

# ON THE VARIATIONAL LIMITS OF LATTICE ENERGIES ON PRESTRAINED ELASTIC BODIES

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ABSTRACT. We study the asymptotic behaviour of the discrete elastic energies in presence of the prestrain metric  $G$ , assigned on the continuum reference configuration  $\Omega$ . When the mesh size of the discrete lattice in  $\Omega$  goes to zero, we obtain the variational bounds on the limiting (in the sense of  $\Gamma$ -limit) energy. In case of the nearest-neighbour and next-to-nearest-neighbour interactions, we derive a precise asymptotic formula, and compare it with the non-Euclidean model energy relative to  $G$ .

## 1. INTRODUCTION

Recently, there has been a growing interest in the study of prestrained materials, i.e. materials which assume non-trivial rest configurations in the absence of exterior forces or boundary conditions. This phenomenon has been observed in contexts such as: naturally growing tissues, torn plastic sheets, specifically engineered polymer gels, and many others. The basic mathematical model, called “incompatible elasticity” has been put forward in [31, 13, 18] and further studied in [24, 22, 23, 4, 25, 26, 11, 12, 19, 20]. In this paper, we pose the following question: is it possible to derive an equivalent continuum mechanics model starting from an appropriate discrete description, by means of a homogenization procedure when the mesh size goes to 0? Discrete-to-continuum limits of this type have been investigated by means of  $\Gamma$ -convergence in a number of areas of application, including nonlinear elasticity [1, 28, 21, 2, 33, 34] and others (see for example [3, 30, 14, 32]).

Discrete lattices may model both the atomic structures and mechanical trusses. The latter case is not restricted to classical material mechanics but it also encompasses biological tissues. For instance, in the cell-to-muscle homogenization problem [8, 16, 29], the muscle tissue of the heart, which forms a thick middle (myocardial) layer between the outer epicardium and the inner endocardium layers, is regarded as a set of basic nodes and fibers suitably arranged. The myocardial fibers consist of myocytes; these are elongated structures which can undergo further elongation/traction as well as angle interaction. It is possible to reconstruct an elastic law for the myocardium from the known behavior of the myocytes [8, 16], and the obtained results are consistent with the experimental measurements in the physiological literature. Further observations [17] confirm that there should be a spatial heterogeneity in the myocardium cells, as a consequence of the temporal heterogeneity. Nevertheless, so far measurements were not precise enough (due to the noise in the diffraction techniques) to give distinct values, and therefore most of the time heterogeneity has been left aside in prior works.

The analysis in the present paper investigates the relation of the continuum limit of the atomistic models taking into account the weighted pairwise interactions of nodes in the lattice, with the continuum elastic energy where all possible interactions are taken into account. We show that,

although the limit model inherits the same structure of the continuum energy, the two models differ by: (i) the relaxation in the density potential which, as one naturally expects, is the quasiconvexification of the original density, and (ii) the new “incompatibility” metric represented by the superposition of traces of the original incompatibility metric, along the admissible directions of interaction.

**1.1. The continuum model  $\mathcal{E}$ .** We now introduce and explain the models involved. The “incompatible elasticity” postulates that the three-dimensional body seeks to realize a configuration with a prescribed Riemannian metric  $G$ , and that the resulting deformation minimizes the energy  $\mathcal{E}$  which in turn measures the deviation of a given deformation from being an orientation-preserving isometric immersion of  $G$ . More precisely, let  $G$  be a smooth Riemannian metric on an open, bounded, connected domain  $\Omega \subset \mathbb{R}^n$ , i.e.  $G \in \mathcal{C}^\infty(\bar{\Omega}, \mathbb{R}^{n \times n})$  and  $G(x)$  is symmetric positive definite for every  $x \in \bar{\Omega}$ . The shape change that occurs during the growth of  $\Omega$  is due to changes in the local stress-free state (for instance, material may be added or removed), and to the accommodation of these changes. Consequently, the gradient of the deformation  $u : \Omega \rightarrow \mathbb{R}^n$  that maps the original stress-free state to the observed state, can be decomposed as:

$$\nabla u = FA,$$

into the growth deformation tensor  $A : \Omega \rightarrow \mathbb{R}^{n \times n}$ , describing the growth from the reference zero-stress state to a new locally stress-free state, and the elastic deformation tensor  $F$ . The elastic energy  $\mathcal{E}$  is then given in terms of  $F$ , by:

$$(1.1) \quad \mathcal{E}(u) = \int_{\Omega} \bar{W}(F) \, dx = \int_{\Omega} \bar{W}(\nabla u A^{-1}) \, dx.$$

Here, the density potential  $\bar{W} : \mathbb{R}^{n \times n} \rightarrow \bar{\mathbb{R}}_+$  satisfies the following assumptions of frame invariance with respect to the group of proper rotations  $SO(n)$ , normalization, and non-degeneracy:

$$(1.2) \quad \forall F \in \mathbb{R}^{n \times n}, R \in SO(n) \quad \bar{W}(RF) = \bar{W}(F), \quad \bar{W}(R) = 0, \quad \bar{W}(F) \geq c \, \text{dist}^2(F, SO(n)),$$

for some uniform constant  $c > 0$ .

