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We derive the equivalent energy of a square lattice that either deforms into the three-dimensional Euclidean space or remains planar. Interactions are not restricted to pairs of points and take into account changes of angles. Under some relationships between the local energies associated with the four vertices of an elementary square, we show that the limit energy can be obtained by mere quasiconvexification of the elementary cell energy and that the limit process does not involve any relaxation at the atomic scale. In this case, it can be said that the Cauchy-Born rule holds true. Our results apply to classical models of mechanical trusses that include torques between adjacent bars and to atomistic models.

Keywords: Lattices, nonlinear elasticity, atomistic models, Cauchy-Born rule

1. Introduction

The justification of the laws of solid mechanics from atomistic models has a long history, starting from the works of Cauchy. To derive macroscopic laws from the microscopic behavior, Cauchy assumed that the deformation at the atomistic scale follows the macroscopic deformation. This approach was later extended by Born who, in the case of complex lattices, considered possible relaxation with respect to the sub-lattice. The Cauchy-Born (CB) rule refers usually to one of those two assumptions (no microscopic relaxation or only sub-lattice relaxation) and even sometimes to weaker forms (see Ref. 24, 22 for additional discussions). Modern treatment of the derivation of continuum theories uses asymptotic procedures and can be divided in two different approaches depending on whether or not the CB rule is assumed to apply. On the one side, a major advantage of using the CB rule at the start is that it allows for the analysis of a large range of atomistic and realistic interactions as done in Blanc, Le Bris and Lions.[8,9,10] In particular, not only atomic interactions, but also quantum interactions (through the free electrons), on deterministic and stochastic lattices are dealt with. On the other side, checking the validity of the Cauchy-Born rule is of major interest. This was investigated by Friesecke and Theil[26] who consider reference configurations that may be stressed and deal with deformations close to rigid motions (see also Conti, Dolzmann, Kirchheim, and Müller[18]). E and Ming[23] examine this topic for small deformation gradients. Independently of the Cauchy-Born rule *per se,* a series of works has been devoted by several researchers to the identification of the limit behavior of a lattice by means of variational techniques. Let us mention that, because of compactness requirements for the use of Γ-convergence, minimal growth assumptions have to be satisfied by the microscopic energies thus restricting the class of microscopic interactions. The limit of a one-dimensional lattice made of atoms subject to nearest-neighbour nonlinear interactions is obtained in Braides, Dal Maso and Garroni[12] where a continuous nonlinear model allowing for softening and fracture (see also Truskinovky[36] and Chambolle[16]) is derived. Generalization to nonlocal interactions and long-range interactions, however still in the case of a scalar-valued state function, can be found in 11 and 14 (see also Ref. 13). Alicandro and Cicalese[4] generalize this approach to the fully vectorial case for discrete energies with superlinear growth, Le Dret and Raoult [29] study the hexagonal case, while results in the same spirit are established for stochastic lattices by Iosifescu, Licht, Michaille[27] in a one-dimensional setting and by Alicandro, Cicalese and Gloria[3] in arbitrary dimension. Note that the latter analysis, that is valid for many interactions, provides results of interest in the purely deterministic case as well. The case of multilayers films is studied in the membrane regime by Friesecke and James[25] and Schmidt[34] under a so-called minimal strain hypothesis that restricts the deformation behavior. The same topic is analysed by Alicandro, Braides and Cicalese[2]. Using another scaling, Schmidt[33] derives plate theories for thin (resp. thick) film-like lattices containing a finite (resp. infinite) number of atomic layers. Finally, linear elasticity is obtained as a limit of discrete models by Braides, Solci, Margherita and Vitali[15] and Schmidt.[35] To end up, let us mention that critical modeling and computational issues, in particular related to special geometries, to dislocations, or to defects, are discussed in Refs. 5, 6, 21, 20 and 25 among others.

In the present paper, we focus on angular interactions, which is essential from a mechanical point of view. Indeed, mechanical networks are stabilized by angular torques. Similarly, several atomistic models include angles between bonds: examples are the Stillinger-Weber potential and the Tersoff potential. Under symmetry assumptions on the angular interactions and superlinear growth assumptions on the atomistic energies, we establish the convergence of the discrete models towards a continuous model and we recover the Cauchy-Born rule. We keep the geometrical setting simple since we consider square lattices that may deform into $\mathbb{R}^2$ or into $\mathbb{R}^3$. Note that angular terms have been considered previously in formal asymptotic derivations in the case of biological tissues[30] and for graphenes[17]. Non pairwise interactions have also been taken into account by Shmidt[35,33] for linear and plate models as well as angular forces in 34, though under a minimal strain hypothesis. Alicandro, Cicalese and Gloria[3] devote special attention to terms accounting for volume changes.

In Section 2, we introduce relationships between the four elementary energies associated with the corners of an elementary cell: for instance, we require the stiffness of opposite angles to be equal. These compatibility conditions are needed to perform the analysis that is detailed here and they are shown to be satisfied by realistic examples. In Section 3.1, we give the continuous expression of the discrete energy. A consequence of the relationships just mentioned is that it reads in terms of a single elementary energy. However, a standard piecewise affine interpolate of a discrete deformation is not sufficient to take into account all angles. We make use of a trick consisting of associating with a given discrete deformation two separate piecewise affine interpolates corresponding to two transverse triangulations. At this stage, we can apply Γ-convergence techniques in $L^p(\omega;\mathbb{R}^n)$ in order to identify a limit model. This is the object of Sections 3.2 to 3.4. Note that an angle between two vectors one of which is zero is not properly defined. As a consequence, we impose the natural requirement that adjacent nodes should not be mapped by the deformation on a single point. Some technicalities are induced that are dealt with in Section 3.2 where we give a density lemma and in Section 3.3 where we show how to extend the microscopic energy to matrices that can admit columns equal to 0. We show in Section 4 that the limit energy is equal to 0 on compressed states. Section 5 summarizes our results with respect to the Cauchy-Born rule.

2. Energy of lattices with three point interactions

Let $\omega =]0, L[^2$ be a square domain in $\mathbb{R}^2$ equipped with an orthonormal basis (e_1, e_2). For any $h > 0$, we consider the lattice $\mathcal{L}^h$ whose reference configuration consists of points $M^h_{ij} = (ih, jh)$, $(i, j) \in \mathbb{N}^2$, that belong to $\bar{\omega}$. In order to avoid technicalities that are not central to our analysis, we restrict to $h = L/N_h$, $N_h \in \mathbb{N}$. The lattice is allowed to deform either into $\mathbb{R}^2$ or into $\mathbb{R}^3$. We let $n = 2$ or 3 and we denote by $|\cdot|$ the Euclidean norm in $\mathbb{R}^n$. We assume that any point M^h_{ij} in $\mathcal{L}^h$ is involved in up to four interactions, each of those bringing three points into play. More precisely, let $\mathcal{E} = \{(e_1, e_2), (e_2, -e_1), (-e_1, -e_2), (-e_2, e_1)\}$ and for $(i, j) \in \{0, 1, \ldots, N_h\}^2$, let $\mathcal{E}^h_{ij} = \{(a, b) \in \mathcal{E}, \{M^h_{ij}, M^h_{ij} + ha, M^h_{ij} + hb\} \subset \bar{\omega}\}$. Clearly, if M^h_{ij} belongs to ω, $\mathcal{E}^h_{ij} = \mathcal{E}$, and if M^h_{ij} belongs to $\partial\omega$, $\mathcal{E}^h_{ij}$ consists of two elements or of one element when M^h_{ij} is a vertex of $\bar{\omega}$. Whenever $(a, b) \in \mathcal{E}^h_{ij}$, any point $M^h_{ij} \in \bar{\omega}$ is supposed to interact with $M^h_{ij} + ha$ and $M^h_{ij} + hb$ by means of a microscopic or elementary energy $w^h_{a,b}$ that acts on the deformed positions $\psi(M^h_{ij}), \psi(M^h_{ij} + ha), \psi(M^h_{ij} + hb)$. As $w^h_{a,b}$ does not depend on (i, j) the lattice is periodic. The global internal lattice energy associated with $\psi : \mathcal{L}^h \mapsto \mathbb{R}^n$ is given by

$$I_h(\psi) = \sum_{i,j=0}^{N_h} \sum_{(a,b)\in\mathcal{E}_{ij}^h} w_{a,b}^h(\psi(M_{ij}^h), \psi(M_{ij}^h + ha), \psi(M_{ij}^h + hb)). \tag{2.1}$$

A mechanically sound requirement is that adjacent nodes should not be sent on a single point; this prevents elementary bars to retract to length 0 or to fold. We assume that the nodes that belong to some part Γ_0 of the boundary are clamped. For definiteness, let $\Gamma_0 := \{0\} \times [0, L]$. The set of admissible deformations is therefore given by

$$\begin{aligned} \mathcal{A}_h^* = \{ &\psi : \mathcal{L}^h \mapsto \mathbb{R}^n; \psi_{|\Gamma_0 \cap \mathcal{L}^h} = \varphi_{0|\Gamma_0 \cap \mathcal{L}^h}, \\ &\forall (k,l), (k',l') \, s.t. \, |k'-k| + |l'-l| = 1, \, \psi(k'h, l'h) \neq \psi(kh, lh)\} \end{aligned} \tag{2.2}$$

where $\varphi_0 : \bar{\omega} \mapsto \mathbb{R}^n$ is a given mapping that is supposed to be one-to-one and affine for simplicity. Note that a two-dimensional lattice deforming in $\mathbb{R}^3$ may fold back on itself. Such deformations should not be ruled out by the modeling and they actually belong to $\mathcal{A}_h^*$.

