{Q}_{\varepsilon_k}(\bar{x}) \right)^\circ.$$

Lemma 4.1. *Let (u_k) be a sequence in $\mathcal{A}_{\varepsilon_k}(g, \partial\Omega_*, \Omega)$.*

(i) If the sequence $(I_k(u_k))$ of energies is bounded, then the sequences $(\|\tilde{u}_k\|_{H^1(\Omega_k')})$, $(\|\bar{\nabla} u_k'\|_{L^2(\Omega_k')})$ and $(\|\bar{\nabla} u_k\|_{L^2(\Omega_k'')})$ are bounded, too.

(ii) If the sequence $(\chi_{\Omega_k'} \delta_k^{-2} \operatorname{dist}^2(Z + \delta_k \bar{\nabla} u_k', \bar{SO}(d)))$ or, equivalently, the sequence $(\chi_{\Omega_k'} \delta_k^{-2} \operatorname{dist}^2(\mathrm{Id} + \delta_k \nabla \tilde{u}_k, SO(d)))$ is equiintegrable on $\mathbb{R}^d$, then both $(\chi_{\Omega_k'} |\bar{\nabla} u_k'|^2)$ and $(\chi_{\Omega_k'} |\nabla \tilde{u}_k|^2)$ are equiintegrable, too.

Proof. (i) If $I_k(u_k) \le C$, then by Lemmas 3.6, 3.2 and 3.7 we also have

$$\begin{aligned} \int_{\Omega_k'} \operatorname{dist}^2(\mathrm{Id} + \delta_k \nabla \tilde{u}_k, SO(d)) &\le C \int_{\Omega_k'} \operatorname{dist}^2(Z + \delta_k \bar{\nabla} u_k', \bar{SO}(d)) + C\delta_k^2 \\ &\le C\varepsilon_k^d \sum_{\bar{x} \in \mathcal{L}'_{\varepsilon_k}(\Omega)^\circ} W_{\mathrm{cell}}(Z + \delta_k \bar{\nabla} u_k(\bar{x})) + C\delta_k^2 \le C\delta_k^2. \end{aligned}$$

(We follow the convention of denoting possibly different constants with the same letter.) Applying the continuum results of [5], in particular Proposition 3.4 and Poincaré's inequality, we find that the $\tilde{u}_k$ are equibounded in $H^1(g, \partial\Omega_*, \Omega)$. By the construction of u_k' and by Lemmas 3.5 and 3.4 we then find that

$$\|\bar{\nabla} u_k\|^2_{L^2(\Omega_k'')} \le C \|\bar{\nabla} u_k'\|^2_{L^2(\Omega_k')} \le C \|\nabla \tilde{u}_k\|^2_{L^2(\Omega_k'')} \le C.$$

(ii) First note that Lemma 3.6 implies that $(\chi_{\Omega_k'} \delta_k^{-2} \operatorname{dist}^2(\mathrm{Id} + \delta_k \nabla \tilde{u}_k, SO(d)))$ is equiintegrable if and only if $(\chi_{\Omega_k'} \delta_k^{-2} \operatorname{dist}^2(Z + \delta_k \bar{\nabla} u_k', \bar{SO}(d)))$ is equiintegrable. This follows from the fact that there is a constant $c > 0$ such that $\delta_k^{-2} \operatorname{dist}^2(Z + \delta_k \bar{\nabla} u_k', \bar{SO}(d)) \ge M$ on a cell Q can only hold if $\delta_k^{-2} \operatorname{dist}^2(\mathrm{Id} + \delta_k \nabla \tilde{u}_k, SO(d)) \ge cM$ on one of the d-simplices on which $\tilde{u}_k$ is interpolated linearly and, vice versa, if $\delta_k^{-2} \operatorname{dist}^2(\mathrm{Id} + \delta_k \nabla \tilde{u}_k, SO(d)) \ge M$, then $\delta_k^{-2} \operatorname{dist}^2(Z + \delta_k \bar{\nabla} u_k', \bar{SO}(d)) \ge cM$ on Q. An analogous argument shows that $(\chi_{\Omega_k'} |\nabla \tilde{u}_k|^2)$ is equiintegrable if and only if $(\chi_{\Omega_k'} |\bar{\nabla} u_k'|^2)$ is equiintegrable.

As a consequence we can refer to the continuum case investigated in Lemma 4.2 in [10], from which it follows that if $(\delta_k^{-2} \operatorname{dist}^2(\mathrm{Id} + \delta_k \nabla \tilde{u}_k, SO(d)))$ is equiintegrable, then so is $(\chi_\Omega |\nabla \tilde{u}_k|^2)$. The claim now follows from Lemmas 3.5 and 3.4. □

Suppose (u_k) is a sequence in $\mathcal{A}_{\varepsilon_k}(g, \partial\Omega_*, \Omega)$ such that $(I_k(u_k))$ is bounded. By Lemma 4.1 we immediately deduce that for a suitable subsequence (not relabeled) $\tilde{u}_k \rightharpoonup u$ in H^1 for some $u \in H^1(g, \partial\Omega_*, \Omega)$. Passing to a further subsequence we also see from Lemma 4.1 that there exists $f \in L^2(\Omega, \mathbb{R}^d)$ such that $\chi_{\Omega_k'} \bar{\nabla} u_k' \rightharpoonup \chi_\Omega f$ in L^2, and so $\chi_{\Omega_k''} \bar{\nabla} u_k \rightharpoonup \chi_\Omega f$ in L^2. Noting that any compact subset of $\overline{\Omega} \setminus (\overline{\partial\Omega \setminus \partial\Omega_*})$ is eventually contained in Ω_k'', we see that $\bar{\nabla} u_k \rightharpoonup f$ in $L^2_{\mathrm{loc}}(\overline{\Omega} \setminus (\overline{\partial\Omega \setminus \partial\Omega_*}))$.

