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ELASTIC LIMIT OF SQUARE LATTICES WITH THREE POINT INTERACTIONS

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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 atomic models.

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

AMS Subject Classification: 74K35, 74B20, 49J45

1. Introduction

Recent years have seen a large body of work by many authors on the derivation of an equivalent continuum model for lattices. We briefly describe below the general approach initiated by Braides and coauthors.[10,11,12,13,3] The case of stochastic lattices can be found in Refs. 5, 8 and 9. As emphasized by Ericksen,[19] a major point is to understand the Cauchy-Born rule and to check its validity; for results in this direction, see also Refs. 18 and 21. Finally, let us mention that critical modeling and computational issues, in particular related to special geometries, to dislocations, or to defects, are discussed in Refs. 6, 7, 16, 17 and 20 among others.

According to the context, lattices may be mechanical trusses made of elastic bars or atomic lattices. The first case is not restricted to classical material mechanics and

encompasses biological tissue models.[14,26] Braides and coauthors devised a general rigorous method that expresses the modeling issue in terms of a convergence analysis and they studied an extensive array of examples. The first ingredient in the method is to introduce a sequence of lattices whose bar lengths – or bond lengths – go to 0, and to specify their mechanical or crystal properties. Then, one can seek for a limit behavior. In order to make the sequence of unknown deformations belong to a single functional space, one has to associate with each lattice deformation – which is defined at lattice nodes only – an extended deformation defined on a continuous surface or on a volumic body that contains the original lattice. In practice, piecewise affine interpolates are used. Formulations in terms of energy infima allow to use Γ-convergence tools. Mathematical key tools are relaxation, quasiconvexification and, when appropriate, homogenization.

The energies of the discrete models contain terms such as the distances between neighboring nodes, or longer range distances. It has been proved, see Ref. 4 and the references already mentioned, that in many cases the limit model consists in minimizing an energy that can be said to be elastic since it reads as the integral over a surface or over a volume of an integrand that depends on the gradient of the limit deformation.

In the present paper, we focus on three point interaction lattices. This allows us to consider lattices whose energies depend on the angles between bonds or bars, which is essential from a mechanical point of view. Indeed, mechanical networks are stabilized by angular torques. Similarly, several atomistic models do not restrict to pairwise interactions: examples are the Stillinger-Weber potential and the Tersoff potential. We keep the geometrical setting simple since we consider square lattices that may deform into $\mathbb{R}^2$ or into $\mathbb{R}^3$. Nevertheless, angular terms induce some difficulties. Let us mention that more complicated discrete structures may lead to a much more intricate description. The case of hexagonal lattices for instance – of particular interest for graphenes or carbon nanotubes – has been recently solved first in a purely pairwise setting.[25]

In the present study, an energy is associated with each triplet of vertices of an elementary subsquare, that is a square with side length equal to the grid size. We assume periodicity of the energies along the lattice. We therefore begin with four energies, referred to as microscopic or elementary energies. In Section 2, we recall some consequences of frame indifference. Moreover, we introduce relationships between the four elementary energies: for instance, we require the stiffnesses 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 we consider angle contribution and 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 technical difficulties are induced that are dealt with in Section 3.3 where we show how to extend the microscopic energy to matrices that can admit columns equal to 0, and in Appendix A where we give a density lemma. We show in Section 4 that the limit energy is equal to 0 on compressed states. Section 5 is devoted to a discussion of the Cauchy-Born rule in the simple framework of square lattices.

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. 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 $(i,j) \in \{0, 1, \dots, N_h\}^2$, 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 $\psi : \mathcal{L}^h = \{M^h_{ij} \in \bar{\omega}\} \mapsto \mathbb{R}^n$ is given by

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

The elementary energies $w^h_{a,b}$ must satisfy the frame indifference principle. For an energy w acting on three points m_0, m_1, m_2, this principle states that

$$\begin{aligned} &\forall \psi : \{m_0, m_1, m_2\} \mapsto \mathbb{R}^n,\ \forall R \in SO(n),\ \forall c \in \mathbb{R}^n, \\ &w(R\psi(m_0) + c, R\psi(m_1) + c, R\psi(m_2) + c) = w(\psi(m_0), \psi(m_1), \psi(m_2)). \end{aligned} \tag{2.2}$$

Let us recall the consequences of frame indifference on the expression of w.

Proposition 2.1. *Let w be a frame indifferent energy. Then, there exists a function $\hat{w} : \mathbb{R}^n \times \mathbb{R}^n \mapsto \mathbb{R}$ satisfying*

$$\forall (u,v) \in (\mathbb{R}^n)^2, \forall R \in SO(n),\ \hat{w}(Ru, Rv) = \hat{w}(u,v) \tag{2.3}$$

such that

$$\forall (x,y,z) \in (\mathbb{R}^n)^3,\ w(x,y,z) = \hat{w}(y-x, z-x). \tag{2.4}$$

Proof. By choosing $R = \mathrm{Id}$ and $c = -\psi(m_0)$ in (2.2), we obtain

$$w(\psi(m_0), \psi(m_1), \psi(m_2)) = w(0, \psi(m_1) - \psi(m_0), \psi(m_2) - \psi(m_0)).$$

Letting $\hat{w}(u,v) = w(0,u,v)$, we can write

$$w(\psi(m_0), \psi(m_1), \psi(m_2)) = \hat{w}(\psi(m_1) - \psi(m_0), \psi(m_2) - \psi(m_0)).$$

Property (2.3) follows immediately from (2.2). □

In the above definitions of elementary energies and of frame indifference, we have ignored possible requirements of no superposition of deformed mechanical nodes or atoms. A reasonable restriction is that adjacent nodes should not be sent on a single point, thus preventing an elementary bar to retract to length 0 or to fold. On the contrary, folds of the lattices inside or outside their plane are perfectly admissible from a modeling point of view and they obey this requirement. Therefore, statement (2.2) is actually restricted to deformations ψ such that $\psi(m_1) \neq \psi(m_0)$, $\psi(m_2) \neq \psi(m_0)$, equation (2.4) to triplets (x,y,z) such that $y \neq x$ and $z \neq x$, and equation (2.3) to pairs (u,v) such that $u \neq 0$ and $v \neq 0$. We recall that one may define in $\mathbb{R}^2$ the oriented angle $\widehat{(u,v)}$ between a nonzero vector u and a nonzero vector v: $\widehat{(u,v)} \in [0, 2\pi[$ and $\widehat{(v,u)} = -\widehat{(u,v)}[2\pi]$. In $\mathbb{R}^3$, the angle $\widehat{(u,v)}$ between two non zero vectors belongs to $[0,\pi]$ and $\widehat{(v,u)} = \widehat{(u,v)}$. The Euclidean norm in $\mathbb{R}^n$ is denoted by $|\cdot|$. Proposition 2.1 can be rephrased as follows.

Corollary 2.1. *Let w be a frame indifferent energy. Then,*

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

$$w(x,y,z) = \check{w}(|y-x|, |z-x|, \widehat{(y-x, z-x)}). \tag{2.5}$$

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

$$\hat{w}(u,v) = \bar{w}(|u|, |v|, u \cdot v). \tag{2.6}$$

Proof. Let $n = 2$ or 3. Let u, v, s, t be four nonzero vectors such that $|s| = |u|$, $|t| = |v|$, $\widehat{(s,t)} = \widehat{(u,v)}$. Then, there exists a direct isometry that maps u on s and v on t. This proves (2.5). If $n = 3$, conditions $|s| = |u|$, $|t| = |v|$, $s \cdot t = u \cdot v$ are sufficient to ensure that $\widehat{(s,t)} = \widehat{(u,v)}$ from which (2.6) follows. □

Remark 2.1. It is seen on (2.6) that, when $n = 3$, invariance of w through $SO(3)$ implies invariance through $O(3)$. The analog is not true when $n = 2$: consider $\hat{w}(u,v) = \det(u,v)$.