From now on we assume all four energies to be frame indifferent. Their domain of definition is the set of triplets (x, y, z) such that $y \neq x$ and $z \neq x$ and frame indifference implies that

$$\forall (x,y,z) \in (\mathbb{R}^n)^3, y \neq x, z \neq x, \; w_{a,b}^h(x,y,z) = \hat{w}_{a,b}^h(y-x, z-x) \tag{2.3}$$

where $\hat{w}_{a,b}^h : (\mathbb{R}^n \setminus \{0\})^2 \mapsto \mathbb{R}$ satisfies

$$\forall (u,v) \in (\mathbb{R}^n \setminus \{0\})^2, \forall R \in SO(n), \; \hat{w}_{a,b}^h(Ru, Rv) = \hat{w}_{a,b}^h(u,v). \tag{2.4}$$

When $n = 2$, we denote by $\widehat{(u,v)} \in [0, 2\pi[$ the oriented angle between two nonzero vectors and, when $n = 3$, we denote by $\widehat{(u,v)} \in [0, \pi]$ the geometric angle. The energies read in the alternative following ways:

- There exists a function $\check{w}_{a,b}^h : \mathbb{R}^{+*} \times \mathbb{R}^{+*} \times [0, 2\pi[\mapsto \mathbb{R}$ if $n = 2$, $\mathbb{R}^{+*} \times \mathbb{R}^{+*} \times [0, \pi] \mapsto \mathbb{R}$ if $n = 3$, such that for all $(x, y, z) \in (\mathbb{R}^n)^3$, $y \neq x, z \neq x$,

$$w_{a,b}^h(x,y,z) = \check{w}_{a,b}^h(|y-x|, |z-x|, \widehat{(y-x, z-x)}). \tag{2.5}$$

- If $n = 3$, there exists a function $\bar{w}_{a,b}^h : \{(d, d', p) \in \mathbb{R}^{+*} \times \mathbb{R}^{+*} \times \mathbb{R}; |p| \leq dd'\} \mapsto \mathbb{R}$ such that for all $(u, v) \in (\mathbb{R}^3 \setminus \{0\})^2$,

$$\hat{w}_{a,b}^h(u,v) = \bar{w}_{a,b}^h(|u|, |v|, u \cdot v). \tag{2.6}$$

It is classically seen on (2.6) that, when $n = 3$, invariance through $SO(3)$ implies invariance through $O(3)$. As well known, equation (2.5) makes clear that changes in the elementary energies are due to changes of lengths between adjacent points and to changes of angles between interacting vectors.

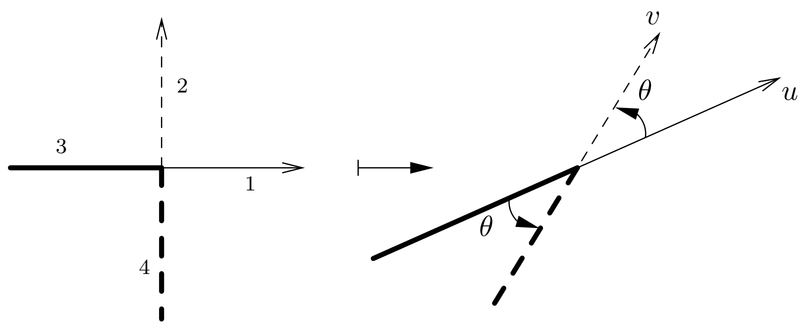

Fig. 1. Deformation of four unit bars by $F = (u, v)$: the stored energy due to the deformed positions of bars 1 and 2 equals the stored energy due to the deformed positions of bars 3 and 4.

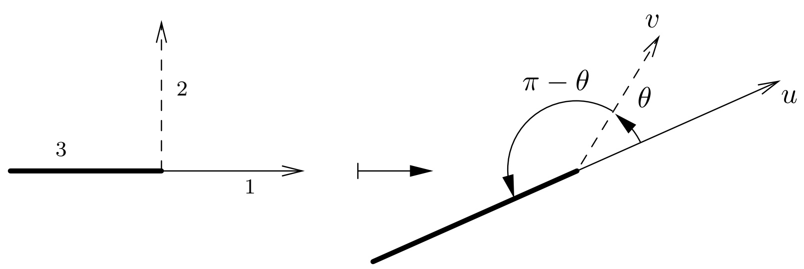

Fig. 2. The stored energy due to the deformed positions of bars 1 and 2 equals the stored energy due to the deformed positions of bars 2 and 3.

In order to perform an asymptotic analysis, we assume that the energies obey the equivalent natural scalings

$$\hat{w}^h_{a,b}(u,v) = h^2 \hat{w}_{a,b}\left(\frac{u}{h}, \frac{v}{h}\right), \ \check{w}^h_{a,b}(d,d',\theta) = h^2 \check{w}_{a,b}\left(\frac{d}{h}, \frac{d'}{h}, \theta\right). \tag{2.7}$$

Note that other scalings could have been chosen leading to other limit models. Finally, in the present study, we restrict our analysis to lattices whose equivalent continuous energy is obtained without homogenization. As will be made clear in the next sections, this can be achieved when the four elementary energies $\hat{w}_{a,b}$, $(a,b) \in \mathcal{E}$, are related through the assumptions

$$\hat{w}_{-e_1,-e_2} = \hat{w}_{e_1,e_2}, \ \hat{w}_{-e_2,e_1} = \hat{w}_{e_2,-e_1}, \ \hat{w}_{e_2,-e_1}(v,-u) = \hat{w}_{e_1,e_2}(u,v), \tag{2.8}$$

or, equivalently, when the four microscopic energies $\check{w}_{a,b}$ satisfy

$$\check{w}_{-e_1,-e_2} = \check{w}_{e_1,e_2}, \ \check{w}_{-e_2,e_1} = \check{w}_{e_2,-e_1}, \ \check{w}_{e_2,-e_1}(d',d,\pi-\theta) = \check{w}_{e_1,e_2}(d,d',\theta). \tag{2.9}$$

The first two assumptions say that opposite pairs have the same mechanical behavior, see Fig. 1. In particular, opposite angles have the same stiffness which usual mechanical devices impose. Note that bars or bonds that are horizontal in the reference configuration may behave differently than vertical bars or bonds. The third assumption correlates adjacent angle stiffness, see Fig. 2.

Let us give some examples. We consider a mechanical truss consisting in a reference configuration of horizontal bars with stiffness k_1^h, of vertical bars with stiffness k_2^h, and of angular springs with stiffness K^h, that make the lattice at rest when bars are orthogonal and of lengths r_1^h and r_2^h. Usually, this is described by

$$\hat{w}_{e_1,e_2}(u,v) = k_1(|u| - r_1)^2 + k_2(|v| - r_2)^2 + K(\cos\widehat{(u,v)})^2, \tag{2.10}$$

and the three corresponding elementary energies that satisfy (2.8). Scalings (2.7) translate in

$$r_1^h = r_1 h,\ r_2^h = r_2 h,\ k_1^h = k_1,\ k_2^h = k_2,\ K^h = Kh^2.$$

Suppose more generally that the angular springs are such that the lattice is at rest when bars $M_{ij}^h M_{i,j+1}^h$ are deformed in bars that make an angle $\gamma \in]0, \pi/2]$ with the undeformed horizontal bars $M_{ij}^h M_{i+1,j}^h$ and consequently an angle $\pi - \gamma$ with the undeformed horizontal bars $M_{ij}^h M_{i-1,j}^h$. Then, one can choose

$$\hat{w}_{e_1,e_2}(u,v) = k_1(|u| - r_1)^2 + k_2(|v| - r_2)^2 + K(\sin(\widehat{(u,v)} - \gamma))^2. \tag{2.11}$$

Note that when $n = 2$, these simple formulations have the drawback to allow the angle between two vectors to enlarge by π at zero cost through a planar rotation although a spring should resist.