To finish the first part of the proof of Theorem 2.6, it remains to show that $f = \nabla u \cdot Z$. Let $V \subset\subset \Omega$. For $i \in \{1, \dots, 2^d\}$ denote by $\bar{\partial}_i u_k$ and f_i the i-th columns of $\bar{\nabla} u_k$ and f, respectively. Note that

$$\bar{\partial}_i u_k(x) \rightharpoonup f_i, \quad \bar{\partial}_1 u_k(x + \varepsilon_k(z_i - z_1)) \rightharpoonup f_1 \quad \text{in } L^2(V).$$

For $x \in V$ compute

$$\begin{aligned}
\bar\partial_i u_k(x) &= \varepsilon_k^{-1}\left(\tilde u_k(\bar x + \varepsilon_k z_i) - \tilde u_k(\bar x)\right)\\
&= \varepsilon_k^{-1}\left(\tilde u_k(\bar x + \varepsilon_k(z_i - z_1) + \varepsilon_k z_1) - \tilde u_k(\bar x + \varepsilon_k(z_i - z_1))\right)\\
&\quad + \varepsilon_k^{-1}\left(\tilde u_k(\bar x + \varepsilon_k(z_i - z_1)) - \tilde u_k(\bar x)\right)\\
&= \bar\partial_1 u_k(\bar x + \varepsilon_k(z_i - z_1))\\
&\quad + \varepsilon_k^{-1}\fint_{A[-\frac{\varepsilon_k}{2},\frac{\varepsilon_k}{2})^d} \tilde u_k(\bar x + \varepsilon_k(z_i - z_1) + \xi) - \tilde u_k(\bar x + \xi)\, d\xi\\
&= \bar\partial_1 u_k(x + \varepsilon_k(z_i - z_1))\\
&\quad + \varepsilon_k^{-1}\left(P_{\varepsilon_k}\tilde u_k(x + \varepsilon_k(z_i - z_1)) - P_{\varepsilon_k}\tilde u_k(x)\right)
\end{aligned}$$

by construction (see (6) and (5)). Now observe that for a test function $\psi \in C_c^\infty(V, \mathbb{R}^d)$

$$\begin{aligned}
&\varepsilon_k^{-1}\int_V \left(P_{\varepsilon_k}\tilde u_k(x + \varepsilon_k(z_i - z_1)) - P_{\varepsilon_k}\tilde u_k(x)\right)\psi(x)\, dx\\
&= \int_V P_{\varepsilon_k}\tilde u_k(x)\frac{\psi(x - \varepsilon_k(z_i - z_1)) - \psi(x)}{\varepsilon_k}\, dx
\end{aligned}$$

for ε_k sufficiently small. Since $\tilde u_k \to u$ in L^2 and $\|P_{\varepsilon_k}\| \le 1$ by Jensen's inequality, the first term $P_{\varepsilon_k}\tilde u_k$ in the integral converges strongly to u. The second term converges to $-\nabla\psi\cdot(z_i - z_1)$ uniformly. Summarizing, we have shown that

$$\int_V (f_i - f_1)(x)\psi(x)\, dx = \int_V u(x)\nabla\psi(x)\cdot(z_i - z_1)\, dx$$

and hence, since V was arbitrary,

$$f_i - f_1 = \nabla u\cdot(z_i - z_1).$$

The claim now follows from

$$\sum_{i=1}^{2^d} f_i = \lim_{k\to\infty}\sum_{i=1}^{2^d}\bar\partial_i u_k = 0 = \sum_{i=1}^{2^d}\nabla u\cdot z_i.$$

□

4.2. **The Gamma-liminf inequality.**

Let $\varepsilon_k^d\sum_{x\in\mathcal{L}_{\varepsilon_k}(\Omega)^\circ\cup\partial\mathcal{L}_{\varepsilon_k}(\Omega)_*}|u_k(x) - P_{\varepsilon_k}u(x)|^2 \to 0$ and assume without loss of generality $I_k(u_k) \le C$, so that by the compactness properties proved in the previous paragraph we may assume that $u_k' \to u$, $\bar\nabla u_k' \rightharpoonup \nabla u\cdot Z$.