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. These are classical ingredients in models for atom lattices as well as in models for mechanical trusses whose bars can elongate or shorten while remaining straight. A standard three point energy is given for (u, v) in $(\mathbb{R}^n \setminus \{0\})^2$ by

$$\begin{aligned}\hat{w}(u, v) &= k_1(|u| - r_1)^2 + k_2(|v| - r_2)^2 + K(\cos\theta)^2 \\ &= k_1(|u| - r_1)^2 + k_2(|v| - r_2)^2 + K\left(\frac{u}{|u|} \cdot \frac{v}{|v|}\right)^2, \end{aligned} \tag{2.7}$$

where θ is the angle between the nonzero vectors u and v, r_1 and r_2 are bar or bond lengths at rest, k_1 and k_2 are bar stiffnesses and K is a spring stiffness. And more generally by

$$\hat{w}(u, v) = g_1(|u|) + g_2(|v|) + g(\theta). \tag{2.8}$$

Although generally continuous on $(\mathbb{R}^n \setminus \{0\})^2$, such energies have no continuous extensions to $(\mathbb{R}^n)^2$ when $g \neq 0$. In (2.7) for instance $\frac{u}{|u|}$ 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 them to $\mathbb{R}^n \times \mathbb{R}^n$.

Let us now apply the previous remarks to lattices $\mathcal{L}^h$. For definiteness, we consider that nodes that belong to the part of the boundary defined by $\Gamma_0 := ([0, L] \times \{L\}) \cup (\{L\} \times [0, L])$ are clamped. As previously mentioned, the deformations are supposed to map adjacent nodes on distinct points. Altogether this leads to the definition of the set of admissible deformations

$$\begin{aligned}&\mathcal{A}_h^* = \{\psi : \mathcal{L}^h \mapsto \mathbb{R}^n; \psi_{|\Gamma_0 \cap \mathcal{L}^h} = \varphi_{0|\Gamma_0 \cap \mathcal{L}^h}, \\ &\forall (k, l), (k', l')\, s.t. \, |k' - k| + |l' - l| = 1,\ \psi(k'h, l'h) \neq \psi(kh, lh)\}\end{aligned} \tag{2.9}$$

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. Regarding the energies w_{ab}^h, we impose as a first requirement that they satisfy the principle of frame indifference that has been discussed above. Therefore, there exist $\hat{w}_{ab}^h$ and $\check{w}_{ab}^h$ – whose domains have been defined in Proposition 2.1 and Corollary 2.1 – such that for all $(x, y, z) \in (\mathbb{R}^n)^3, y \neq x, z \neq x$,

$$w_{ab}^h(x, y, z) = \hat{w}_{ab}^h(y - x, z - x) = \check{w}_{ab}^h(|y - x|, |z - x|, \theta). \tag{2.10}$$

The second assumption on the energies concerns their behavior with respect to h: we assume that they obey the natural scaling

$$\hat{w}_{ab}^h(u, v) = h^2 \hat{w}_{ab}\left(\frac{u}{h}, \frac{v}{h}\right) \tag{2.11}$$

which, with obvious notations, expresses equivalently as

$$\check{w}_{ab}^h(d, d', \theta) = h^2 \check{w}_{ab}\left(\frac{d}{h}, \frac{d'}{h}, \theta\right).$$

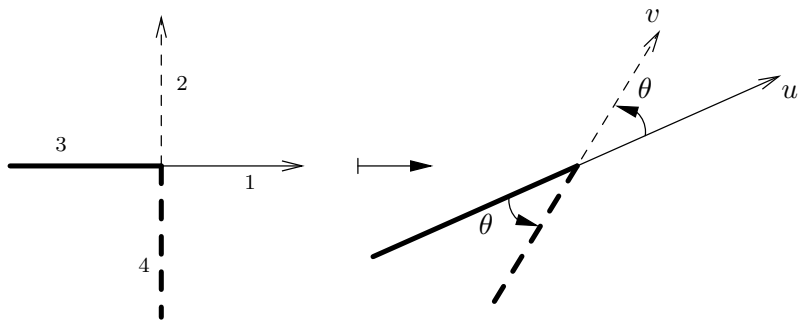

Fig. 1. Deformation of four unit bars by $F = (u, v)$: the stored energy due to the deformed positions of bars 1 and 2 equals the stored energy due to the deformed positions of bars 3 and 4.

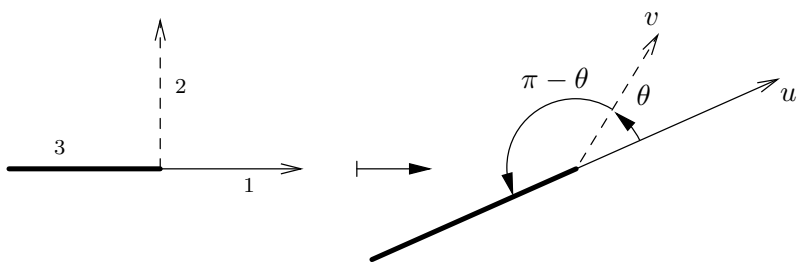

Fig. 2. The stored energy due to the deformed positions of bars 1 and 2 equals the stored energy due to the deformed positions of bars 2 and 3.

For (2.7) for instance, this means that

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

Note that other scalings could have been chosen leading to other limit models. Third, 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

$$\hat{w}_{-e_1,-e_2} = \hat{w}_{e_1,e_2},\ \hat{w}_{-e_2,e_1} = \hat{w}_{e_2,-e_1},\ \hat{w}_{e_2,-e_1}(v, -u) = \hat{w}_{e_1,e_2}(u, v), \tag{2.12}$$

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

$$\check{w}_{-e_1,-e_2} = \check{w}_{e_1,e_2},\ \check{w}_{-e_2,e_1} = \check{w}_{e_2,-e_1},\ \check{w}_{e_2,-e_1}(d', d, \pi-\theta) = \check{w}_{e_1,e_2}(d, d', \theta). \tag{2.13}$$

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 stiffnesses in a natural way, 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 that make the lattice at rest when bars are orthogonal. Then, the elementary energies may be chosen of the form (2.7) with

$$\hat{w}_{e_1,e_2}(u,v) = k_1(|u|-r_1)^2 + k_2(|v|-r_2)^2 + K(\cos\widehat{(u,v)})^2, \tag{2.14}$$

$$\hat{w}_{e_2,-e_1}(v,u) = k_1(|u|-r_1)^2 + k_2(|v|-r_2)^2 + K(\cos\widehat{(v,u)})^2, \tag{2.15}$$

$$\hat{w}_{-e_1,-e_2}(u,v) = k_1(|u|-r_1)^2 + k_2(|v|-r_2)^2 + K(\cos\widehat{(u,v)})^2, \tag{2.16}$$

$$\hat{w}_{-e_2,e_1}(v,u) = k_1(|u|-r_1)^2 + k_2(|v|-r_2)^2 + K(\cos\widehat{(v,u)})^2, \tag{2.17}$$

and conditions (2.12) are satisfied. 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

$$\hat{w}_{e_1,e_2}(u,v) = k_1(|u|-r_1)^2 + k_2(|v|-r_2)^2 + K(\sin(\widehat{(u,v)}-\gamma))^2, \tag{2.18}$$

$$\hat{w}_{e_2,-e_1}(v,u) = k_1(|u|-r_1)^2 + k_2(|v|-r_2)^2 + K(\sin(\widehat{(v,u)}+\gamma-\pi))^2, \tag{2.19}$$

$$\hat{w}_{-e_1,-e_2}(u,v) = k_1(|u|-r_1)^2 + k_2(|v|-r_2)^2 + K(\sin(\widehat{(u,v)}-\gamma))^2, \tag{2.20}$$

$$\hat{w}_{-e_2,e_1}(v,u) = k_1(|u|-r_1)^2 + k_2(|v|-r_2)^2 + K(\sin(\widehat{(v,u)}+\gamma-\pi))^2, \tag{2.21}$$

and conditions (2.12) are satisfied as well. 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.