Observe that:  $\mathcal{E}(u) = 0$  is equivalent to  $\nabla u(x) \in SO(n)A(x)$  for almost every  $x \in \Omega$ . Further, in view of the polar decomposition theorem, the same condition is equivalent to:  $(\nabla u)^T \nabla u = A^T A$  and  $\det \nabla u > 0$  in  $\Omega$ , i.e.  $\mathcal{E}(u) = 0$  if and only if  $u$  is an isometric immersion of the imposed Riemannian metric  $G = A^T A$ . Hence, when  $G$  is not realizable (i.e. when its Riemann curvature tensor does not vanish identically in  $\Omega$ ), there is no  $u$  with  $\mathcal{E}(u) = 0$ . It has further been proven in [24] that in this case:  $\inf\{\mathcal{E}(u); u \in W^{1,2}(\Omega, \mathbb{R}^n)\} > 0$  as well, which points to the existence of residual non-zero strain at free equilibria of  $\mathcal{E}$ .

Given  $G$ , we will call  $A = \sqrt{G}$ , and without loss of generality we always assume that  $A$  is symmetric and strictly positive definite in  $\Omega$ .

**1.2. The discrete model  $E_\epsilon$ .** We now describe the discrete model whose asymptotic behavior we intend to study. The total stored discrete energy of a given deformation acting on the atoms of the lattice in  $\Omega$ , is defined to be the superposition of the energies weighting the pairwise interactions between the atoms, with respect to  $G$ . More precisely, given  $\epsilon > 0$  and a discrete map  $u_\epsilon : \epsilon\mathbb{Z}^n \cap \Omega \rightarrow \mathbb{R}^n$ , let:

$$(1.3) \quad E_\epsilon(u_\epsilon) = \sum_{\xi \in \mathbb{Z}^n} \sum_{\alpha \in R_\epsilon^\xi(\Omega)} \epsilon^n \psi(|\xi|) \left| \frac{|u_\epsilon(\alpha + \epsilon\xi) - u_\epsilon(\alpha)|}{\epsilon |A(\alpha)\xi|} - 1 \right|^2,$$

where  $R_\epsilon^\xi(\Omega) = \{\alpha \in \epsilon\mathbb{Z}^n : [\alpha, \alpha + \epsilon\xi] \subset \Omega\}$  denotes the set of lattice points interacting with the node  $\alpha$ , and where a smooth cut-off function  $\psi : \mathbb{R}_+ \rightarrow \mathbb{R}$  allows only for interactions with finite range:

$$\psi(0) = 0 \quad \text{and} \quad \exists M > 0 \quad \forall n \geq M \quad \psi(n) = 0.$$

The energy in (1.3) measures the discrepancy between lengths of the actual displacements between the nodes  $x = \alpha + \epsilon\xi$  and  $y = \alpha$  due to the deformation  $u_\epsilon$ , and the ideal displacement length  $\langle G(\alpha)(x - y), (x - y) \rangle^{1/2} = \epsilon|A(\alpha)\xi|$ . Note that the measure of this discrepancy in terms of the ratio  $\frac{l}{l_0}$  of the actual length  $l = |u_\epsilon(\alpha + \epsilon\xi) - u_\epsilon(\alpha)|$  and the ideal length  $l_0 = \epsilon|A(\alpha)\xi|$  is present in the reconstruction of an elastic law for the myocardium from the known behavior of the myocytes in [8] (formula (11)).

When  $\epsilon \rightarrow 0$  and when sampling on sufficiently many interaction directions  $\xi$ , one might expect that (1.3) will effectively measure the discrepancy between all lengths  $|u(x) - u(y)|$  and the ideal lengths  $|A(x)(x - y)|$  determined by the imposed metric, as in (1.1). For  $G = \text{Id}$ , it has been proven in [1] that this is indeed the case, as well as that the  $\Gamma$ -limit  $\mathcal{F}$  of  $E_\epsilon$  has the form:  $\mathcal{F}(u) = \int_\Omega f(\nabla u) dx$  with the limiting density  $f$  frame invariant and quasiconvex.

**1.3. The main results and the organization of the paper.** Towards studying the energies (1.3), we first derive an integral representation for  $E_\epsilon$  by introducing a family of lattices determined by each length of the admissible interactions (when  $\psi \neq 0$ ); this is done in sections 2 and 3. Since the general formula for the integral representation uses quite involved notation, we first present its simpler versions, valid in cases of the nearest-neighbour and next-to-nearest-neighbour interactions. For each lattice, we define its  $n$ -dimensional triangulation and, as usual in the lattice analysis, we associate with it the piecewise affine maps matching with the original discrete deformations at each node.