Using Lemma 3.7 and Lemma 3.2 (set $V_k = V_{\varepsilon_k}$) we can compute

$$\begin{aligned}
I_k(u_k) &= \delta_k^{-2}\varepsilon_k^d\sum_{\bar x\in\mathcal{L}'_{\varepsilon_k}(\Omega)} W_{\varepsilon_k}(\bar x, \varepsilon_k(Z + \delta_k\bar\nabla u_k(\bar x)))\\
&\ge \delta_k^{-2}\varepsilon_k^d\sum_{\bar x\in\mathcal{L}'_{\varepsilon_k}\cap\Omega''} W_{\mathrm{cell}}(Z + \delta_k\bar\nabla u_k(\bar x))\\
&\ge \frac{\delta_k^{-2}}{\det A}\int_{V_k} W_{\mathrm{cell}}(Z + \delta_k\bar\nabla u_k(x))\, dx\\
&\quad + c\delta_k^{-2}\int_{\Omega'_k\setminus V_k}\mathrm{dist}^2(Z + \delta_k\bar\nabla u_k'(x), \bar{SO}(d))\, dx
\end{aligned}$$

for some $c > 0$. By Assumption 2.1 we can write $W_{\mathrm{cell}}(Z+F) = \frac{1}{2}Q_{\mathrm{cell}}(F) + \omega(F)$ with $\sup\{\frac{\omega(F)}{|F|^2} : |F| \le \rho\} \to 0$ as $\rho \to 0$. Let (η_k) be a sequence of positive numbers and set $\chi_k(x) := \chi_{[0,\eta_k)}(|\bar\nabla u_k(x)|)$. Using Lemma 3.7 once more, we find

$$\begin{aligned} I_k(u_k) &\ge \frac{\delta_k^{-2}}{\det A}\int_{V_k} \chi_k(x) W_{\mathrm{cell}}(Z+\delta_k\bar\nabla u_k(x))\,dx \\ &\quad + c\delta_k^{-2}\int_{\Omega_k'} (1-\chi_k(x))\,\mathrm{dist}^2(Z+\delta_k\bar\nabla u_k'(x), S\bar O(d))\,dx \\ &= \frac{1}{2\det A}\int_{V_k}\chi_k(x)\left(Q_{\mathrm{cell}}(\bar\nabla u_k(x)) + \delta_k^{-2}\omega(\delta_k\bar\nabla u_k(x))\right)\,dx \\ &\quad + c\delta_k^{-2}\int_{\Omega_k'} (1-\chi_k(x))\,\mathrm{dist}^2(Z+\delta_k\bar\nabla u_k'(x), S\bar O(d))\,dx, \end{aligned}$$

where the second term inside the first integral can be bounded by

$$\chi_k|\bar\nabla u_k|^2\frac{\omega(\delta_k\bar\nabla u_k)}{|\delta_k\bar\nabla u_k|^2}.$$

Now if η_k is such that $\eta_k \to \infty$ and $\eta_k\delta_k \to 0$, then, since $\chi_{\Omega_k'}|\bar\nabla u_k'|$ is bounded in L^2 and $\chi_{\Omega_k'}\chi_k\frac{\omega(\delta_k\bar\nabla u_k)}{|\delta_k\bar\nabla u_k|^2}$ converges to zero uniformly as $k\to\infty$, we deduce that

$$\begin{aligned} \liminf_{k\to\infty} I_k(u_k) &\ge \liminf_{k\to\infty}\frac{1}{2\det A}\int_\Omega Q_{\mathrm{cell}}\left(\chi_{V_k}(x)\chi_k(x)\bar\nabla u_k(x)\right)\,dx \\ &\quad + c\liminf_{k\to\infty}\delta_k^{-2}\int_{\Omega_k'}(1-\chi_k(x))\,\mathrm{dist}^2(Z+\delta_k\bar\nabla u_k'(x), S\bar O(d))\,dx. \end{aligned}$$

Now observe that $\chi_{V_k}\chi_k$ converges to 1 boundedly in measure, so

$$\chi_{V_k}\chi_k\bar\nabla u_k \rightharpoonup \nabla u\cdot Z \quad \text{in } L^2(\Omega).$$

By lower semicontinuity we obtain

$$\begin{aligned} \liminf_{k\to\infty} I_k(u_k) &\ge \frac{1}{2\det A}\int_\Omega Q_{\mathrm{cell}}(\nabla u\cdot Z)\,dx \\ &\quad + c\liminf_{k\to\infty}\delta_k^{-2}\int_{\Omega_k'}(1-\chi_k(x))\,\mathrm{dist}^2(Z+\delta_k\bar\nabla u_k'(x), S\bar O(d))\,dx. \quad (9) \end{aligned}$$

Since the latter term is non-negative and $F\mapsto Q_{\mathrm{cell}}(F\cdot Z)$ vanishes on antisymmetric matrices (see (4)), the lower bound in Theorem 2.6 is proved. □

The benefit of proving a sharper estimate in (9) than needed to obtain the Γ-lim inf inequality is seen in the proof of the following observation.

Lemma 4.2. *For a recovery sequence (u_k) the terms $\chi_{\Omega_k'}\delta_k^{-2}\,\mathrm{dist}^2(Z+\delta_k\bar\nabla u_k', S\bar O(d))$ are equiintegrable.*

Proof. Suppose this were not the case. Then there exists $\gamma > 0$ such that for each $m\in\mathbb{N}$ we find $k = k(m)\in\mathbb{N}$ such that

$$\int_{\{|\bar\nabla u_k'|>m\}\cap\Omega_k'}\delta_k^{-2}\,\mathrm{dist}^2(Z+\delta_k\bar\nabla u_k', S\bar O(d)) \ge \gamma.$$