Finally, lattices are submitted to external loads acting on nodes $M_{ij}^h, (i,j) \in \{0,\dots,N_h-1\}^2$ that read

$$L_h(\psi) = h^2 \sum_{i,j=0}^{N_h-1} f(ih,jh)\cdot\psi(ih,jh)$$

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 sequence of problems whose unknowns belong to a single functional space. We follow

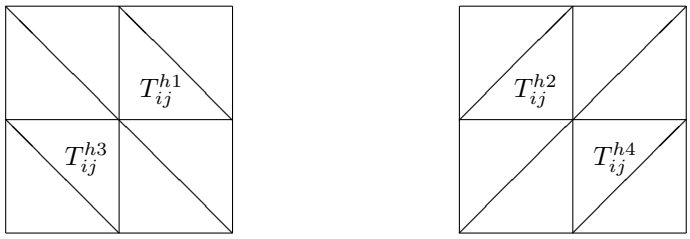

Fig. 3. Left: triangulation $\mathcal{T}_1^h$, Right: triangulation $\mathcal{T}_2^h$

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 (2.4), and from the scaling assumption (2.11), 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, as seen in Remark 2.1, or $n = 2$

and $-\operatorname{Id}$ belongs to $SO(n)$. From the first assumption in (2.12), we derive that

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

Therefore 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. We obtain

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

Similarly,

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

From the frame indifference principle, this transforms as

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

We now use the second assumption in (2.12) and we gather all terms in $I_h(\psi)$ containing $\hat{w}_{e_2,-e_1}$ or $\hat{w}_{-e_2,e_1}$. We obtain

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

Finally, using the third assumption in (2.12), 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 (2.12) have been necessary to arrive at an integral formulation that makes use of a single elementary energy. If, for instance, opposite angles have distinct stiffnesses, 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

$$J_h = I_h - L_h.$$

The set $\mathcal{A}_h^*$ can be redefined as

$$\begin{aligned}\mathcal{A}_h^* = \{&\psi \in \mathcal{C}^0(\bar{\omega};\mathbb{R}^n);\ \forall\, T \in \mathcal{T}_h^1, \psi_{|T} \in \mathbb{P}_1(T;\mathbb{R}^n), \psi_{|\Gamma_0} = \varphi_{0|\Gamma_0},\\ &\forall (k,l),(k',l')\ s.t.\ |k'-k| + |l'-l| = 1,\ \psi(k'h,l'h) \neq \psi(kh,lh)\},\end{aligned} \tag{3.3}$$

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

$$\varphi_h \in \mathcal{A}_h^*,\ \forall \psi \in \mathcal{A}_h^*,\ J_h(\varphi_h) \leq J_h(\psi) + s(h), \tag{3.4}$$

where $s(h) \geq 0$, $s(h) \to 0$ when $h \to 0$. For the reader's convenience, we recall that I_h is given on $\mathcal{A}_h^*$ by (3.2) and that

$$L_h(\psi) = h^2 \sum_{i,j=0}^{N_h-1} f(ih,jh) \cdot \psi(ih,jh). \tag{3.5}$$

In the sequel, we will use occasionally the set $\mathcal{A}_h$ which does not require the deformations to be locally one-to-one:

$$\mathcal{A}_h = \{\psi \in \mathcal{C}^0(\bar{\omega};\mathbb{R}^n);\ \forall\, T \in \mathcal{T}_1^h, \psi_{|T} \in \mathbb{P}_1(T;\mathbb{R}^n), \psi_{|\Gamma_0} = \varphi_{0|\Gamma_0}\}. \tag{3.6}$$

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, with no lack of generality, that $\hat{w} : \mathbb{M}_{n\times 2}^* \mapsto \mathbb{R}$ is a continuous nonnegative function such that for any $F = (u,v) \in \mathbb{M}_{n\times 2}^*$,

$$\alpha(||F||^p - 1) \leq \hat{w}(F) \leq \beta(||F||^p + 1), \tag{3.7}$$

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

$$\forall \psi \in L^p(\omega;\mathbb{R}^n) \setminus \mathcal{A}_h^*,\ J_h(\psi) = +\infty. \tag{3.8}$$

Obviously, φ_h solves (3.4) if and only it satisfies

$$\varphi_h \in L^p(\omega;\mathbb{R}^n),\ \forall \psi \in L^p(\omega;\mathbb{R}^n),\ J_h(\varphi_h) \leq J_h(\psi) + s(h). \tag{3.9}$$

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*. We let

$$W^{1,p}_{\Gamma_0}(\omega;\mathbb{R}^n) = \{\psi \in W^{1,p}(\omega;\mathbb{R}^n); \psi_{|\Gamma_0} = \varphi_{0|\Gamma_0}\}.$$

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 (3.9).*

- *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 emphasize the fact that dealing with the loading term is straightforward in usual Γ-convergence proofs, that is in a "continuous-to-continuous" setting. Here, the discrete-to-continuous process imposes some care in characterizing the loading term behavior. This will be seen again in Section 3.3 for the proof of Proposition 3.3. In order not to be distracted from the main topic of the paper which is the behavior of the internal energy, we gather technical approximation lemmas in Appendix A.

Proof. Let $\psi = \varphi_0$ in (3.9). 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, since for any h, $L_h(\varphi_0)$ is a Riemann sum associated with $f \cdot \varphi_0$, the sequence $L_h(\varphi_0)$ is bounded. In addition, $s(h)$ goes to 0. 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 A.1,

$$\forall h,\ 2\int_\omega \hat{w}(\nabla\varphi_h(x))\,dx \leq C + C_2||\varphi_h||_{L^p(\omega;\mathbb{R}^n)}.$$

The coerciveness inequality in (3.7) and Poincaré's inequality provide the first assertions of Proposition 3.1. The second point is standard. □

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. *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 $L^p(\omega;\mathbb{R}^n)$. The proof of the following technical lemma which actually gives a stronger result is given in Appendix A.

Lemma 3.1. *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 $W^{1,p}(\omega;\mathbb{R}^n)$.*

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 3.1. 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 A.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 Lemma 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 3.2. *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

$$\|\nabla\tilde{\psi}_h\|_{L^p(\omega;\mathbb{M}_{n\times 2})} = \|\nabla\psi_h\|_{L^p(\omega;\mathbb{M}_{n\times 2})}. \tag{3.10}$$

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 the whole of $\mathbb{M}_{n\times 2}$ by letting

$$\forall F\in\mathbb{M}_{n\times 2},\ \hat{W}(F) = \begin{cases}\hat{w}(F) \text{ on } \mathbb{M}^*_{n\times 2},\\ \beta(||F||^p+1) \text{ on } \mathbb{M}_{n\times 2}\setminus\mathbb{M}^*_{n\times 2}.\end{cases} \tag{3.11}$$

Obviously,

$$\forall F\in\mathbb{M}_{n\times 2},\ \alpha(||F||^p-1)\le\hat{W}(F)\le\beta(||F||^p+1), \tag{3.12}$$

and $J_h(\psi_h)$ reads

$$J_h(\psi_h) = 2\,K(\psi_h) + 2\,K(\tilde{\psi}_h) - L_h(\psi_h) \tag{3.13}$$

where K is defined on $W^{1,p}_{\Gamma_0}(\omega;\mathbb{R}^n)$ by

$$\forall\psi\in W^{1,p}_{\Gamma_0}(\omega;\,\mathbb{R}^n),\ K(\psi) = \int_\omega \hat{W}(\nabla\psi(x)\,dx. \tag{3.14}$$

As can be expected, the quasiconvex envelope $Q\hat{W}$ of $\hat{W}$ will be of use in the sequel. We recall that a Borel measurable and locally integrable function $z:\mathbb{M}_{n\times 2}\mapsto\mathbb{R}$ is

quasiconvex if for a domain $d \subset \mathbb{R}^2$, for all $F \in M_{n\times 2}$, and for all $\psi \in W_0^{1,\infty}(d;\mathbb{R}^n)$,

$$z(F) \leq \frac{1}{|d|}\int_d z(F+\nabla\psi(x))\,dx,$$

and that the property does not depend on d. The quasiconvex envelope of $\hat{W}$ is classically defined[15] by

$$Q\hat{W}(F) = \sup\{z(F);\ z : \mathbb{M}_{n\times 2} \mapsto \mathbb{R},\ z \,\text{quasiconvex}, z \leq \hat{W}\} \tag{3.15}$$

and it satisfies

$$\forall F \in \mathbb{M}_{n\times 2},\ 0 \leq Q\hat{W}(F) \leq \beta(||F||^p + 1). \tag{3.16}$$