A final comment on the energies is that they have no continuous extension to $(\mathbb{R}^n)^2$. Indeed, in (2.10) for instance, $\cos\widehat{(u,v)} = \frac{u}{|u|} \cdot \frac{v}{|v|}$ and $\frac{u}{|u|}$ may converge to any unit vector or not converge at all when u goes to 0. We will see in the sequel how to properly extend a class of more general energies to $\mathbb{R}^n \times \mathbb{R}^n$.

We complete the problem setting by assuming that the lattices are submitted to external loads acting on the nodes of $\mathcal{L}_h$ of the form

$$L_h(\psi) = h^2 \sum_{M \in \mathcal{L}^h} f(M) \cdot \psi(M), \tag{2.12}$$

where f is – say – a continuous function on $\bar{\omega}$ with values in $\mathbb{R}^n$. The total energy of $\mathcal{L}^h$ when deformed by ψ is $J_h(\psi) = I_h(\psi) - L_h(\psi)$ and we seek for the limit behavior of the minimizers φ_h of J_h on $\mathcal{A}_h^*$. Actually, $\mathcal{A}_h^*$ is not a closed subset of the finite dimensional space consisting of mappings from $\mathcal{L}^h$ into $\mathbb{R}^n$, therefore the existence of a minimizer is not obvious even for smooth energies, and we will be interested in almost minimizers.

3. Convergence results

3.1. *Problem reformulation*

It is customary in lattice analysis to associate with each mapping defined on the lattice nodes a piecewise affine function defined on $\bar{\omega}$. This allows to deal with a se-

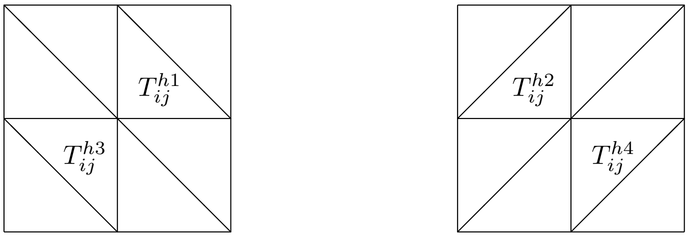

Fig. 3. Left: triangulation $\mathcal{T}_1^h$, Right: triangulation $\mathcal{T}_2^h$

quence of problems whose unknowns belong to a single functional space. We follow this classical trick and we introduce a first triangulation $\mathcal{T}_1^h$ of $\bar{\omega}$ consisting of triangles T_{ij}^{h1} and T_{ij}^{h3}, see Fig. 3: T_{ij}^{h1} is the triangle with vertices $M_{ij}^h, M_{i+1,j}^h, M_{i,j+1}^h$ and T_{ij}^{h3} the triangle with vertices $M_{ij}^h, M_{i-1,j}^h, M_{i,j-1}^h$. From (2.1) and (2.3), and from the scaling assumption (2.7), we have

$$I_h(\psi) = h^2 \sum_{i,j=0}^{N_h} \sum_{(a,b)\in\mathcal{E}_{ij}^h} \hat{w}_{a,b}\Big(\frac{\psi(M_{ij}^h + ha) - \psi(M_{ij}^h)}{h}, \frac{\psi(M_{ij}^h + hb) - \psi(M_{ij}^h)}{h}\Big) \tag{3.1}$$

where $\psi : \mathcal{L}^h \mapsto \mathbb{R}^n$ can be identified with the unique continuous function on $\bar{\omega}$, affine on all triangles T_{ij}^{h1} and T_{ij}^{h3}, that coincides with ψ at each node. In the above sum, let us consider terms corresponding to $(a, b) = (e_1, e_2)$. As ψ is affine on T_{ij}^{h1}, its partial derivatives are constant on T_{ij}^{h1} and they coincide with the difference quotients along e_1 and e_2. Using the fact that T_{ij}^{h1} is of area $h^2/2$, we can write

$$h^2 \hat{w}_{e_1,e_2}\Big(\frac{\psi(M_{ij}^h + he_1) - \psi(M_{ij}^h)}{h}, \frac{\psi(M_{ij}^h + he_2) - \psi(M_{ij}^h)}{h}\Big) = 2\int_{T_{ij}^{h1}} \hat{w}_{e_1,e_2}(\nabla\psi(x))\,dx.$$

Similarly,

$$h^2 \hat{w}_{-e_1,-e_2}\Big(\frac{\psi(M_{ij}^h - he_1) - \psi(M_{ij}^h)}{h}, \frac{\psi(M_{ij}^h - he_2) - \psi(M_{ij}^h)}{h}\Big) = 2\int_{T_{ij}^{h3}} \hat{w}_{-e_1,-e_2}(-\nabla\psi(x))\,dx.$$

From the frame indifference principle, we have

$$\hat{w}_{-e_1,-e_2}(-\nabla\psi(x)) = \hat{w}_{-e_1,-e_2}(\nabla\psi(x)).$$

Indeed, either $n = 3$ and $\hat{w}$ is left $O(n)$-invariant, or $n = 2$ and $-\,\mathrm{Id}$ belongs to $SO(n)$. Using the first assumption in (2.8) that relates $\hat{w}_{-e_1,-e_2}$ and $\hat{w}_{e_1,e_2}$, we obtain that the subsum $I_h^1(\psi)$ of all terms containing $\hat{w}_{e_1,e_2}$ or $\hat{w}_{-e_1,-e_2}$ in (3.1) reads simply

$$I_h^1(\psi) = 2 \int_\omega \hat{w}_{e_1,e_2}(\nabla\psi(x))\,dx.$$

Let us turn to terms corresponding to $(a,b) = (e_2,-e_1)$. They involve the pair $(\frac{\psi(M_{ij}^h+he_2)-\psi(M_{ij}^h)}{h}, \frac{\psi(M_{ij}^h-he_1)-\psi(M_{ij}^h)}{h})$ which does not correspond to finite differences of ψ on a single triangle of $\mathcal{T}_1^h$. Therefore, we introduce a new triangulation $\mathcal{T}_2^h$, transverse to the previous one, consisting of triangles T_{ij}^{h2} with vertices $M_{ij}^h, M_{i,j+1}^h, M_{i-1,j}^h$ and T_{ij}^{h4} with vertices $M_{ij}^h, M_{i,j-1}^h, M_{i+1,j}^h$, see Fig. 3. We denote by $\tilde{\psi}$ the unique continuous function on $\bar{\omega}$, affine on all triangles T_{ij}^{h2} and T_{ij}^{h4}, that coincides with ψ at each node. Then,

$$\begin{aligned} h^2\hat{w}_{e_2,-e_1}\Big(\frac{\psi(M_{ij}^h+he_2)-\psi(M_{ij}^h)}{h}, \frac{\psi(M_{ij}^h-he_1)-\psi(M_{ij}^h)}{h}\Big) \\ = 2\int_{T_{ij}^{h2}} \hat{w}_{e_2,-e_1}(\partial_2\tilde{\psi}(x), -\partial_1\tilde{\psi}(x))\,dx. \end{aligned}$$

Similarly,

$$\begin{aligned} h^2\hat{w}_{-e_2,e_1}\Big(\frac{\psi(M_{ij}^h-he_2)-\psi(M_{ij}^h)}{h}, \frac{\psi(M_{ij}^h+he_1)-\psi(M_{ij}^h)}{h}\Big) \\ = 2\int_{T_{ij}^{h4}} \hat{w}_{-e_2,e_1}(-\partial_2\tilde{\psi}(x), \partial_1\tilde{\psi}(x))\,dx. \end{aligned}$$

From the frame indifference principle and the second assumption in (2.8), all terms in $I_h(\psi)$ containing $\hat{w}_{e_2,-e_1}$ or $\hat{w}_{-e_2,e_1}$ combine in

$$I_h^2(\psi) = 2\int_\omega \hat{w}_{e_2,-e_1}(\partial_2\tilde{\psi}(x), -\partial_1\tilde{\psi}(x))\,dx.$$

Finally, using the third assumption in (2.8), we have

$$I_h(\psi) = 2\int_\omega \hat{w}(\nabla\psi(x))\,dx + 2\int_\omega \hat{w}(\nabla\tilde{\psi}(x))\,dx \tag{3.2}$$

where, for short, $\hat{w} = \hat{w}_{e_1,e_2}$. We emphasize the fact that all assumptions in (2.8) have been necessary to arrive at an integral formulation that makes use of a single elementary energy. If, for instance, opposite angles have distinct stiffness, the analysis we give below does not apply and some homogenization technique has to be incorporated in the limit process.