Without loss of generality we may choose $k(m)$ such that $k(1) < k(2) < \dots$ and $m\delta_{k(m)} \le m^{-1}$. Now choose η_k as the inverse of $m\mapsto k(m)$ wherever it is defined,

i.e., such that $\eta_{k(m)} = m$, and note that $\delta_{k(m)}\eta_{k(m)} = m\delta_{k(m)} \le m^{-1} = \eta_{k(m)}^{-1}$. Then for the subsequence $(u'_{k(m)})$ we have

$$\int_{\{|\bar\nabla u'_{k(m)}|>\eta_{k(m)}\}\cap\Omega'_{k(m)}} \delta_{k(m)}^{-2}\,\mathrm{dist}^2(Z+\delta_{k(m)}\bar\nabla u'_{k(m)}, S\bar O(d)) \ge \gamma.$$

Taking the lim inf of this expression we find by using (9) that

$$\liminf_{k\to\infty} I_k(u_k) \ge I(u) + c\gamma.$$

This contradicts the fact that (u_k) is a recovery sequence for u. □

Lemma 4.3. *If (u_k) is a recovery sequence, then $(\chi_{\Omega'_k}|\nabla\tilde u_k|^2)$ and $(\chi_{\Omega'_k}|\bar\nabla u'_k|^2)$ are equiintegrable.*

Proof. Immediate from Lemma 4.1(ii) and Lemma 4.2. □

4.3. **Recovery sequences.** By density it suffices to provide recovery sequences for $u \in W^{1,\infty}(\Omega,\mathbb{R}^d)$ with $u = g$ on $\partial\Omega_*$. Extending u we may assume that $u \in W^{1,\infty}(\mathbb{R}^d,\mathbb{R}^d)$. Recall the definition of P_ε from (5) and define lattice displacements $u_k \in \mathcal{A}_{\varepsilon_k}(g,\partial\Omega_*,\Omega)$ by

$$u_k(x) = \begin{cases} P_{\varepsilon_k}u(x), & \text{for } x \in \mathcal{L}_{\varepsilon_k}\setminus\partial\mathcal{L}_{\varepsilon_k}(\Omega)_*,\\ g(x), & \text{for } x\in\partial\mathcal{L}_{\varepsilon_k}(\Omega)_*\end{cases} \tag{10}$$

(and interpolate to obtain $\tilde u_k : \Omega'_k \to \mathbb{R}^d$ as before).

Lemma 4.4. *Let (u_k) be the sequence of functions defined in (10). Then $u_k \to u$ in the sense of Definition 2.5, $\chi_{\Omega'_k}\bar\nabla u_k \to \chi_\Omega\nabla u\cdot Z$ strongly in L^2 and $\tilde u_k \to u$ strongly in $H^1(\Omega)$.*

Proof. Note first that $\|\bar\nabla u_k\|_{L^\infty}$ is bounded. This is easily seen on lattice cells not neighboring a Dirichlet boundary cell and on Dirichlet boundary cells it follows from $\nabla g \in L^\infty$. If $Q = Q_{\varepsilon_k}(\bar x)$ and $Q' = Q_{\varepsilon_k}(\bar x')$ are cells with $\overline{Q}\cap\overline{Q'} \ne \emptyset$ and $\bar x' \in \partial\mathcal{L}'_{\varepsilon_k}(\Omega)_*$, then by the remark below Definition 2.3 and by Definition 2.4(i) there exists $a \in \mathbb{R}^d$ with $|a|$ bounded independently of $\bar x$, $\bar x'$ and ε_k such that $\bar x' + \varepsilon_k a \in \partial\Omega_*$. For all pairs of corners $(\bar x+\varepsilon_k z_i, \bar x+\varepsilon_k z_j)$ of Q we have

$$\begin{aligned}&|u_k(\bar x+\varepsilon_k z_i) - u_k(\bar x+\varepsilon_k z_j)|\\ &\le |u_k(\bar x+\varepsilon_k z_i) - u(\bar x'+\varepsilon_k a)| + |u_k(\bar x+\varepsilon_k z_j) - u(\bar x'+\varepsilon_k a)|.\end{aligned}$$

Since $u(\bar x'+\varepsilon_k a) = g(\bar x'+\varepsilon_k a)$, the estimate now also follows on Q from $u, g \in W^{1,\infty}$.

Since $u_k = P_{\varepsilon_k}u$ on all inner cells and $\|\bar\nabla u_k\|_{L^\infty}$ is bounded, we have

$$\varepsilon_k^d \sum_{x\in\mathcal{L}_{\varepsilon_k}\cap\Omega} |u_k(x) - P_{\varepsilon_k}u(x)| \le C\varepsilon_k \to 0$$

as $k\to\infty$, i.e, $u_k \to u$.

Let $U_k = P_{\varepsilon_k}\nabla u(\cdot + (\frac{\varepsilon_k}{2},\dots,\frac{\varepsilon_k}{2}))$. In order to see that $\bar\nabla u_k \to \nabla u\cdot Z$ in L^2, it suffices to show that $\bar\nabla u_k - U_k\cdot Z \to 0$, because $U_k\cdot Z \to \nabla u\cdot Z$ in L^2. Choose $c>0$ such that $V_k := \{x\in\Omega : \mathrm{dist}(x,\partial\Omega) > c\varepsilon_k\}$ satisfies $\partial\mathcal{L}_{\varepsilon_k}(\Omega)\cap V_k \ne \emptyset$. Since