Since $\hat{W}$ takes finite values only, all functions z in (3.15) 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 $W^{1,p}_{\Gamma_0}(\omega;\mathbb{R}^n)$, $J_0(\psi) \geq 4\int_\omega Q\hat{W}(\nabla\psi(x))\,dx - \int_\omega f(x)\cdot\psi(x)\,dx$.*

Proof. Let us first mention that the limit behavior of the loading term $L_h(\psi_h)$ in (3.13) is studied in Appendix A. Lemma A.2 shows that $L_h(\psi_h)$ converges to $\int_\omega f(x)\cdot\psi(x)\,dx$. 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 (3.16). It has been proved[2,15] that the quasiconvexity of $Q\hat{W}$ implies that H is sequentially weakly lower semicontinuous on $W^{1,p}(\omega;\mathbb{R}^n)$. Obviously,

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

and

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

since by Lemma 3.2 both sequences ψ_h and $\tilde{\psi}_h$ converge weakly to ψ. □

3.4. *Bound from above*

As mentioned previously, it remains to prove that the inequality in Proposition 3.3 is actually an identity.

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

Proof. By the definition of Γ-convergence, $J_0(\psi) \leq \liminf J_h(\psi_h)$ for any sequence ψ_h that converges to ψ in $L^p(\omega;\mathbb{R}^n)$. From Lemma 3.1, 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 3.2, 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 3.2 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. Therefore, there exist $g \in L^p(\omega;\mathbb{R})$ and a subsequence labelled by h' such that

$$\nabla\psi_{h'} \to \nabla\psi \text{ a.e.}, \quad \|\nabla\psi_{h'}\|_{\mathbb{M}_{n\times 2}} \leq g \text{ a.e.} \tag{3.17}$$

$$\nabla\tilde{\psi}_{h'} \to \nabla\psi \text{ a.e.}, \quad \|\nabla\tilde{\psi}_{h'}\|_{\mathbb{M}_{n\times 2}} \leq g \text{ a.e.} \tag{3.18}$$

Since $\psi_{h'}$ belongs to $\mathcal{A}^*_{h'}$, we have again

$$J_{h'}(\psi_{h'}) = 2\,K(\psi_{h'}) + 2\,K(\tilde{\psi}_{h'}) - L_h(\psi_{h'})$$

where K is given by (3.14). We recall that $\hat{W}$ is not continuous on $\mathbb{M}_{n\times 2}$, but that it coincides on $\mathbb{M}^*_{n\times 2}$ with $\hat{w}$ which is continuous. 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 into 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,

$$K(\psi_{h'}) + K(\tilde{\psi}_{h'}) = X_{h'} + Y_{h'}, \tag{3.19}$$

where

$$X_{h'} = \int_{\omega_1}\Big(\hat{W}(\nabla\psi_{h'}(x)) + \hat{W}(\nabla\tilde{\psi}_{h'}(x))\Big)\,dx = \int_{\omega_1}\Big(\hat{w}(\nabla\psi_{h'}(x)) + \hat{w}(\nabla\tilde{\psi}_{h'}(x))\Big)\,dx,$$

since $\psi_{h'}(x)$ belongs to $\mathcal{A}^*_{h'}$, and

$$Y_{h'} = \int_{\omega_2}\Big(\hat{W}(\nabla\psi_{h'}(x)) + \hat{W}(\nabla\tilde{\psi}_{h'}(x))\Big)\,dx.$$

The second inequality in (3.7) and property (3.17)-(3.18) on the one hand allow to use the dominated convergence theorem on ω_1, thus proving that

$$X_{h'} \to 2\int_{\omega_1} \hat{w}(\nabla\psi(x))\,dx = 2\int_{\omega_1} \hat{W}(\nabla\psi(x))\,dx. \tag{3.20}$$

On the other hand, by (3.11),

$$Y_{h'} \leq Z_{h'} := \beta\int_{\omega_2} \Big((\|\nabla\psi_{h'}(x)\|^p_{\mathbb{M}_{n\times 2}} + 1) + (\|\nabla\tilde{\psi}_{h'}(x)\|^p_{\mathbb{M}_{n\times 2}} + 1)\Big)\,dx. \tag{3.21}$$

It is immediately checked that $Z_{h'}$ converges to

$$Z := 2\,\beta\int_{\omega_2} (\|\nabla\psi(x)\|^p_{\mathbb{M}_{n\times 2}} + 1)\,dx = 2\int_{\omega_2} \hat{W}(\nabla\psi(x))\,dx. \tag{3.22}$$

Therefore,

$$\liminf(X_{h'} + Y_{h'}) \leq 2\int_{\omega} \hat{W}(\nabla\psi(x))\,dx. \tag{3.23}$$

At this point, we can say that

$$\forall\psi \in W^{1,p}_{\Gamma_0}(\omega;\mathbb{R}^n),\ J_0(\psi) \leq\ G_0(\psi), \tag{3.24}$$

where $G_0(\psi) = 4\int_\omega \hat{W}(\nabla\psi(x))\,dx - \int_\omega f(x)\cdot\psi(x)\,dx$. Since J_0 is sequentially weakly lower semicontinuous on $W^{1,p}_{\Gamma_0}(\omega;\mathbb{R}^n)$, it follows that $J_0 \leq \Gamma\text{-}G_0$ where $\Gamma\text{-}G_0$ is the sequential weak lower semicontinuous envelope of G_0 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, positive and satisfying (3.7), the sequential weak lower semicontinuous envelope of K defined by $K(\psi) = \int_\omega \hat{W}(\nabla\psi(x))\,dx$ is given by $\Gamma\text{-}K(\psi) = \int_\omega Q\hat{W}(\nabla\psi(x))\,dx$. Although less known, the result remains true when $\hat{W}$ is no longer continuous, but Borel measurable, see Theorem 9.1 in Ref. 15. 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 $W^{1,p}_{\Gamma_0}(\omega;\mathbb{R}^n)$,*

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

4. Properties of the limit energy

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

We investigate the invariance properties of the limit energy obtained in Theorem 3.1. We recall that $\hat{w} : \mathbb{M}^*_{n\times 2} = (\mathbb{R}^n \setminus \{0\}) \times (\mathbb{R}^n \setminus \{0\}) \mapsto \mathbb{R}$ has been supposed to be frame indifferent, see Proposition 2.1, and that $\hat{W}$ has been defined by

$$\forall F \in \mathbb{M}_{n\times 2},\ \hat{W}(F) = \begin{cases} \hat{w}(F) \text{ on } \mathbb{M}^*_{n\times 2}, \\ \beta(||F||^p + 1) \text{ on } \mathbb{M}_{n\times 2} \setminus \mathbb{M}^*_{n\times 2}. \end{cases} \tag{4.1}$$

Proposition 4.1. *The limit energy $4Q\hat{W}$ is frame indifferent in the sense that for any $R \in SO(n)$ and for any F in $\mathbb{M}_{n\times 2}$, $Q\hat{W}(RF) = Q\hat{W}(F)$.*

Proof. Let $R \in SO(n)$. Since $\hat{w}$ is frame indifferent, we can write that

$$\forall F = (u, v) \in \mathbb{M}^*_{n\times 2},\ \hat{w}(Ru, Rv) = \hat{w}(u, v),$$

with which it is immediately seen on (4.1) that

$$\forall F = (u, v) \in \mathbb{M}_{n\times 2},\ \hat{W}(RF) = \hat{W}(F).$$

The result follows from definition (3.15) since when $F \mapsto z(F)$ is quasiconvex, so is $F \mapsto z(RF)$. □

We denote by $\mathbb{S}^2_+$ the set of 2×2 symmetric, positive-semidefinite matrices.