We are now in a position to study the behavior of almost minimizers ψ_h on $\mathcal{A}_h^*$ of

$$J_h = I_h - L_h,$$

where L_h is given by (2.12). The set $\mathcal{A}_h^*$ can be redefined as

$$\begin{aligned} \mathcal{A}_h^* = \{\psi \in \mathcal{C}^0(\bar{\omega};\mathbb{R}^n);\ \forall T \in \mathcal{T}_h^1, \psi_{|T} \in \mathbb{P}_1(T;\mathbb{R}^n), \psi_{|\Gamma_0} = \varphi_{0|\Gamma_0}, \\ \forall (k,l),(k',l')\ s.t.\ |k'-k|+|l'-l| = 1,\ \psi(k'h,l'h) \neq \psi(kh,lh)\}, \end{aligned}$$

where $\mathbb{P}_1(T;\mathbb{R}^n)$ is the set of polynomials of degree lower or equal to one with values in $\mathbb{R}^n$. Functions φ_h satisfy

$$\varphi_h \in \mathcal{A}_h^*,\ \forall\psi \in \mathcal{A}_h^*,\ J_h(\varphi_h) \leq J_h(\psi) + s(h), \tag{3.3}$$

where $s(h) \geq 0$, $s(h) \to 0$ when $h \to 0$. In the sequel, we will use occasionally the set $\mathcal{A}_h$ which does not require the deformations to be locally one-to-one:

$$\mathcal{A}_h = \{\psi \in \mathcal{C}^0(\bar{\omega};\mathbb{R}^n);\ \forall\, T \in \mathcal{T}_1^h, \psi_{|T} \in \mathbb{P}_1(T;\mathbb{R}^n), \psi_{|\Gamma_0} = \varphi_{0|\Gamma_0}\}. \tag{3.4}$$

3.2. **Γ-*convergence setting***

We identify a matrix F in $\mathbb{M}_{n\times 2}$ with the pair (u,v) of its column vectors and we let $\mathbb{M}_{n\times 2}^* = (\mathbb{R}^n \setminus \{0\}) \times (\mathbb{R}^n \setminus \{0\})$. From now on, we assume that $\hat{w} : \mathbb{M}_{n\times 2}^* \mapsto \mathbb{R}$ is a continuous nonnegative function such that for any $F = (u,v) \in \mathbb{M}_{n\times 2}^*$,

$$\alpha(||F||^p - 1) \leq \hat{w}(F) \leq \beta(||F||^p + 1), \tag{3.5}$$

where $\alpha > 0,\ \beta > 0,\ p > 1$. A natural functional space for the deformations is therefore $W^{1,p}(\omega;\mathbb{R}^n)$ and Γ-convergence may be achieved in $L^p(\omega;\mathbb{R}^n)$. To this end, we extend energies J_h as customary by letting

$$\forall\psi \in L^p(\omega;\mathbb{R}^n) \setminus \mathcal{A}_h^*,\ J_h(\psi) = +\infty. \tag{3.6}$$

Obviously, φ_h solves (3.3) if and only it satisfies

$$\varphi_h \in L^p(\omega;\mathbb{R}^n),\ \forall\psi \in L^p(\omega;\mathbb{R}^n),\ J_h(\varphi_h) \leq J_h(\psi) + s(h). \tag{3.7}$$

We extract from J_h a Γ-convergent subsequence for the $L^p(\omega;\mathbb{R}^n)$-topology and we call J_0 its Γ-limit. As usual, the uniqueness of J_0 will make the extraction of this subsequence unnecessary *a posteriori*.

Proposition 3.1. *Let φ_h be a sequence of almost minimizers in $L^p(\omega;\mathbb{R}^n)$, that is to say a sequence satisfying (3.7).*

- *It is a bounded sequence in $W^{1,p}(\omega;\mathbb{R}^n)$ and there exist $\varphi \in W^{1,p}(\omega;\mathbb{R}^n)$ and a subsequence that we still label by h such that $\varphi_h \to \varphi$ in $L^p(\omega;\mathbb{R}^n)$ and $\varphi_h \rightharpoonup \varphi$ in $W^{1,p}(\omega;\mathbb{R}^n)$,*
- *φ minimizes J_0 on $L^p(\omega;\mathbb{R}^n)$.*

Before proving Proposition 3.1, let us give a technical result on the loading term. The first assertion of Lemma 3.1 will be used in the proof of Proposition 3.1 and the second assertion will be used in Section 3.3 for the proof of Proposition 3.3.

Lemma 3.1. *There exists $C > 0$ such that*

$$\forall h,\ \forall\varphi_h \in \mathcal{A}_h,\ |L_h(\varphi_h)| \leq C\|\varphi_h\|_{L^1(\omega;\mathbb{R}^3)}. \tag{3.8}$$

Moreover, if a sequence of functions $\varphi_h \in \mathcal{A}_h$ converges to φ in $L^1(\omega;\mathbb{R}^3)$, then $L_h(\varphi_h)$ converges to $\int_\omega f \cdot \varphi\, dx$.

Proof. As classically done in the finite element theory for instance, by relying on the equivalence of norms in finite dimension and rescaling, we obtain that

$$\exists C>0, \forall h,\ \forall T\in\mathcal{T}_h^1,\ \forall\psi\in\mathbb{P}_1(T;\mathbb{R}^n),\ h^2\sum_{M\in\mathcal{V}(T)}|\psi(M)|\le C\int_T|\psi|\,dx, \qquad (3.9)$$

where $\mathcal{V}(T)$ stands for the set of vertices of T. This immediately induces that

$$\exists C>0, \forall h,\ \forall\varphi_h\in\mathcal{A}_h,\ h^2\sum_{M\in\mathcal{L}_h}|\varphi_h(M)|\le C\|\varphi_h\|_{L^1(\omega;\mathbb{R}^n)}. \qquad (3.10)$$

Estimate (3.8) is a direct consequence of (2.12) and (3.10).

It remains to prove the second part of the Lemma. Let $\varphi_h\in\mathcal{A}_h$ be a sequence converging to φ in $L^1(\omega;\mathbb{R}^3)$. We have to prove that $L_h(\varphi_h)-\int_\omega f\cdot\varphi\,dx$ converges to 0. This immediately amounts to proving that

$$e_h := L_h(\varphi_h)-\int_\omega f\cdot\varphi_h\,dx$$

converges to 0. We split e_h in two parts, thus obtaining

$$e_h = h^2\sum_{M\in\mathcal{L}^h} f(M)\cdot\varphi_h(M)-\sum_{T\in\mathcal{T}_h^1}\int_T f\cdot\varphi_h\,dx = e_h^1+e_h^2$$

with

$$e_h^1 := h^2\sum_{M\in\mathcal{L}^h} f(M)\cdot\varphi_h(M)-\frac{h^2}{6}\sum_{T\in\mathcal{T}_h^1}\sum_{M\in\mathcal{V}(T)} f(M)\cdot\varphi_h(M),$$

$$e_h^2 := \sum_{T\in\mathcal{T}_h^1} e_{h,T}^2, \quad e_{h,T}^2 := \frac{h^2}{6}\sum_{M\in\mathcal{V}(T)} f(M)\cdot\varphi_h(M)-\int_T f\cdot\varphi_h\,dx.$$

It is easily seen that interior nodes $M=(ih,jh), i,j\neq 0, N_h$, contribute in a equal way to both sums in e_h^1. Therefore, letting $\partial\mathcal{L}^h=\mathcal{L}^h\cap\partial\omega$,

$$e_h^1 = h^2\sum_{M\in\partial\mathcal{L}^h} c_M f(M)\cdot\varphi_h(M),$$

where $c_M=\frac{1}{2},\frac{2}{3}$, or $\frac{5}{6}$. It follows that

$$|e_h^1|\le h^2\sum_{T\in\partial\mathcal{T}_1^h}\sum_{M\in\mathcal{V}(T)}|\varphi_h(M)|,$$

where $\partial\mathcal{T}_1^h$ is the set of triangles in $\mathcal{T}_1^h$ that have at least one vertex on $\partial\omega$. Denoting by o_h the union of these triangles and using (3.9) again, we obtain

$$|e_h^1|\le C\|\varphi_h\|_{L^1(o_h;\mathbb{R}^3)}.$$

Since φ_h converges in $L^1(\omega;\mathbb{R}^3)$ and since the measure of o_h goes to 0, we have $\|\varphi_h\|_{L^1(o_h;\mathbb{R}^3)}\to 0$ which proves that e_h^1 converges to 0.