$\bar\nabla u_k$ and U_k are constant on lattice cells, we have

$$\begin{aligned}
&\|\bar\partial_i u_k - \bar\partial_1 u_k - U_k\cdot(z_i-z_1)\|^2_{L^2(\Omega'_k)}\\
&\le C\varepsilon_k^d \sum_{\bar x\in\mathcal{L}'_{\varepsilon_k}\cap V_k} \left|\bar\partial_i u_k(\bar x) - \bar\partial_1 u_k(\bar x) - U_k(\bar x)\cdot(z_i-z_1)\right|^2 + C\varepsilon_k\\
&= C\varepsilon_k^d \sum_{\bar x\in\mathcal{L}'_{\varepsilon_k}\cap V_k} \left| \fint_{A[0,\varepsilon_k)^d} \left(\frac{u(\bar x+\varepsilon_k z_i+\xi) - u(\bar x+\varepsilon_k z_1+\xi)}{\varepsilon_k} \right.\right.\\
&\qquad\qquad \left.\left. - \nabla u(\bar x+\xi)\cdot(z_i-z_1)\right) d\xi \right|^2 + C\varepsilon_k\\
&\le C\int_\Omega \left| \frac{u(\xi+\varepsilon_k z_i) - u(\xi+\varepsilon_k z_1)}{\varepsilon_k} - \nabla u(\xi)\cdot(z_i-z_1)\right|^2 d\xi + C\varepsilon_k
\end{aligned}$$

by Jensen's inequality. This is easily seen to tend to 0 as $\varepsilon_k\to 0$ (see, e.g., Lemma A.2 in [9]). Since $\sum_{i=1}^{2^d}\bar\partial_i u_k = 0$ for all k and $\sum_{i=1}^{2^d} z_i = 0$, it follows that $\bar\nabla u_k \to \nabla u\cdot Z$. (It is not hard to see that this also implies that $\nabla\tilde u_k\to\nabla u$, see, e.g., Lemma A.1 in [9].) □

We finish the proof of Theorem 2.6 by showing that u_k as defined above is a recovery sequence for u. By Lemma 4.4 it remains to prove that $\limsup_{k\to\infty} I_k(u_k)\le I(u)$.

The terms $W_{\text{surface}}(\mathcal{I}_{\varepsilon_k}(\bar x), Z+\delta_k\bar\nabla u_k(\bar x))$ on boundary cells are uniformly bounded. If W_{surface} and W_{cell} are compatible, they are even bounded by $C\delta_k^2$ for some $C>0$. It follows that

$$I_k(u_k)\le \frac{1}{\det A}\int_\Omega \delta_k^{-2} W_{\text{cell}}(Z+\delta_k\bar\nabla u_k(x))\,dx + C\delta_k^{-2}\varepsilon_k,$$

where the error term can be improved to $C\varepsilon_k$ for W_{surface} and W_{cell} compatible.

Since $F\mapsto \delta_k^{-2}W_{\text{cell}}(Z+\delta_k F)$ converges uniformly on compacta to $\frac12 Q_{\text{cell}}$ and the error terms $C\delta_k^{-2}\varepsilon_k$ (resp. $C\varepsilon_k$) converge to zero, we obtain from Lemma 4.4

$$\limsup_{k\to\infty} I_k(u_k)\le \frac{1}{2\det A}\int_\Omega Q_{\text{cell}}(\nabla u(x)\cdot Z)\,dx.$$

□

Proof of Theorem 2.7. Let (u_k) be a recovery sequence for u. Strong convergence $\bar\nabla u'_k\to\nabla u\cdot Z$ follows from a convexity argument and equiintegrability of the discrete gradients of recovery sequences proved in Lemma 4.3 (also compare [10]).

For V_k as in the proof of Lemma 4.4 we have

$$\begin{aligned}
I_k(u_k) - I(\tilde u_k) \ge{}& \frac{1}{\det A}\int_{V_k\cap\{|\bar\nabla u_k|\le M\}} \left(\delta_k^{-2}W_{\text{cell}}(Z+\delta_k\bar\nabla u_k) - \frac12 Q_{\text{cell}}(\nabla\tilde u_k\cdot Z)\right)\\
&- \frac{1}{\det A}\int_{(V_k\cap\{|\bar\nabla u_k|>M\})\cup(\Omega\setminus V_k)} \frac12 Q_{\text{cell}}(\nabla\tilde u_k\cdot Z)
\end{aligned}$$

for all $M>0$. Sending first k and then M to ∞, since $F\mapsto\delta_k^{-2}W_{\text{cell}}(Z+\delta_k F)$ converges uniformly on compacta to $\frac12 Q_{\text{cell}}$, we obtain

$$I(u) - \limsup_{k\to\infty} I(\tilde u_k)\ge \liminf_{k\to\infty} I_k(u_k) - I(\tilde u_k)\ge 0 \tag{11}$$

by Lemma 4.4 and equiintegrability of $(|\nabla \tilde{u}_k|^2)$. But Q_{cell} grows quadratically on the subspace perpendicular to infinitesimal rotations and translations. In particular,

$$\frac{1}{2}Q_{\text{cell}}(F \cdot Z) \geq c \left| \frac{F^T + F}{2} \right|^2$$

and so

$$\begin{aligned} & c \int_\Omega |e(\tilde{u}_k) - e(u)|^2 \\ & \leq \frac{1}{2 \det A} \int_\Omega Q_{\text{cell}}(\nabla \tilde{u}_k \cdot Z) - 2Q_{\text{cell}}(\nabla \tilde{u}_k \cdot Z, \nabla u \cdot Z) + Q_{\text{cell}}(\nabla u \cdot Z). \end{aligned}$$