Corollary 4.1. *If $n = 3$, there exists $\tilde{Y} : \mathbb{S}^2_+ \mapsto \mathbb{R}$ such that $\forall F \in \mathbb{M}_{3\times 2}$, $Q\hat{W}(F) = \tilde{Y}(F^T F)$. In particular, $Q\hat{W}$ is left $O(3)$-invariant.*

Proof. We have already noticed in the proof of Corollary 2.1 that for F and G in $\mathbb{M}_{3\times 2}$ such that $F^T F = G^T G$, there exists R in $SO(3)$ such that $G = RF$. □

From now on, we will concentrate on the main example we gave in Section 2. Namely, an energy corresponding to rest bar lengths r_1, r_2 and to rest values for the four angles around a node given in trigonometric order by γ, $\pi - \gamma$, γ, $\pi - \gamma$. In other words, see (2.14), (2.18),

$$\hat{w}(u, v) = k_1(|u| - r_1)^2 + k_2(|v| - r_2)^2 + K(\sin(\theta - \gamma))^2, \tag{4.2}$$

where θ is the angle between u and v. When $\gamma = \pi/2$, (4.2) reads

$$\hat{w}(u, v) = k_1(|u| - r_1)^2 + k_2(|v| - r_2)^2 + K(\cos\theta)^2. \tag{4.3}$$

The energy given by (4.2) makes clear that Corollary 4.1 has no counterpart for $n = 2$. Indeed, $\hat{w}$ is not left invariant through the planar reflections R_δ of axis δ except when $\gamma = \pi/2$. This is meaningful from a modeling point of view: in order to mechanically bring within their plane two interacting bonds or bars onto their images through R_δ a torque has to be exerted and the angular spring should resist. One may wonder why the same definition (4.2) provides an invariant energy when $n = 3$. From a modeling point of view, sending – as just described – two bars defining a plane P onto their images through a planar reflection in P is perfectly admissible since it can be obtained through the rotation in $\mathbb{R}^3$ with axis δ and angle π. This rotation acts out of the plane P. From a calculation point of view, this is alternatively seen directly on (4.2): indeed, when $n = 3$, θ belongs to $[0, \pi]$ and $\sin(\theta - \gamma)$ expresses in terms of $\cos\theta$.

We now turn to identifying a subset of $\mathbb{M}_{n\times 2}$ on which $Q\hat{W}$ vanishes. Whenever $Q\hat{W}$ is left $O(n)$-invariant, we can use Pipkin's argument. Indeed, it has been proved

in Ref. 24 by extending Pipkin's idea that for any $Y : \mathbb{M}_{n\times 2} \mapsto \mathbb{R}$, $n = 2, 3$, that is left $O(n)$-invariant (and consequently reads $Y(F) = \tilde{Y}(F^T F)$) and rank 1 convex, the mapping $\tilde{Y} : \mathbb{S}^2_+ \mapsto \mathbb{R}$ satisfies

$$\forall C, S \in \mathbb{S}^2_+,\ \tilde{Y}(C) \leq \tilde{Y}(C + S). \tag{4.4}$$

From now on, we let $Y = Q\hat{W}$ and when $\hat{W}$ is $O(n)$-invariant (hence $Q\hat{W}$ is), we write $\hat{W}(F) = \tilde{W}(F^T F)$ and $Y(F) = Q\hat{W}(F) = \tilde{Y}(F^T F)$. Obviously, $\tilde{Y} \leq \tilde{W}$.

Let us start with the energy (4.3). We recall that the singular values $v_1(G)$, $v_2(G)$ of G in $\mathbb{M}_{n\times 2}$ are the square roots of the eigenvalues of $G^T G$.

Proposition 4.2. *Let $n = 2, 3$ and let $\hat{w}$ be given by (4.3). 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 $Q\hat{W}(F) = 0$. If $r_1 = r_2$, any F such that $v_i(F) \leq r_1$, $i = 1, 2$, satisfies $Q\hat{W}(F) = 0$. If r_1, r_2 are arbitrary, any $F = (u, v)$ such that $|u| \leq r_1$, $|v| \leq r_2$ and $u \cdot v = 0$ satisfies $Q\hat{W}(F) = 0$.*

Proof. Let $F \in \mathbb{M}^*_{n\times 2}$ such that $G := F\,\mathrm{diag}(1/r_1, 1/r_2)$ satisfies $v_i(G) \leq 1$, $i = 1, 2$. Let us show that $S := \mathrm{diag}(r_1^2, r_2^2) - F^T F$ belongs to $\mathbb{S}^2_+$. We remark that

$$\forall \eta \in \mathbb{R}^2,\ \eta^T G^T G \eta = |G\eta|^2 \leq \|G\|_2^2 |\eta|^2 \leq |\eta|^2 = \eta^T \eta.$$

Defining ξ in $\mathbb{R}^2$ through $\eta = \mathrm{diag}(r_1, r_2)\xi$, we have $F\xi = G\eta$. Hence,

$$\forall \xi \in \mathbb{R}^2,\ \xi^T F^T F \xi \leq \xi^T \mathrm{diag}(r_1^2, r_2^2)\xi.$$

This proves that S is positive-semidefinite. As a consequence,

$$\tilde{Y}(F^T F) \leq \tilde{Y}(\mathrm{diag}(r_1^2, r_2^2)) \leq \tilde{W}(\mathrm{diag}(r_1^2, r_2^2)) = \hat{W}(\mathrm{diag}(r_1, r_2)) = 0.$$

The first claim is proved. The other two claims are easy particular cases. □

Remark 4.1. The example $r_1 = 1$, $r_2 = 2$, $|u| = 1/2$, $|v| = 1/2$ and $\widehat{(u, v)} = \pi/4$ shows that there exist matrices F with non orthogonal column vectors such that $Q\hat{W}(F) = 0$.

Let us now turn to the energy (4.2) with arbitrary $\gamma \in]0, \pi/2]$. In this more general case, we can prove that the limit energy vanishes on a subset of matrices whose column vectors make an angle equal to γ.

Proposition 4.3. *Let $n = 2, 3$ and let $\hat{w}$ be given by (4.2). Any matrix $F = (u, v)$ such that $|u| = tr_1$, $|v| = tr_2$ with $t < 1$, and $\widehat{(u, v)} = \gamma$ satisfies $Q\hat{W}(F) = 0$.*

Proof. Let $F = (u, v)$ such that $|u| = tr_1$, $|v| = tr_2$ with $t < 1$ and $\widehat{(u, v)} = \gamma$. Let $S = (s_{ij})$, $i, j = 1, 2$, be the symmetric matrix given by $s_{ii} = (1 - t^2)r_i^2$, $s_{12} = (1 - t^2)r_1 r_2 \cos\gamma$. It is clearly seen on the one hand that S is positive-semidefinite and on the other hand that $D := F^T F + S$, whose entries are $d_{ii} = r_i^2$, $d_{12} = r_1 r_2 \cos\gamma$, satisfies $\tilde{W}(D) = 0$. Therefore,

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

The result follows. □

If $n = 2$, definition (4.2) has the drawback of allowing the same energy to pairs (u, v) and $(-u, v)$. As a consequence, we can show that $Q\hat{W}(F)$ is actually equal to 0 on a larger set.