As for e_h^2, for any T in $\mathcal{T}_h^1$, we decompose $e_{h,T}^2$ as follows. Letting G be any point in T,

$$e_{h,T}^2 = \frac{h^2}{6} \sum_{M \in \mathcal{V}(T)} (f(M) - f(G)) \cdot \varphi_h(M) + \left(\frac{h^2}{6} f(G) \cdot \sum_{M \in \mathcal{V}(T)} \varphi_h(M) - \int_T f \cdot \varphi_h \, dx \right).$$

Since the quadrature formula

$$\int_T \psi \, dx = \frac{|T|}{3} \sum_{M \in \mathcal{V}(T)} \psi(M)$$

is exact for every ψ in $\mathbb{P}_1(T; \mathbb{R}^n)$, we have

$$e_{h,T}^2 = \frac{h^2}{6} \sum_{M \in \mathcal{V}(T)} (f(M) - f(G)) \cdot \varphi_h(M) + \int_T (f(G) - f) \cdot \varphi_h \, dx.$$

Therefore, using (3.10),

$$|e_h^2| \leq (C+1) \max_{(M,M'), |M-M'| \leq \sqrt{2}h} |f(M) - f(M')| \, \|\varphi_h\|_{L^1(\omega;\mathbb{R}^n)}.$$

The result follows. $\square$

Proof. [**of Proposition 3.1**] Let $\psi = \varphi_0$ in (3.7). We have $J_h(\varphi_h) \leq J_h(\varphi_0) + s(h)$. As we made the simplifying assumption that φ_0 is affine and one-to-one, φ_0 belongs to $\mathcal{A}_h^*$ for any h, and $J_h(\varphi_0) = I_h(\varphi_0) - L_h(\varphi_0)$ where I_h is given by (3.2). The first term $I_h(\varphi_0)$ is constant and $L_h(\varphi_0)$ is bounded by Lemma 3.1 for instance. Therefore, $J_h(\varphi_h) \leq C < +\infty$ from which we deduce by (3.2) and the positiveness of $\hat{w}$ that

$$\forall h, \ 2 \int_\omega \hat{w}(\nabla \varphi_h(x)) \, dx \leq C + L_h(\varphi_h).$$

Therefore, by Lemma 3.1,

$$\forall h, \ 2 \int_\omega \hat{w}(\nabla \varphi_h(x)) \, dx \leq C(1 + ||\varphi_h||_{L^p(\omega;\mathbb{R}^n)}).$$

The coerciveness inequality in (3.5) and Poincaré's inequality provide the first assertions of Proposition 3.1. The second point is standard. $\square$

Remark 3.1. The above proof immediately shows that every sequence $\psi_h \in L^p(\omega; \mathbb{R}^n)$ such that $J_h(\psi_h) \leq C < +\infty$ for all h, which necessarily consists of elements of $\mathcal{A}_h^*$, is bounded in $W^{1,p}(\omega; \mathbb{R}^n)$.

The aim is to identify J_0. We begin our analysis by characterizing the domain where J_0 takes finite values. The following result is classical.

Proposition 3.2. *Let* $W^{1,p}_{\Gamma_0}(\omega; \mathbb{R}^n) = \{\psi \in W^{1,p}(\omega; \mathbb{R}^n); \psi_{|\Gamma_0} = \varphi_{0|\Gamma_0}\}$. *For all* ψ *in* $L^p(\omega; \mathbb{R}^n) \setminus W^{1,p}_{\Gamma_0}(\omega; \mathbb{R}^n)$, $J_0(\psi) = +\infty$.

Proof. We proceed by contradiction. Suppose $J_0(\psi) < +\infty$. Since J_h Γ-converges to J_0 for the $L^p(\omega;\mathbb{R}^n)$-topology, there exists a sequence ψ_h in $L^p(\omega;\mathbb{R}^n)$ such that $\psi_h \to \psi$ in $L^p(\omega;\mathbb{R}^n)$ and $J_h(\psi_h) \to J_0(\psi) < +\infty$. Obviously $J_h(\psi_h)$ is bounded from above. Therefore, from Remark 3.1, we deduce that ψ_h converges weakly to ψ in $W^{1,p}(\omega;\mathbb{R}^n)$ which states in particular that ψ belongs to $W^{1,p}_{\Gamma_0}(\omega;\mathbb{R}^n)$. □

Let us now prove that conversely J_0 is finite on $W^{1,p}_{\Gamma_0}(\omega;\mathbb{R}^n)$. When the sequence of problems under study does not arise from discrete models but from continuous models, it usually suffices to let $\psi_h = \psi$ and to simply write that, by mere definition of Γ-convergence, $J_0(\psi) \leq \liminf J_h(\psi) < +\infty$. This does not work here since, in general, ψ does not belong to $\mathcal{A}_h^*$ and $J_h(\psi)$ is not finite. We therefore need a density result of $\mathcal{A}_h^*$ into $L^p(\omega;\mathbb{R}^n)$.

Lemma 3.2. *For any ψ in $W^{1,p}_{\Gamma_0}(\omega;\mathbb{R}^n)$, there exists a sequence ψ_h such that $\psi_h \in \mathcal{A}_h^*$ and $\psi_h \to \psi$ in $W^{1,p}(\omega;\mathbb{R}^n)$.*

Proof. Classical results in interpolation theory prove that any ψ in $W^{1,p}_{\Gamma_0}(\omega;\mathbb{R}^n)$ can be written as the limit in $W^{1,p}(\omega;\mathbb{R}^n)$ of a sequence $\psi_h \in \mathcal{A}_h$. To prove the lemma, it suffices to check that $\mathcal{A}_h^*$ is dense in $\mathcal{A}_h$, or equivalently that $\mathcal{B}_h := \mathcal{A}_h \backslash \mathcal{A}_h^*$ has an empty interior. Obviously,

$$\mathcal{B}_h = \cup_{\{(k,l),(k',l'),\,|k'-k|+|l'-l|=1\}}\{\psi_h \in \mathcal{A}_h; \psi_h(k,l) = \psi_h(k',l')\}.$$

Therefore, $\mathcal{B}_h$ is the finite union of affine subspaces of codimension $n > 0$, which implies that $(\mathcal{B}_h)^\circ = \emptyset$. □

Corollary 3.1. *J_0 is finite on $W^{1,p}_{\Gamma_0}(\omega;\mathbb{R}^n)$.*

Proof. Let ψ be in $W^{1,p}_{\Gamma_0}(\omega;\mathbb{R}^n)$, and let ψ_h be chosen according to Lemma 3.2. Then, $J_0(\psi) \leq \liminf J_h(\psi_h)$. As ψ_h converges to ψ not only in $L^p(\omega;\mathbb{R}^n)$, but also in $W^{1,p}(\omega;\mathbb{R}^3)$, we can say that $I_h(\psi_h)$ is bounded. By Lemma 3.1, $L_h(\psi_h)$ is bounded as well. Therefore, $J_h(\psi_h)$ is bounded and the result follows. □

3.3. *Bound from below*

This section is devoted to finding a bound from below for J_0 on $W^{1,p}_{\Gamma_0}(\omega;\mathbb{R}^n)$. As will be shown in the next section, this bound will turn out to be sufficiently precise to be actually equal to J_0.

Let ψ in $W^{1,p}_{\Gamma_0}(\omega;\mathbb{R}^n)$. There exists a sequence ψ_h in $L^p(\omega;\mathbb{R}^n)$ such that $\psi_h \to \psi$ in $L^p(\omega;\mathbb{R}^n)$ and $J_h(\psi_h) \to J_0(\psi) < +\infty$. From Remark 3.1, we derive that (a subsequence still denoted) ψ_h belongs to $\mathcal{A}_h^*$ and converges weakly to ψ in $W^{1,p}(\omega;\mathbb{R}^n)$. In order to analyze $J_h(\psi_h)$, we need some information on the behavior of the sequence $\tilde{\psi}_h$ which is used in the definition (3.2) of $I_h(\psi_h)$.

Lemma 3.3. *For any sequence ψ_h in $\mathcal{A}_h$ such that ψ_h converges to ψ strongly in $L^p(\omega;\mathbb{R}^n)$ and weakly in $W^{1,p}(\omega;\mathbb{R}^n)$, the sequence $\tilde{\psi}_h$ converges to ψ strongly* *in* $L^p(\omega;\mathbb{R}^n)$ *and weakly in* $W^{1,p}(\omega;\mathbb{R}^n)$ *as well. Moreover,* $\|\nabla\tilde{\psi}_h\|_{L^p(\omega;\mathbb{M}_{n\times 2})} = \|\nabla\psi_h\|_{L^p(\omega;\mathbb{M}_{n\times 2})}$.