By Lemma 4.1 $\nabla \tilde{u}_k$ converges weakly to ∇u, so (11) implies

$$\limsup_{k \to \infty} c \int_\Omega |e(\tilde{u}_k) - e(u)|^2 = 0.$$

The strong convergence of $\nabla \tilde{u}_k$ to ∇u in $L^2(\Omega)$ now follows from Korn's inequality. By Lemma 4.3 we now deduce that in fact $\chi_{\Omega'_k} \nabla \tilde{u}_k$ and $\chi_{\Omega'_k} \bar{\nabla} u_k$ converge to $\chi_\Omega \nabla u$ and $\chi_\Omega \nabla u \cdot Z$ strongly in $L^2(\mathbb{R}^d)$, respectively. Using again that any compact subset of $\overline{\Omega} \setminus (\overline{\partial\Omega \setminus \partial\Omega_*})$ is eventually contained in Ω''_k and $\bar{\nabla} u'_k = \bar{\nabla} u_k$ on Ω''_k, we conclude the proof. □

Proof of Corollary 2.8. Just note that I has a unique minimizer w by strict convexity of Q_{cell} on symmetric matrices and Korn's inequality. So if (w_k) is a sequence of almost minimizers of I_k, then (w_k) is a recovery sequence for w. The claim thus follows from Theorem 2.7. □

5. **Examples.** In this section we give some examples of atomic interactions to which the results of the previous sections apply. Motivated by the investigations in [8, 2, 9] we examine mass spring models: lattices of atoms whose energy is given by springs between nearest and next nearest neighbors. We also provide explicit formulas for the (partly well-known) limiting functionals, which can be derived by elementary calculations.

5.1. **The triangular lattice in 2D.** The nearest neighbor interaction

$$E_\varepsilon(y) = \frac{\varepsilon^2}{2} \sum_{\substack{x_1, x_2 \in \mathcal{L}_\varepsilon \cap \Omega \\ |x_1 - x_2| = \varepsilon}} \frac{K}{2} \left(\frac{|y(x_1) - y(x_2)|}{\varepsilon} - 1 \right)^2,$$

on the triangular lattice $\mathcal{L} = A\mathbb{Z}^2 = \begin{pmatrix} 1 & \frac{1}{2} \\ 0 & \frac{\sqrt{3}}{2} \end{pmatrix} \mathbb{Z}^2$ in 2D for deformations that are locally orientation preserving, i.e., whose affine interpolation has nonnegative determinant on each triangle of the induced triangulation, has been analyzed by Braides, Solci and Vitali in [2]. We include it here for the sake of completeness.

Denoting the i-th column of $F \in \mathbb{R}^{2\times 4}$ by F_i and choosing the numbering of z_i such that $Z = \frac{1}{2} A \begin{pmatrix} -1 & 1 & 1 & -1 \\ -1 & -1 & 1 & 1 \end{pmatrix}$, the associated cell energy is given by

$$\begin{aligned} W_{\text{cell}}(F) = \frac{K}{4} \Big(& (|F_2 - F_1| - 1)^2 + (|F_3 - F_2| - 1)^2 \\ & + (|F_4 - F_3| - 1)^2 + (|F_1 - F_4| - 1)^2 + 2(|F_4 - F_2| - 1)^2 \Big) \end{aligned}$$

on orientation preserving discrete gradients. W_{surface} (compatible with W_{cell}) is defined appropriately. This is an admissible cell energy, and we have thus re-derived the limiting functional

$$I(u) = \frac{1}{2\det A}\int_\Omega Q_{\text{cell}}(e(u)\cdot Z) = \frac{\sqrt{3}K}{8}\int_\Omega 2|e(u)|^2 + (\operatorname{trace} e(u))^2$$

from [2].

5.2. **A mass spring model in 2D.** The following energy functional has been introduced and studied by Friesecke and Theil in [8]. Let $\mathcal{L} = \mathbb{Z}^2$. For a deformation $y : \mathcal{L}_\varepsilon \cap \Omega \to \mathbb{R}^2$ let

$$E_\varepsilon(y) = \frac{\varepsilon^2}{2}\sum_{\substack{x_1,x_2\in\mathcal{L}_\varepsilon\cap\Omega\\ |x_1-x_2|=\varepsilon}} \frac{K_1}{2}\left(\frac{|y(x_1)-y(x_2)|}{\varepsilon} - a_1\right)^2 + \frac{\varepsilon^2}{2}\sum_{\substack{x_1,x_2\in\mathcal{L}_\varepsilon\cap\Omega\\ |x_1-x_2|=\sqrt{2}\varepsilon}} \frac{K_2}{2}\left(\frac{|y(x_1)-y(x_2)|}{\varepsilon} - a_2\right)^2 + \sum_{\bar{x}\in\mathcal{L}'_\varepsilon(\Omega)}\chi(\bar{\nabla}y(\bar{x}))$$

with $\chi = 0$ on orientation preserving cell deformations and $= \infty$ otherwise. (We will only need that χ is zero in a neighborhood of $\bar{SO}(2)$ and positive ($\geq c > 0$) on $\bar{O}(2)\setminus\bar{SO}(2)$.