Proposition 4.4. *Let $n = 2$. Then $Q\hat{W}(F) = 0$ as soon as $|u| \leq r_1$, $|v| \leq r_2$, and $\widehat{(u, v)} = \gamma$ or $\pi + \gamma$.*

Proof. We proceed in two steps. First, we show that $Q\hat{W}(F) \leq k_2(|v| - r_2)^2$ for matrices $F = (u, v)$ such that $|u| \leq r_1$ and $\widehat{(u, v)} = \gamma$ or $\gamma + \pi$. To this aim, we let $G = (-r_1 u/|u|, v)$, $H = (r_1 u/|u|, v)$ and $t = |u|/r_1$. Observe that $\mathrm{rank}(H - G) \leq 1$. Obviously, $F = (\frac{1}{2} - \frac{t}{2})G + (\frac{1}{2} + \frac{t}{2})H$. Either, the column vectors in H make an angle equal to γ and the column vectors in G make an angle equal to $\gamma + \pi$, or conversely; in both cases the angular term in $\hat{W}$ equals 0. By the rank 1 convexity of $Q\hat{W}$, we obtain

$$Q\hat{W}(F) \leq \frac{1-t}{2}\hat{W}(G) + \frac{1+t}{2}\hat{W}(H) = k_2(|v| - r_2)^2. \tag{4.5}$$

Now, we take $F = (u, v)$ such that $|u| \leq r_1$, $|v| \leq r_2$, and $\widehat{(u, v)} = \gamma$ or $\pi + \gamma$. We let $G = (u, -r_2 v/|v|)$, $H = (u, r_2 v/|v|)$ and $t = |v|/r_2$. From (4.5), we know that $Q\hat{W}(G)$ and $Q\hat{W}(H)$ are both equal to 0. By the rank 1 convexity of $Q\hat{W}$ again, we obtain

$$Q\hat{W}(F) \leq \frac{1-t}{2}\hat{W}(G) + \frac{1+t}{2}\hat{W}(H) = 0. \tag{4.6}$$ □

Let us end up this section by some comments. First, Propositions 4.2 to 4.4 exhibit compressed states with limit energy equal to 0. Related results were given in Ref. 1 for strings, then in Refs. 23, 22 for membranes with altogether different proofs. Second, minimizers of the limit problem may be non unique. In particular, when submitted to appropriate compression on its boundary, a planar lattice may either remain in its plane or achieve zero energy by out-of-plane deformations that may conserve bond lengths.

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 stiffnesses k_i, $i = 1, 2$. Obviously, $\hat{W}$ is right invariant through the planar rotations of angle $m\pi/2$, $m \in \mathbb{N}$.

Proposition 4.5. *Let $n = 2, 3$ and $\hat{w}$ be given by (4.3) 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_{ij}, $i,j = 1,2$, are the coefficients of $C = F^TF$ and $\tilde{y}$ satisfies $\tilde{y}(c_{11}, c_{22}, c_{12}) = \tilde{y}(c_{22}, c_{11}, -c_{12})$.

Proof. Let $R(\pi/2)$ (resp. $R(3\pi/2)$) be the plane rotation with angle $\pi/2$ (resp. $3\pi/2$). We recall the representation formula for quasiconvex envelopes,[15]

$$Q\hat{W}(F) = \inf\left\{\frac{1}{|B(0,1)|}\int_{B(0,1)} \hat{W}(F + \nabla\psi(x))\,dx;\ \psi \in W_0^{1,\infty}(B(0,1);\mathbb{R}^n)\right\}.$$

Then,

$$\begin{aligned} Q\hat{W}(FR(\pi/2)) &= \inf_{\psi\in W_0^{1,\infty}(B(0,1);\mathbb{R}^n)} \frac{1}{|B(0,1)|}\int_{B(0,1)} \hat{W}(FR(\pi/2) + \nabla\psi(x))\,dx \\ &= \inf_{\psi\in W_0^{1,\infty}(B(0,1);\mathbb{R}^n)} \frac{1}{|B(0,1)|}\int_{B(0,1)} \hat{W}(F + \nabla\psi(x)R(3\pi/2))\,dx \\ &= \inf_{\psi'\in W_0^{1,\infty}(B(0,1);\mathbb{R}^n)} \frac{1}{|B(0,1)|}\int_{B(0,1)} \hat{W}(F + \nabla\psi'(x))\,dx. \end{aligned}$$

The last equality has been obtained by letting $\psi' = \psi \circ R(3\pi/2)$. As we integrate over the unit ball, ψ' belongs to $W_0^{1,\infty}(B(0,1);\mathbb{R}^n)$ if and only if ψ does. It follows that for any $F \in \mathbb{M}_{n\times 2}$, $Q\hat{W}(FR(\pi/2)) = Q\hat{W}(F)$. We have seen in Subsection 4.1 that $Q\hat{W}$ is left $O(n)$-invariant and reads $Q\hat{W}(F) = \tilde{Y}(F^TF)$. Now, let us define $\tilde{y}$ by $\tilde{y}(c_{11}, c_{22}, c_{12}) = \tilde{Y}(C)$ for $C = (c_{ij})$ symmetric semi-definite positive. Let $D = (d_{ij})$ with $d_{11} = c_{22}$, $d_{22} = c_{11}$, $d_{12} = -c_{12}$. Let F such that $C = F^TF$ and let $G = FR(\pi/2)$. Then $D = G^TG$, hence $\tilde{Y}(C) = \tilde{Y}(D)$ and the result follows. □

5. Cauchy-Born rule

Cauchy-Born rule is a generic name for a variety of statements that relate the macroscopic description of the deformation of a crystalline solid and the individual placement of its atoms. We refer to Ericksen[19] for an account of the pioneering statements by Cauchy, then by Born, as well as for a list of references that includes recent works devoted to prove, disprove or determine the range of validity of the rule.[21,18] It is very likely that Cauchy-Born rule was originally meant for planar deformations of plane lattices and for three-dimensional deformations of three-dimensional lattices. In its simplest and more restrictive form, the 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 simple lattices, alternatively called 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). It is

immediately computed and usually denoted as $W_{CB}(F)$. The density thus obtained is not quasiconvex in general. Then affine deformations φ_F do not minimize the internal energy among deformations with boundary conditions $\varphi_F(x)$ on the whole of the boundary. Therefore, 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 exist. They allow for atom relaxation over a range of cells which gives rise to homogenized energy densities W_{hom}. They can also allow for atom relaxation inside the elementary cell, specially for complex lattices.[18,25] 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 (2.13) 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 a realistic case where both minimization at the cell level and homogenization are required, we refer to Le Dret and Raoult[25] where hexagonal lattices are studied.

A. Approximation results

As mentioned in the main body of the paper, dealing with the loading term requires some technical lemmas that we gather in the present section. Lemma A.1 below gives a bound from above for $L_h(\psi_h)$ and is useful for the proof of Proposition 3.1.

Lemma A.1. *There exist $C_1 > 0$ and $C_2 > 0$ such that*

$$\forall h,\, \forall \psi_h \in \mathcal{A}_h,\, \left[\sum_{i,j=0}^{N_h-1} h^2 |\psi_h(ih, jh)|^p\right]^{1/p} \leq C_1\, ||\psi_h||_{L^p(\omega;\mathbb{R}^n)} \tag{A.1}$$

and

$$\forall h,\, \forall \psi_h \in \mathcal{A}_h,\, L_h(\psi_h) \leq C_2\, ||\psi_h||_{L^p(\omega;\mathbb{R}^n)}. \tag{A.2}$$

Proof. The proof uses arguments that are classical in the finite element theory. Let $\hat{T}$ be the unit rectangular triangle. From the equivalence of all norms on $\mathbb{P}_1(\hat{T};\mathbb{R}^n)$, we derive that

$$\exists C_1 > 0, \forall \hat{\chi} \in \mathbb{P}_1(\hat{T};\mathbb{R}^n), |\hat{\chi}(0,0)|^p + |\hat{\chi}(1,0)|^p + |\hat{\chi}(0,1)|^p \leq C_1^p \|\hat{\chi}\|^p_{L^p(\hat{T};\mathbb{R}^n)}. \tag{A.3}$$

Let ψ_h in $\mathcal{A}_h$. First, we transform the $L^p(\omega;\mathbb{R}^n)$-norm of ψ_h into norms on $\hat{T}$. Indeed,

$$||\psi_h||^p_{L^p(\omega;\mathbb{R}^n)} = \sum_{T\in\mathcal{T}_1^h} ||\psi_{h|T}||^p_{L^p(T;\mathbb{R}^n)} = h^2 \sum_{T\in\mathcal{T}_1^h} ||\widehat{\psi_{h|T}}||^p_{L^p(\hat{T};\mathbb{R}^n)} \tag{A.4}$$

where for any $T = T_{ij}^{h1}$ in $\mathcal{T}_1^h$, $\widehat{\psi_{h|T}}$ is the unique affine function defined on $\hat{T}$ such that $\widehat{\psi_{h|T}}(0,0) = \psi_h(M_{ij}^h)$, $\widehat{\psi_{h|T}}(1,0) = \psi_h(M_{i+1,j}^h)$, $\widehat{\psi_{h|T}}(0,1) = \psi_h(M_{i,j+1}^h)$ and for any $T = T_{ij}^{h3}$ in $\mathcal{T}_1^h$, $\widehat{\psi_{h|T}}$ is the unique affine function defined on $\hat{T}$ such that