Proof. Let Q^h_{ij} be the square with vertices $M^h_{ij}, M^h_{(i+1),j}, M^h_{(i+1),(j+1)}, M^h_{i,(j+1)}$. We divide Q^h_{ij} into triangles T^{h1}_{ij} and $T^{h3}_{(i+1),(j+1)}$ that have been defined in Section 3.1 and into triangles $T^{h2}_{(i+1),j}$ and $T^{h4}_{i,(j+1)}$ as well. Restricted to T^{h1}_{ij} (resp. $T^{h3}_{(i+1),(j+1)}$), $\partial_1\psi_h$ is a constant vector that is equal to $\partial_1\tilde{\psi}_h$ restricted to $T^{h2}_{(i+1),j}$ (resp. $T^{h4}_{i,(j+1)}$). Therefore,

$$\begin{aligned}\int_{Q^h_{ij}} |\partial_1\psi_h|^p\,dx &= \int_{T^{h1}_{ij}\cup T^{h3}_{(i+1),(j+1)}} |\partial_1\psi_h|^p\,dx \\ &= \int_{T^{h2}_{(i+1),j}\cup T^{h4}_{i,(j+1)}} |\partial_1\tilde{\psi}_h|^p\,dx = \int_{Q^h_{ij}} |\partial_1\tilde{\psi}_h|^p\,dx.\end{aligned}$$

Similar equalities hold for the derivatives with respect to x_2. Upon adding the equalities for all squares Q^h_{ij}, we obtain

$$\|\nabla\tilde{\psi}_h\|_{L^p(\omega;\mathbb{M}_{n\times 2})} = \|\nabla\psi_h\|_{L^p(\omega;\mathbb{M}_{n\times 2})}. \tag{3.11}$$

Hence, $\|\nabla\tilde{\psi}_h\|_{L^p(\omega;\mathbb{M}_{n\times 2})}$ is bounded. As $\tilde{\psi}_h$ coincides with φ_0 on Γ_0, we derive from the equivalence of the semi-norm $|\cdot|_{W^{1,p}(\omega;\mathbb{R}^n)}$ and of the norm $\|\cdot\|_{W^{1,p}(\omega;\mathbb{R}^n)}$ on $W^{1,p}_{\Gamma_0}(\omega;\mathbb{R}^n)$ that $\tilde{\psi}_h$ is bounded in $W^{1,p}(\omega;\mathbb{R}^n)$.

Let us now prove that $\chi_h := \tilde{\psi}_h - \psi_h$ converges to 0 in $L^p(\omega;\mathbb{R}^n)$. Since ψ_h and $\tilde{\psi}_h$ coincide on the vertices on any Q^h_{ij} defined above, they coincide on the edges of Q^h_{ij}. In other words, χ_h is equal to 0 on ∂Q^h_{ij}. We use Poincaré's inequality on the unit square and we obtain its scaled version

$$\|\chi_h\|_{L^p(Q^h_{ij};\mathbb{R}^n)} \le h\,\|\nabla\chi_h\|_{L^p(Q^h_{ij};\mathbb{M}_{n\times 2})}$$

which implies that $\|\chi_h\|_{L^p(\omega;\mathbb{R}^n)} \le h\|\nabla\chi_h\|_{L^p(\omega;\mathbb{M}_{n\times 2})}$. Using the first part of the proof, it is immediately seen that $\tilde{\psi}_h$ converges to ψ in $L^p(\omega;\mathbb{R}^n)$. In addition, since $\tilde{\psi}_h$ is a bounded sequence in $W^{1,p}(\omega;\mathbb{R}^n)$, it converges weakly to ψ in $W^{1,p}(\omega;\mathbb{R}^n)$. □

Let us now proceed to study the limit behavior of $J_h(\psi_h)$. To this aim, we extend $\hat{w}$ to $\mathbb{M}_{n\times 2}$ by letting

$$\forall F\in\mathbb{M}_{n\times 2},\ \hat{W}(F) = \begin{cases}\hat{w}(F) \text{ on } \mathbb{M}^*_{n\times 2},\\ \beta(||F||^p+1) \text{ on } \mathbb{M}_{n\times 2}\setminus\mathbb{M}^*_{n\times 2}.\end{cases} \tag{3.12}$$

Note that $\hat{W}$ is not necessarily continuous on the whole of $\mathbb{M}_{n\times 2}$ and that

$$\forall F\in\mathbb{M}_{n\times 2},\ \alpha(||F||^p-1) \le \hat{W}(F) \le \beta(||F||^p+1). \tag{3.13}$$

The quasiconvex envelope of $\hat{W}$ is classically defined[19] by

$$Q\hat{W}(F) = \sup\{z(F);\ z:\mathbb{M}_{n\times 2}\mapsto\mathbb{R},\ z\,\text{quasiconvex}, z\le\hat{W}\} \tag{3.14}$$

and it satisfies

$$\forall F \in \mathbb{M}_{n\times 2},\ 0 \le Q\hat{W}(F) \le \beta(||F||^p + 1). \tag{3.15}$$

Since $\hat{W}$ takes finite values only, all functions z in (3.14) are continuous: indeed, rank-one convex functions that are finite valued are continuous. Therefore, $Q\hat{W}$ is lower semicontinuous, hence Borel measurable.

Proposition 3.3. *For all ψ in $W^{1,p}_{\Gamma_0}(\omega;\mathbb{R}^n)$, $J_0(\psi) \ge 4\int_\omega Q\hat{W}(\nabla\psi(x))\,dx - \int_\omega f(x)\cdot\psi(x)\,dx$.*

Proof. From (3.2) and because ψ_h belongs to $\mathcal{A}_h^*$ and $\hat{w}$ and $\hat{W}$ coincide on $\mathbb{M}^*_{n\times 2}$, $J_h(\psi_h)$ reads

$$J_h(\psi_h) = 2\int_\omega \hat{W}(\nabla\psi_h(x))\,dx + 2\int_\omega \hat{W}(\nabla\tilde{\psi}_h(x))\,dx - L_h(\psi_h).$$

Let

$$H : \psi \in W^{1,p}(\omega;\mathbb{R}^n) \mapsto H(\psi) = \int_\omega Q\hat{W}(\nabla\psi(x))\,dx \in \mathbb{R},$$

which is well defined since $Q\hat{W}$ is Borel measurable and satisfies (3.15). It has been proved[1,19] that the quasiconvexity of $Q\hat{W}$ implies that H is sequentially weakly lower semicontinuous on $W^{1,p}(\omega;\mathbb{R}^n)$. Obviously,

$$J_h(\psi_h) \ge 2\,H(\psi_h) + 2\,H(\tilde{\psi}_h) - L_h(\psi_h).$$

Therefore, using Lemma 3.1 for the loading term,

$$\begin{aligned} J_0(\psi) = \lim J_h(\psi_h) &\ge \liminf(2\,H(\psi_h) + 2\,H(\tilde{\psi}_h)) - \lim L_h(\psi_h) \\ &\ge 2\left(\liminf H(\psi_h) + \liminf H(\tilde{\psi}_h)\right) - \int_\omega f(x)\cdot\psi(x)\,dx \\ &\ge 4\,H(\psi) - \int_\omega f(x)\cdot\psi(x)\,dx, \end{aligned}$$

since by Lemma 3.3 both sequences ψ_h and $\tilde{\psi}_h$ converge weakly to ψ. □

3.4. *Bound from above*

It remains to prove that the inequality in Proposition 3.3 is actually an identity.

Proposition 3.4. *For all ψ in $W^{1,p}_{\Gamma_0}(\omega;\mathbb{R}^n)$, $J_0(\psi) \le 4\int_\omega Q\hat{W}(\nabla\psi(x))\,dx - \int_\omega f(x)\cdot\psi(x)\,dx$.*

Proof. By the definition of Γ-convergence, $J_0(\psi) \le \liminf J_h(\psi_h)$ for any sequence ψ_h that converges to ψ in $L^p(\omega;\mathbb{R}^n)$. From Lemma 3.2, we can choose a sequence $\psi_h \in \mathcal{A}_h^*$ that converges strongly to ψ in $W^{1,p}(\omega;\mathbb{R}^n)$. From Lemma 3.3, we know that $\tilde{\psi}_h$ converges weakly to ψ in $W^{1,p}(\omega;\mathbb{R}^n)$. In fact, it converges strongly as well.

Indeed, it suffices to show that $\|\tilde{\psi}_h\|_{W^{1,p}(\omega;\mathbb{R}^n)} \to \|\psi\|_{W^{1,p}(\omega;\mathbb{R}^n)}$. Actually, from Lemma 3.3 again,

$$\begin{aligned}\|\tilde{\psi}_h\|^p_{W^{1,p}(\omega;\mathbb{R}^n)} &= \|\tilde{\psi}_h\|^p_{L^p(\omega;\mathbb{R}^n)} + \|\nabla\tilde{\psi}_h\|^p_{L^p(\omega;\mathbb{M}_{n\times 2})}\\ &= \|\tilde{\psi}_h\|^p_{L^p(\omega;\mathbb{R}^n)} + \|\nabla\psi_h\|^p_{L^p(\omega;\mathbb{M}_{n\times 2})}\\ &\to \|\psi\|^p_{L^p(\omega;\mathbb{R}^n)} + \|\nabla\psi\|^p_{L^p(\omega;\mathbb{M}_{n\times 2})}\end{aligned}$$

which proves the claim.