Denoting the i-th column $F\cdot z_i$ of $F\in\mathbb{R}^{2\times 4}$ by F_i, the associated cell energy is given by

$$W_{\text{cell}}(F) = \frac{1}{4}\sum_{|z_i-z_j|=1}\frac{K_1}{2}(|F_i-F_j|-a_1)^2 + \frac{1}{2}\sum_{|z_i-z_j|=\sqrt{2}}\frac{K_2}{2}(|F_i-F_j|-a_2)^2 + \chi(F),$$

the surface energy expressions are defied appropriately.

We choose units such that $K_1a_1 + \sqrt{2}K_2a_2 = K_1 + 2K_2$, i.e., such that Z is a stationary point of W_{cell} (with $\mu := W_{\text{cell}}(Z) = K_1(1-a_1)^2 + K_2(\sqrt{2}-a_2)^2$). In [8] it is shown that indeed for a parameter region (open with respect to the constraint $K_1a_1 + \sqrt{2}K_2a_2 = K_1 + 2K_2$) W_{cell} grows quadratically on the subspace perpendicular to infinitesimal translations and rotations. Now note that Theorems 2.6 and 2.7 apply to the energy functional E^μ_ε that arises from E_ε by replacing W_{cell} with $W_{\text{cell}} - \mu$. The limiting linear energy functional is given by

$$I(u) = \frac{1}{2}\int_\Omega Q_{\text{cell}}(e(u)\cdot Z),$$

where the quadratic form $\mathbb{R}^{2\times 2}_{\text{sym}} \ni F \mapsto Q_{\text{cell}}(F\cdot Z)$ is given by

$$F \mapsto K_1a_1|F|^2 + \frac{a_2K_2}{2}(\operatorname{trace} F)^2 + 2(\sqrt{2}a_2K_2 - a_1K_1)f_{12}^2.$$

Remarks. (i) Note that for $a_1 \neq 1$, $a_2 \neq \sqrt{2}$ the bulk and surface contributions are not compatible and $\mu > 0$. Our result can be interpreted as a Γ-development of the functionals $u \mapsto E_{\varepsilon_k}(\mathrm{Id} + \delta_k u)$: Subtracting the zeroth order constant Γ-limit $\mu|\Omega|$, the above calculated Γ-limit is just the Γ-limit of

$$u \mapsto \delta_k^{-2}\left(E_{\varepsilon_k}(\mathrm{Id}+\delta_k u) - \mu|\Omega|\right) = \delta_k^{-2}E^\mu_{\varepsilon_k}(\mathrm{Id}+\delta_k u) + C\varepsilon_k\delta_k^{-2}.$$

(See, e.g., [1] for the notion of development by Γ-convergence.)

(ii) If $a_1 = 1$, $a_2 = \sqrt{2}$, we have $\mu = 0$. In this case $W_{\rm cell}$ and $W_{\rm surface}$ are compatible.

5.3. **A mass spring model in 3D.** The following energy functional has been investigated in [9] for $a_1 = 1$, $a_2 = \sqrt{2}$. Let $\mathcal{L} = \mathbb{Z}^3$. For a deformation $y : \mathcal{L}_\varepsilon \cap \Omega \to \mathbb{R}^3$ let

$$E_\varepsilon(y) = \frac{\varepsilon^3}{2} \sum_{\substack{x_1,x_2 \in \mathcal{L}_\varepsilon \cap \Omega \\ |x_1 - x_2| = \varepsilon}} \frac{K_1}{2} \left(\frac{|y(x_1) - y(x_2)|}{\varepsilon} - a_1 \right)^2 + \frac{\varepsilon^3}{2} \sum_{\substack{x_1,x_2 \in \mathcal{L}_\varepsilon \cap \Omega \\ |x_1 - x_2| = \sqrt{2}\varepsilon}} \frac{K_2}{2} \left(\frac{|y(x_1) - y(x_2)|}{\varepsilon} - a_2 \right)^2 + \sum_{\bar{x} \in \mathcal{L}'_\varepsilon(\Omega)} \chi(\bar{\nabla} y(\bar{x})).$$

The non-negative term χ is assumed to be non-zero only for deformations which are not locally orientation preserving, in particular it is zero in a neighborhood of $S\bar{O}(3)$ and positive ($\geq c > 0$) on $\bar{O}(3) \setminus S\bar{O}(3)$.

The associated cell energy on $\mathbb{R}^{3\times 8}$ is given by

$$W_{\rm cell}(F) = \frac{1}{8} \sum_{|z_i - z_j| = 1} \frac{K_1}{2} (|F_i - F_j| - a_1)^2 + \frac{1}{4} \sum_{|z_i - z_j| = \sqrt{2}} \frac{K_2}{2} (|F_i - F_j| - a_2)^2 + \chi(F),$$

the surface energy is chosen appropriately.

In [9] it is shown that for $a_1 = 1$, $a_2 = \sqrt{2}$, $W_{\rm cell}$ is an admissible cell energy in the sense of Assumption 2.1 for all $K_1, K_2 > 0$. Noting that for $a_1 \neq 1$, $a_2 \neq \sqrt{2}$ the cell energy can be written as a sum of 2D cell energies over the cube's faces as in the previous example, a necessary condition that $W_{\rm cell}$ be equilibrated on Z is that $\frac{K_1}{4} a_1 + \sqrt{2} \frac{K_2}{2} a_2 = \frac{K_1}{4} + 2 \frac{K_2}{2}$, i.e., $K_1 a_1 + 2\sqrt{2} K_2 a_2 = K_1 + 4K_2$.