$\widehat{\psi_{h|T}}(0,0) = \psi_h(M^h_{ij})$, $\widehat{\psi_{h|T}}(1,0) = \psi_h(M^h_{i-1,j})$, $\widehat{\psi_{h|T}}(0,1) = \psi_h(M^h_{i,j-1})$. Then, by (A.3) and by (A.4),

$$\begin{aligned} C_1^p\,||\psi_h||^p_{L^p(\omega;\mathbb{R}^n)} &\geq h^2 \sum_{T\in\mathcal{T}_1^h} (|\widehat{\psi_{h|T}}(0,0)|^p + |\widehat{\psi_{h|T}}(1,0)|^p + |\widehat{\psi_{h|T}}(0,1)|^p) \\ &\geq h^2 \sum_{T^{h1}_{ij}\in\mathcal{T}_1^h} (|\psi_h(M^h_{ij})|^p + |\psi_h(M^h_{i+1,j})|^p + |\psi_h(M^h_{i,j+1})|^p) \\ &+ h^2 \sum_{T^{h3}_{ij}\in\mathcal{T}_1^h} (|\psi_h(M^h_{ij})|^p + |\psi_h(M^h_{i-1,j})|^p + |\psi_h(M^h_{i,j-1})|^p) \end{aligned}$$

which provides

$$C_1^p\,||\psi_h||^p_{L^p(\omega;\mathbb{R}^n)} \geq h^2 \sum_{i,j=0}^{N_h-1} |\psi_h(ih,jh)|^p \tag{A.5}$$

that is the first assertion of Lemma A.1. Now, letting $\frac{1}{q}+\frac{1}{p}=1$, $\alpha=\frac{2}{q}$, $\beta=\frac{2}{p}$, we derive from Hölder's inequality that

$$\begin{aligned} L_h(\psi_h) &= \sum_{i,j=0}^{N_h-1} (h^\alpha f(ih,jh))\cdot(h^\beta\psi_h(ih,jh)) \\ &\leq \left[\sum_{i,j=0}^{N_h-1} h^2|f(ih,jh)|^q\right]^{1/q} \left[\sum_{i,j=0}^{N_h-1} h^2|\psi_h(ih,jh)|^p\right]^{1/p} \leq C_2\,||\psi_h||_{L^p(\omega;\mathbb{R}^n)}. \end{aligned}$$ □

We now turn to the precise limit behavior of $L_h(\psi_h)$ when ψ_h converges in some sense. This result is needed for Propositions 3.3 and 3.4. It is worth noticing that for proving that $L_h(\psi_h)$ converges to $\int_\omega f(x)\cdot\psi(x)\,dx$ we not only rely on the L^p-convergence of ψ_h, but we make use of the boundedness of the gradients.

Lemma A.2. *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 $L_h(\psi_h)$ converges to $\int_\omega f(x)\cdot\psi(x)\,dx$.*

Proof. Let us write

$$L_h(\psi_h) - \int_\omega f(x)\cdot\psi(x)\,dx = E_h(\psi_h) + F_h(\psi_h)$$

with

$$E_h(\psi_h) = L_h(\psi_h) - \int_\omega f(x)\cdot\psi_h(x)\,dx,\ F_h(\psi_h) = \int_\omega f(x)\cdot(\psi_h(x)-\psi(x))\,dx.$$

From the L^p-convergence of ψ_h towards ψ, we derive immediately that $F_h(\psi_h)$ goes

to 0 when h goes to 0. We rewrite $E_h(\psi_h)$ in the following way

$$\begin{aligned} E_h(\psi_h) &= h^2 \sum_{i,j=0}^{N_h-1} f(ih,jh)\cdot\psi_h(ih,jh) - \int_\omega f(x)\cdot\psi_h(x)\,dx \\ &= \int_\omega (\Pi_0^h f\cdot\Pi_0^h\psi_h - f\cdot\psi_h)(x)\,dx \end{aligned}$$

where $\Pi_0^h : w\in\mathcal{C}^0(\bar\omega;\mathbb{R}^n)\mapsto\Pi_0^h(w)\in(\mathbb{R}^n)^{N_h^2}$ is the interpolation operator defined by $\Pi_0^h(w)$ is constant on each subsquare $[ih,(i+1)h[\times[jh,(j+1)h[$ and $\Pi_0^h(w) = w(ih,jh)$ on that subsquare. We now split $E_h(\psi_h)$ in two terms:

$$E_h(\psi_h) = \int_\omega (\Pi_0^h f - f)\cdot\Pi_0^h\psi_h\,dx + \int_\omega f\cdot(\Pi_0^h\psi_h - \psi_h)\,dx. \tag{A.6}$$

As f is assumed to be continuous on $\overline{\omega}$, $\Pi_0^h f - f$ converges to 0 in $L^\infty(\omega;\mathbb{R}^n)$ and, by (A.1), $\Pi_0^h\psi_h$ is bounded in $L^p(\omega;\mathbb{R}^n)$. Therefore, the first term in (A.6) goes to 0. The convergence to 0 of the second term follows from the fact that $\Pi_0^h\psi_h - \psi_h$ converges to 0 in $L^p(\omega;\mathbb{R}^n)$. This can be seen as an exercise in the spirit of finite element approximation results that we detail here for the reader convenience. Let Q_{ij}^h be the square with vertices M_{ij}^h, $M_{i+1,j}^h$, $M_{i,j+1}^h$, $M_{i+1,j+1}^h$. Then,

$$\begin{aligned} ||\psi_h - \Pi_0^h\psi_h||^p_{L^p(\omega;\mathbb{R}^n)} &= \sum_{i,j=0}^{N_h-1} ||\psi_{h|Q_{ij}^h} - \psi_h(M_{ij}^h)||^p_{L^p(Q_{ij}^h;\mathbb{R}^n)} \\ &= h^2 \sum_{i,j=0}^{N_h-1} ||(\breve\psi_h^{ij} - \breve\psi_h^{ij}(0,0))||^p_{L^p([0,1]^2;\mathbb{R}^n)} \end{aligned}$$

where for any $\breve x$ in $[0,1]^2$, $\breve\psi_h^{ij}(\breve x) = \psi_h(M_{ij}^h + h\breve x)$. The subterms are estimated as follows:

$$\begin{aligned} \breve\psi_h^{ij}(\breve x) - \breve\psi_h^{ij}(0,0) &= \breve\psi_h^{ij}(\breve x) - \breve\psi_h^{ij}(\breve x_1,0) + \breve\psi_h^{ij}(\breve x_1,0) - \breve\psi_h^{ij}(0,0) \\ &= \int_{\breve u=0}^{\breve x_2} \partial_2\breve\psi_h^{ij}(\breve x_1,\breve u)\,d\breve u + \int_{\breve t=0}^{\breve x_1} \partial_1\breve\psi_h^{ij}(\breve t,0)\,d\breve t. \end{aligned}$$