Since ψ_h belongs to $\mathcal{A}_h^*$, we have

$$J_h(\psi_h) = I_h(\psi_h) - L_h(\psi_h) \text{ with } I_h(\psi_h) = 2\int_\omega \Big(\hat{w}(\nabla\psi_h(x)) + \hat{w}(\nabla\tilde{\psi}_h(x))\Big)\,dx.$$

We choose an element δ_1 (resp. δ_2) in the $\mathcal{L}^p$ class of $\partial_1\psi$ (resp. $\partial_2\psi$) and we decompose ω in two measurable subsets defined by

$$\omega_1 = \{x \in \omega; \delta_1(x) \neq 0 \,\text{and}\, \delta_2(x) \neq 0\},\ \omega_2 = \omega \setminus \omega_1.$$

Clearly, $I_h(\psi_h) = X_h + Y_h$ where

$$X_h = 2\int_{\omega_1} \Big(\hat{w}(\nabla\psi_h(x)) + \hat{w}(\nabla\tilde{\psi}_h(x))\Big)\,dx,$$

and

$$Y_h = 2\int_{\omega_2} \Big(\hat{w}(\nabla\psi_h(x)) + \hat{w}(\nabla\tilde{\psi}_h(x))\Big)\,dx.$$

Since $\nabla\psi_h$ converges to $\nabla\psi$ in $L^p(\omega;\mathbb{R}^n)$, from any subsequence of $\nabla\psi_h$ we can extract a subsequence $\nabla\psi_{h'}$ that converges almost everywhere towards $\nabla\psi$ and such that $\|\nabla\psi_{h'}\|_{\mathbb{M}_{n\times 2}} \leq g$ where $g \in L^p(\omega;\mathbb{R})$. The continuity of $\hat{w}$ on $\mathbb{M}^*_{n\times 2}$ and the second inequality in (3.5) allow to use the dominated convergence theorem on ω_1, thus proving that

$$\int_{\omega_1} \hat{w}(\nabla\psi_{h'}(x))\,dx \to \int_{\omega_1} \hat{w}(\nabla\psi(x))\,dx.$$

Furthermore, as the limit does not depend on the extracted subsequence, the whole sequence $\int_{\omega_1} \hat{w}(\nabla\psi_h)\,dx$ converges. Since the same result applies to $\int_{\omega_1} \hat{w}(\nabla\tilde{\psi}_h)\,dx$, we obtain that

$$X_h \to 4\int_{\omega_1} \hat{w}(\nabla\psi(x))\,dx = 4\int_{\omega_1} \hat{W}(\nabla\psi(x))\,dx, \tag{3.16}$$

by the definition of ω_1 and by (3.12). Now, by (3.5),

$$Y_h \leq Z_h := 2\,\beta\int_{\omega_2} (\|\nabla\psi_h(x)\|^p + \|\nabla\tilde{\psi}_h(x)\|^p + 2)\,dx. \tag{3.17}$$

The right-hand side converges to

$$Z := 4\,\beta\int_{\omega_2} (\|\nabla\psi(x)\|^p + 1)\,dx = 4\int_{\omega_2} \hat{W}(\nabla\psi(x))\,dx, \tag{3.18}$$

by the definition of ω_2 and by (3.12). Therefore,

$$\liminf(X_h + Y_h) \le 4 \int_\omega \hat{W}(\nabla\psi(x))\,dx. \tag{3.19}$$

At this point, we can say that

$$\forall\psi \in W^{1,p}_{\Gamma_0}(\omega;\mathbb{R}^n),\ J_0(\psi) \le G(\psi), \tag{3.20}$$

where $G(\psi) = 4\int_\omega \hat{W}(\nabla\psi(x))\,dx - \int_\omega f(x)\cdot\psi(x)\,dx$. Since J_0 is sequentially weakly lower semicontinuous on $W^{1,p}_{\Gamma_0}(\omega;\mathbb{R}^n)$, it follows that J_0 is smaller than the sequential weak lower semicontinuous envelope of G on $W^{1,p}_{\Gamma_0}(\omega;\mathbb{R}^n)$. It is well known that for $\hat{W} : \mathbb{M}_{n\times 2} \mapsto \mathbb{R}$ continuous, nonnegative, and satisfying $\hat{W}(F) \le \beta(||F||^p + 1)$, the sequential weak lower semicontinuous envelope of the mapping $\psi \mapsto \int_\omega \hat{W}(\nabla\psi(x))\,dx$ is the mapping $\psi \mapsto \int_\omega Q\hat{W}(\nabla\psi(x))\,dx$. Although less known, the result remains true when $\hat{W}$ is no longer continuous, but Borel measurable, see Theorem 9.1 in Ref. 19. This applies here and ends the proof of Proposition 3.4. □

To conclude this section, we can state the result we aimed at.

Theorem 3.1. *For all ψ in $W^{1,p}_{\Gamma_0}(\omega;\mathbb{R}^n)$,*

$$J_0(\psi) = 4\int_\omega Q\hat{W}(\nabla\psi(x))\,dx - \int_\omega f(x)\cdot\psi(x)\,dx.$$

Remark 3.2. Let

$$\overline{W} = \inf\{z : \mathbb{M}_{n\times 2} \to \mathbb{R} \ :\ z \text{ upper semicontinous on } \mathbb{M}_{n\times 2} \text{ and } z \ge \hat{w} \text{ on } \mathbb{M}^*_{n\times 2}\}$$

be the upper semicontinuous envelope of $\hat{w}$ on $\mathbb{M}_{n\times 2}$. Theorem 3.1 remains true if $\hat{W}$ is replaced by any upper semicontinuous function greater or equal than $\overline{W}$ with at most p-polynomial growth at infinity. It is readily checked that all such extensions have the same quasiconvex envelope.

4. Properties of the limit energy

4.1. *Frame-indifference and states with zero energy*

Standard arguments show that the limit energy obtained in Theorem 3.1 inherits the frame-indifference property of $\hat{w}$. In other words, for any $R \in SO(n)$ and for any F in $\mathbb{M}_{n\times 2}$, $Q\hat{W}(RF) = Q\hat{W}(F)$. In cases when $\hat{w}$ is left-$O(n)$ invariant (if $n = 3$ this is implied by left-$SO(n)$ invariance), so is $Q\hat{W}$. Therefore, in such cases, there exists $\tilde{Y} : \mathbb{S}^2_+ \mapsto \mathbb{R}$ such that for all F in $\mathbb{M}_{n\times 2}$, $Q\hat{W}(F) = \tilde{Y}(F^TF)$ where $\mathbb{S}^2_+$ denotes the set of symmetric, positive-semidefinite matrices.

We now turn to identifying a subset of $\mathbb{M}_{n\times 2}$ on which $Q\hat{W}$ vanishes. Note that similar issues are studied in the general case of multi-well energies in Ref. 7. Let us first give a general result. Singular values of a $n \times 2$ matrix are denoted by v_i, $i = 1, 2$, and the spectral radius of a 2×2 matrix is denoted by ρ.

Proposition 4.1. *Suppose that $\hat{w}$ is left-$O(n)$ invariant and let F_0 be such that $\hat{w}(F_0) = 0$. Then, $Q\hat{W}(F) = 0$ for all matrices F in $\mathbb{M}_{n\times 2}$ such that $|F\xi| \leq |F_0\xi|$ for all ξ in $\mathbb{R}^2$. In particular, if $n = 2$, and F_0 is an invertible matrix, then $Q\hat{W}(F) = 0$ for all matrices F in $\mathbb{M}_{2\times 2}$ such that $v_i(FF_0^{-1}) \leq 1$, $i = 1, 2$.*

Proof. It has been proved in Ref. 28 by extending an idea due to Pipkin[32], that for any $Y : \mathbb{M}_{n\times 2} \mapsto \mathbb{R}$ that is left $O(n)$-invariant and rank 1 convex, the mapping $\tilde{Y} : \mathbb{S}^2_+ \mapsto \mathbb{R}$ such that $Y(F) = \tilde{Y}(F^TF)$ satisfies

$$\forall C, S \in \mathbb{S}^2_+,\ \tilde{Y}(C) \leq \tilde{Y}(C + S). \tag{4.1}$$

Let $F \in \mathbb{M}_{n\times 2}$ such that $|F\xi| \leq |F_0\xi|$ for all ξ in $\mathbb{R}^2$. Therefore, $S := F_0^TF_0 - F^TF$ belongs to $\mathbb{S}^2_+$. By applying (4.1) to $Y = Q\hat{W}$, we obtain,

$$Q\hat{W}(F) = \tilde{Y}(F^TF) \leq \tilde{Y}(F^TF + S) = \tilde{Y}(F_0^TF_0) \leq \hat{W}(F_0) = 0.$$

The second statement is proved by noticing that $|F\xi| \leq |F_0\xi|$ for all ξ in $\mathbb{R}^2$ if and only if $\rho((FF_0^{-1})^TFF_0^{-1}) \leq 1$. □

Let us now concentrate on the examples we listed in Section 2. We first consider energies with rest angle $\frac{\pi}{2}$.