For given K_1, K_2, a perturbation argument – using that the in-plane displacements on every face are minimized precisely on the unit square by our previous example – shows that (up to a constant) $W_{\rm cell}$ still is an admissible energy function for small deviations from the perfectly equilibrated system if $K_1 a_1 + 2\sqrt{2} K_2 a_2 = K_1 + 4K_2$. So again our results of the previous sections apply (after subtracting the zeroth order term $\mu|\Omega|$, $\mu = K_1(1 - a_1)^2 + 3K_2(\sqrt{2} - a_2)^2$).

The quadratic form $\mathbb{R}^{3\times 3}_{\rm sym} \ni F \mapsto Q_{\rm cell}(F \cdot Z)$ is given by

$$F \mapsto \left(K_1 + \left(4 - \frac{3a_2}{\sqrt{2}} \right) K_2 \right) |F|^2 + \frac{a_2 K_2}{\sqrt{2}} (\operatorname{trace} F)^2 + \left(\sqrt{2} a_2 K_2 - 2 a_1 K_1 \right) \left(f_{12}^2 + f_{13}^2 + f_{23}^2 \right).$$

5.4. **bcc crystals.** Although the bcc crystal $\mathcal{L} = \mathcal{K} \cup \mathcal{M}$ with $\mathcal{K} = \mathbb{Z}^3$ and $\mathcal{M} = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})^T + \mathbb{Z}^3$ is a Bravais-lattice (spanned, e.g., by $(1,0,0)^T, (0,1,0)^T, (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})^T$),

the nearest and next-nearest neighbor pair interaction functional

$$E_\varepsilon(y) = \frac{\varepsilon^3}{2} \sum_{\substack{x_1,x_2\in\mathcal{L}_\varepsilon\cap\Omega \\ |x_1-x_2|=\frac{\sqrt{3}\varepsilon}{2}}} \frac{K_1}{2}\left(\frac{|y(x_1)-y(x_2)|}{\varepsilon}-\frac{\sqrt{3}}{2}\right)^2 + \frac{\varepsilon^3}{2} \sum_{\substack{x_1,x_2\in\mathcal{L}_\varepsilon\cap\Omega \\ |x_1-x_2|=\varepsilon}} \frac{K_2}{2}\left(\frac{|y(x_1)-y(x_2)|}{\varepsilon}-1\right)^2$$

(with orientation preserving condition) cannot be decomposed in the form (2) as a sum of suitable cell energies over the lattice unit cells.

However, since the individual interactions are equilibrated in the reference configuration, we can still apply our results to derive the limiting linear theory: Assume that boundary conditions are prescribed for every boundary atom $\partial\mathcal{K}_\varepsilon(\Omega)$ and $\partial\mathcal{M}_\varepsilon(\Omega)$ of $\Omega\cap\varepsilon\mathcal{K}$ and of $\Omega\cap\varepsilon\mathcal{M}$, respectively. For $F\in\mathbb{R}^{3\times 8}$, $c\in\mathbb{R}^3$, let

$$\tilde{W}_{\mathrm{cell}}(F,c) = \frac{1}{2}\sum_{1\le i\le 8}\frac{K_1}{2}\left(|F_i-c|-\frac{\sqrt{3}}{2}\right)^2 + \frac{1}{8}\sum_{|z_i-z_j|=1}\frac{K_2}{2}\left(|F_i-F_j|-1\right)^2+\chi(F),$$

χ as before. Then $W_{\mathrm{cell}}(F) := \min_{c\in\mathbb{R}^3}\tilde{W}_{\mathrm{cell}}(F_1-c,\dots,F_8-c)$ is an admissible cell energy function and – up to boundary terms –

$$E_\varepsilon(y) \ge \sum_{\bar{x}\in(\mathbb{Z}^3)'_\varepsilon(\Omega)} W_{\mathrm{cell}}(\bar{\nabla}y_1(\bar{x})) + \sum_{\bar{x}\in(\mathbb{Z}^3)''_\varepsilon(\Omega)} W_{\mathrm{cell}}(\bar{\nabla}y_2(\bar{x})), \tag{12}$$

where y_1, y_2 denote the restrictions of y to the sets $\mathcal{K}'_\varepsilon(\Omega)$ and $\mathcal{M}'_\varepsilon(\Omega)$, respectively (cf. Definition 2.3). A simple convexity argument shows that, in the limit $\bar{\nabla}y\approx\nabla\tilde{y}\cdot Z$, we obtain $W_{\mathrm{cell}}(\bar{\nabla}y)=\tilde{W}_{\mathrm{cell}}(\bar{\nabla}y,0)$ and the lower bound (12) becomes sharp.

As a consequence, the result of the preceding sections also apply here, and we obtain the limiting functional

$$I(u) = \frac{1}{2\det\mathrm{Id}}\int_\Omega 2Q_{\mathrm{cell}}(e(u)\cdot Z) = \int_\Omega Q_{\mathrm{cell}}(e(u)\cdot Z)$$

with

$$Q_{\mathrm{cell}}(F\cdot Z) = K_2|F|^2 + K_1(\operatorname{trace}F)^2 + (4K_1-2K_2)(f_{12}+f_{13}+f_{23})^2$$

for $F\in\mathbb{R}^{3\times 3}$ symmetric.

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