Then,

$$\begin{aligned} &\exists\breve C,\ \forall h,\ \forall(i,j),\ \forall\breve x\in[0,1]^2, \\ &\quad |\breve\psi_h^{ij}(\breve x) - \breve\psi_h^{ij}(0,0)|^p \le \breve C\Big(\int_{\breve u=0}^1 |\partial_2\breve\psi_h^{ij}(\breve x_1,\breve u)|^p\,d\breve u + \int_{\breve t=0}^1 |\partial_1\breve\psi_h^{ij}(\breve t,0)|^p\,d\breve t\Big) \\ &\quad\quad \le \breve C\Big(\int_{\breve u=0}^1 |\partial_2\breve\psi_h^{ij}(\breve x_1,\breve u)|^p\,d\breve u + |\partial_1\breve\psi_h^{ij}(0,0)|^p\Big) \end{aligned}$$

since $\partial_1\breve\psi_h^{ij}(\breve t,0)$ does not depend on t. By integrating over $[0,1]^2$, it follows that there exists $\breve C$ such that for all h, for all (i,j),

$$\|\breve\psi_h^{ij} - \breve\psi_h^{ij}(0,0)\|^p_{L^p([0,1]^2;\mathbb{R}^n)} \le \breve C\,\|\nabla\breve\psi_h^{ij}\|^p_{L^p([0,1]^2;\mathbb{R}^n)}$$

where we used again the fact that $\partial_1 \breve{\psi}_h^{ij}$ is constant on the unit rectangular triangle $\hat{T}$. By returning to ω,

$$||\psi_h - \Pi_0^h \psi_h||^p_{L^p(\omega;\mathbb{R}^n)} \leq \breve{C} h^2 ||\nabla \psi_h||^p_{L^p(\omega;\mathbb{R}^n)}. \qquad \square$$

As a final result, let us prove Lemma 3.1 that we reformulate below. We recall that $W^{1,p}_{\Gamma_0}(\omega;\mathbb{R}^n) = \{\psi \in W^{1,p}(\omega;\mathbb{R}^n); \psi_{|\Gamma_0} = \varphi_{0|\Gamma_0}\}$ and we let

$$W^{1,p}_{0,\Gamma_0}(\omega;\mathbb{R}^n) = \{w \in W^{1,p}(\omega;\mathbb{R}^n); w_{|\Gamma_0} = 0\}$$

and

$$\mathcal{V}_h = \{w \in \mathcal{C}^0(\bar{\omega};\mathbb{R}^n); \forall T \in \mathcal{T}_1^h, w_{|T} \in \mathbb{P}_1(T;\mathbb{R}^n), w_{|\Gamma_0} = 0\}.$$

Lemma A.3. *Any v in $W^{1,p}_{0,\Gamma_0}(\omega;\mathbb{R}^n)$ is the $W^{1,p}$-limit of a sequence in $\mathcal{V}_h$. Any ψ in $W^{1,p}_{\Gamma_0}(\omega;\mathbb{R}^n)$ is the $W^{1,p}$-limit of a sequence ψ_h in $\mathcal{A}_h^*$.*

Proof. Let Π_1^h be the $\mathbb{P}_1$-interpolation operator associated with $\mathcal{T}_1^h$. Standard results show that, for any w in $W^{2,p}(\omega;\mathbb{R}^n)$, $\Pi_1^h w$ converges to w. If in addition $w_{|\Gamma_0} = 0$, then $\Pi_1^h w_{|\Gamma_0} = 0$ as well. Therefore, any w in $(W^{2,p} \cap W^{1,p}_{0,\Gamma_0})(\omega;\mathbb{R}^n)$ is the limit of a sequence w_h, $h \to 0$ with $w_h \in \mathcal{V}_h$. Now, any v in $W^{1,p}_{0,\Gamma_0}(\omega;\mathbb{R}^n)$ is the limit of a sequence w_n, $n \to +\infty$, such that w_n belongs to $(W^{2,p} \cap W^{1,p}_{0,\Gamma_0})(\omega;\mathbb{R}^n)$. Upon extracting a diagonal sequence (recall that $h = L/N_h$ with N_h an integer), we prove the first assertion of Lemma A.3.

Let ψ in $W^{1,p}_{\Gamma_0}(\omega;\mathbb{R}^n)$ and define $v = \psi - \varphi_0$. Obviously, v belongs to $W^{1,p}_{0,\Gamma_0}(\omega;\mathbb{R}^n)$ and we have just proved that v is the $W^{1,p}$-limit of v_h, v_h in $\mathcal{V}_h$. Therefore, $\psi_h := \varphi_0 + v_h$ belongs to $\mathcal{A}_h$ and converges to ψ in $W^{1,p}(\omega;\mathbb{R}^n)$. Let us show that functions ψ_h can be slightly modified into functions ψ_h^* that are pairwise one-to-one and that still converge to ψ. We actually prove a stronger result since we obtain functions ψ_h^* whose restrictions to the set of nodes are one-to-one. Let

$$P_h = \{\big((k,l),(k',l')\big) \in \{\{0,\ldots,N_h\}^2\}^2;\ \psi_h(kh,lh) \neq \psi_h(k'h,l'h)\}.$$

The set P_h is nonempty since $\psi_h = \varphi_0$ on Γ_0. Let

$$C_h = \min_{P_h} |(\psi_h(k'h,l'h) - \psi_h(kh,lh)|.$$

By construction, C_h is strictly positive. Moreover, since on Γ_0, $|\psi_h(kh,lh) \neq \psi_h(k'h,l'h)| \leq K_0 h$ where $K_0 = \|\nabla\varphi_0\|$, we know that $C_h \leq K_0 h$. Finally, let $\varepsilon_h = \frac{C_h}{2\sqrt{2}L}$. Note that ε_h goes to 0 when h goes to 0. Letting $id : (x_1,x_2) \in \bar{\omega} \mapsto (x_1,x_2,0) \in \mathbb{R}^n$, we define ψ_h^* as follows:

$$\psi_h^* = \psi_h + \varepsilon_h id \text{ on } [0, L-h]^2,\ \psi_h^* = \varphi_0 \text{ on } \Gamma_0$$

and ψ_h^* is globally continuous and affine on each triangle in $\mathcal{T}_1^h$. Since ψ_h and id are affine per triangle, there is no contradiction in the previous requirements. Let us check that the restriction of ψ_h^* to the set of nodes is one-to-one. Suppose that

$\psi_h^*(kh, lh) = \psi_h^*(k'h, l'h)$ with $(k, l), (k', l') \in \{0, \dots, N_h\}^2$. Our aim is to show that $(k, l) = (k', l')$. We distinguish several cases:

Case 1: (kh, lh) and $(k'h, l'h)$ belong to $[0, L-h]^2$. Then

- either $\psi_h(kh, lh) = \psi_h(k'h, l'h)$ and the assumption on ψ_h^* implies that $\varepsilon_h(kh, lh, 0) = \varepsilon_h(k'h, l'h, 0)$, whence $(k, l) = (k', l')$ because $\varepsilon_h \neq 0$,

- or $\psi_h(kh, lh) \neq \psi_h(k'h, l'h)$ and the assumption on ψ_h^* implies that $\psi_h(kh, lh) - \psi_h(k'h, l'h) = \varepsilon_h((k'-k)h, (l'-l)h, 0)$. Therefore, $|\psi_h(kh, lh) - \psi_h(k'h, l'h)| \leq \varepsilon_h L\sqrt{2} < \frac{C_h}{2}$ which is contradictory with the definition of C_h.

Case 2: (kh, lh) and $(k'h, l'h)$ belong to Γ_0. Since ψ_h^* coincides with φ_0 on Γ_0, obviously $(k, l) = (k', l')$.

Case 3: $(kh, lh) \in [0, L-h]^2$ and $(k'h, l'h)$ on Γ_0. Then,

$$(\psi_h + \varepsilon_h id)(kh, lh) = \varphi_0(k'h, l'h) = \psi_h(k'h, l'h).$$

Therefore, $|\psi_h(kh, lh) - \psi_h(k'h, l'h)| \leq \varepsilon_h L\sqrt{2}$ and the argument is the same as in Case 1.

The previous considerations show that ψ_h^* belongs to $\mathcal{A}_h^*$. We still have to prove that ψ_h^* converges to ψ in $W^{1,p}(\omega; \mathbb{R}^n)$. Recall that ψ_h converges to ψ and that ε_h converges to 0. Therefore, $\psi_h + \varepsilon_h id$ converges to ψ in $W^{1,p}(\omega; \mathbb{R}^n)$. This remains true for ψ_h^* which differs from $\psi_h + \varepsilon_h id$ on two bands of width h only. □

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