Corollary 4.1. *Let $\hat{w}$ be any left-$O(n)$ invariant elementary energy that vanishes on matrices $F = [u, v]$ such that $|u| = r_1$, $|v| = r_2$, u and v orthogonal, for instance $\hat{w}$ be given by (2.10). Then, for any $F \in \mathbb{M}^*_{n\times 2}$ such that $v_i(F\,\mathrm{diag}(1/r_1, 1/r_2)) \leq 1$, $i = 1, 2$, one has $Q\hat{W}(F) = 0$. In terms of the column vectors u and v of F, this can be rephrased as $Q\hat{W}(F) = 0$ when $|u| \leq r_1$ and $(\frac{u}{r_1} \cdot \frac{v}{r_2})^2 \leq (1 - \frac{|u|^2}{r_1^2})(1 - \frac{|v|^2}{r_2^2})$.*

Proof. For $n = 2$, let $F_0 = \mathrm{diag}(r_1, r_2)$, for $n = 3$, let F_0 be the 3×2 matrix whose columns are $(r_1, 0, 0)^T$ and $(0, r_2, 0)^T$. In both cases, $\hat{W}(F_0) = 0$. From Proposition 4.1, we infer that $Q\hat{W}(F) = 0$ for all matrices F in $\mathbb{M}_{n\times 2}$ such that

$$\forall \xi = (\xi_1, \xi_2) \in \mathbb{R}^2,\ \xi^TF^TF\xi \leq r_1^2\xi_1^2 + r_2^2\xi_2^2,$$

which is easily seen to be equivalent to $\rho(G^TG) \leq 1$ where $G = F\,\mathrm{diag}(1/r_1, 1/r_2)$. The second statement is obtained by letting $D = G^TG$ and recalling that $\rho(D)$ is smaller or equal to 1 if and only if $d_{11} \leq 1$ and $d_{12}^2 \leq (1 - d_{11})(1 - d_{22})$ where we have set $D = (d_{ij}), i, j = 1, 2$. □

Examples of matrices $F = [u, v]$ that satisfy conditions $v_i(F\,\mathrm{diag}(1/r_1, 1/r_2)) \leq 1$, $i = 1, 2$, are matrices with orthogonal column vectors such that $|u| \leq r_1$ and $|v| \leq r_2$. States with non orthogonal column vectors inducing an energy equal to 0 exist as well. Indeed, if $r_1 = r_2 = r$, then all matrices such that $v_i(F) \leq r$, $i = 1, 2$, satisfy $QW(F) = 0$. If $r_1 \neq r_2$, an example is given by $r_1 = 1$, $r_2 = 2$, $|u| = 1/2$, $|v| = 1/2$ and $\widehat{(u, v)} = \pi/4$.

Let now the elementary energy be given by (2.11) with a rest angle γ not necessarily equal to $\frac{\pi}{2}$ (or more generally a frame indifferent energy that vanishes on matrices $F = [u, v]$ such that $|u| = r_1$, $|v| = r_2$, $\widehat{(u, v)} = \gamma$). Proposition 4.1 can be applied only if $n = 3$. Let F_0^γ be the 3×2 matrix whose columns are $(r_1, 0, 0)^T$ and $(r_2 \cos\gamma, r_2 \sin\gamma, 0)^T$. Obviously, $\hat{w}(F_0^\gamma) = 0$. Proposition 4.1 and computations similar to previous ones provide the following result where $\bar{F}_0^\gamma$ is the 2×2 matrix whose columns are $(r_1, 0)^T$ and $(r_2 \cos\gamma, r_2 \sin\gamma)^T$.

Proposition 4.2. *Let $n = 3$ and let the elementary energy be given by (2.11), $\gamma \neq 0$. Then for any $F \in \mathbb{M}^*_{n\times 2}$ such that $v_i(F\,(\bar{F}_0^\gamma)^{-1}) \leq 1$, $i = 1, 2$, one has $Q\hat{W}(F) = 0$. In terms of the column vectors u and v of F, letting $u' = \frac{u}{r_1}$, $v' = \frac{v}{r_2}$, this can be rephrased as $QW(F) = 0$ as soon as $|u'| \leq 1$ and*

$$\left(\frac{u' \cdot v'}{\sin\gamma} - |u'|^2 \cot\gamma\right)^2 \leq (1 - |u'|^2)\left(1 - |u'|^2 \cot^2\gamma - \frac{|v'|^2}{\sin^2\gamma} + 2u' \cdot v' \frac{\cos\gamma}{\sin^2\gamma}\right). \tag{4.2}$$

We leave it to the reader to check that matrices whose column vectors satisfy $|u'| = |v'| \leq 1$ and $\widehat{(u, v)} = \gamma$ are such that $Q\hat{W}(F) = 0$. It is readily seen as well that for any given angle between u and v, for $|u'|$ given such that $|u'| \leq \sin\gamma$, equation (4.2) is satisfied for $|v'|$ small enough.

When $n = 2$, using the fact that $\hat{w}$ defined by (2.11) allows the same energy to pairs (u, v) and $(-u, v)$, we can show by using twice a rank 1 convexity argument that $Q\hat{W}(F) = 0$ for all u and v such that $|u| \leq r_1$, $|v| \leq r_2$, and $\widehat{(u, v)} = \gamma$ or $\pi + \gamma$.

4.2. *Symmetry properties*

We examine the symmetry properties of the limit energy corresponding to a rest angle equal to $\pi/2$ and, for definiteness, to equal rest lengths and equal stiffness k_i, $i = 1, 2$. Obviously, $\hat{W}$ is right invariant through the planar rotations of angle $m\pi/2$, $m \in \mathbb{N}$. Straightforward arguments lead to the following result.

Proposition 4.3. *Let $n = 2, 3$, and $\hat{w}$ be given by (2.10) with $r_1 = r_2$, $k_1 = k_2$. The envelope $Q\hat{W}$ is right invariant through the planar rotations of angle $m\pi/2$, $m \in \mathbb{N}$. Moreover it can be expressed under the form $Q\hat{W}(F) = \tilde{y}(c_{11}, c_{22}, c_{12})$ where $C = F^T F = (c_{ij}), i, j = 1, 2$, and $\tilde{y}$ satisfies $\tilde{y}(c_{11}, c_{22}, c_{12}) = \tilde{y}(c_{22}, c_{11}, -c_{12})$.*

5. Cauchy-Born rule

As explained in the introduction, in its simplest and more restrictive form, the Cauchy-Born rule stipulates that if a crystal lattice is submitted to an affine deformation of the whole of its boundary, then all atoms undergo the same deformation. An immediate extension of this formulation consists in saying first that, as long as plasticity or dislocation effects do not occur and for general boundary conditions, the behavior of a lattice can be approximated by the behavior of a homogeneous, elastic, solid with energy density W, and second in giving a formula for deriving W from the lattice constants. For Bravais lattices, a first guess is that $W(F)$ is directly obtained as the energy of a single cell submitted to the deformation $\varphi_F : x \mapsto Fx$ (or equivalently as the mean value over an increasing domain of the energy due to φ_F). This density $W_{CB}(F)$ is not quasiconvex in general. Then affine deformations φ_F do not necessarily minimize the internal energy among deformations with boundary conditions $\varphi_F(x)$ on the whole of the boundary. A second guess consists in considering that the proper energy is given by QW_{CB}, a process usually known as macroscopic relaxation. More refined theories have emerged: they allow for atom relaxation over a range of cells which gives rise to homogenized energy densities W_{hom} in the spirit of Muller[31] for cellular materials. They can also allow for atom relaxation inside the elementary cell, specially for complex lattices.[22] The magnitude of the several energies just mentioned is decreasing $W_{CB} \geq QW_{CB} \geq W_{hom}$.

In the present paper, we have shown that under assumptions (2.9) the equivalent internal energy density of a square lattice with active angles is actually given by QW_{CB}. In this sense, we say that for such lattices the Cauchy-Born rule holds true. For cases where homogenization is required, possibly including minimization at the cell level, we refer to 3 that considers general geometries and to Le Dret and Raoult [29] who focus on hexagonal lattices.

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