In section 4 we derive the lower and upper bounds  $I_Q$  and  $I$  of the  $\Gamma$ -limit  $\mathcal{F}$  of  $E_\epsilon$ , as  $\epsilon \rightarrow 0$ , in terms of the superposition of integral energies defined effectively on the  $W^{1,2}$  deformations of  $\Omega$ . The disparity between the upper and lower bounds reflects the fact that each lattice in the discrete description gives rise, in general, to a distinct recovery sequence of the associated  $\Gamma$ -limit. This is hardly surprising, since the operation of taking the lsc envelope of an integral energy is not additive (nor is the operation of quasiconvexification of its density).

On the other hand, each term in  $I_Q$  and  $I$  has the structure as in (1.1), but with  $G$  replaced by other effective metric induced by the distinct lattices. In case of only nearest-neighbour or next-to-nearest-neighbour interactions all the effective metrics coincide with one residual metric  $\bar{G}$ . This further allows to obtain the formula for  $\mathcal{F}$ , which is accomplished in section 5. In section 6 we compare  $\mathcal{F}$  with  $\mathcal{E}$  through a series of examples. We note, in particular, that the realisability of  $G$  does not imply the realisability of  $\bar{G}$ , neither the converse of this statement is true.

Finally, in the Appendix section 7 we gather some classical facts on  $\Gamma$  convergence and convexity, which we use in the proofs of this note.

Let us conclude by remarking that a continuum finite range interaction model, in the spirit of (1.3), can be posed similarly to the models considered recently in [5, 7, 27], by:

$$\tilde{E}_\epsilon(u) = \int_\Omega \int_\Omega \psi\left(\frac{|x - y|}{\epsilon}\right) \left| \frac{|u(x) - u(y)|}{|A(x)(x - y)|} - 1 \right|^2 dx dy.$$

It would be interesting to find the  $\Gamma$ -limit of  $\tilde{E}_\epsilon$ , as  $\epsilon \rightarrow 0$  and compare it with both  $\mathcal{E}$  and  $\mathcal{F}$ .

1.4. **Notation.** Throughout the paper,  $\Omega$  is an open bounded subset of  $\mathbb{R}^n$ . For  $s > 0$ , we denote:

$$\Omega_s = \{x \in \Omega; \text{dist}(x, \partial\Omega) > s\}.$$

The standard triangulation of the  $n$ -dimensional cube  $C_n = [0, 1]^n$  is defined as follows. For all permutations  $\pi \in S_n$  of  $n$  elements, let  $T^\pi$  be the  $n$ -simplex obtained by:

$$T^\pi = \{(x_1, \dots, x_n) \in C_n; x_{\pi(1)} \geq \dots \geq x_{\pi(n)}\}.$$

Note that  $T^\pi$  is the convexification of its vertices:

$$T^\pi = \text{conv}\left\{0, e_{\pi(1)}, e_{\pi(1)} + e_{\pi(2)}, \dots, e_{\pi(1)} + \dots + e_{\pi(n)} = e_1 + \dots + e_n\right\},$$

and that all simplices  $T^\pi$  have 0 and  $(1, \dots, 1) = e_1 + \dots + e_n$  as common vertices. The collection of  $n!$  simplices  $\{T^\pi\}_{\pi \in S_n}$  constitutes the standard triangulation of  $C_n$ , which can also be naturally extended to each cell  $\alpha + \epsilon C_n$  where  $\alpha \in \epsilon\mathbb{Z}^n$ :

$$T_\alpha^\pi = \text{conv}\left\{\alpha, \left\{\alpha + \epsilon \sum_{i=1}^j e_{\pi(i)}\right\}_{j=1}^n\right\}.$$

When  $\pi = (i_1, \dots, i_n)$  we shall also write  $T_\alpha^{(i_1, \dots, i_n)} = T_\alpha^\pi = \text{conv}\left\{\alpha, \left\{\alpha + \epsilon \sum_{k=1}^j e_{i_k}\right\}_{j=1}^n\right\}$ . Moreover, we call:

$$(1.4) \quad \mathcal{T}_{\epsilon, n} = \{T_\alpha^\pi; \alpha \in \epsilon\mathbb{Z}^n, \pi \in S_n\}.$$

Finally, by  $C$  we denote any universal constant, depending on  $\Omega$  and  $W$ , but independent of other involved quantities at hand.

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## 2. INTEGRAL REPRESENTATION OF DISCRETE ENERGIES (1.3) - SPECIAL CASES

Since the general formula for the integral representation of  $E_\epsilon$ , given in section 3, uses a somewhat involved notation which may obscure the construction, we first present its simpler versions, valid in cases of the near and next-to-nearest-neighbour interactions, which we further discuss in sections 5 and 6.

2.1. **Case 1: nearest-neighbour interactions in  $\mathbb{R}^2$ .** Let  $\Omega \subset \mathbb{R}^2$  and assume that  $\psi(1) = 1$  and  $\psi(|\xi|) = 0$  for  $|\xi| \geq \sqrt{2}$ . The energy (1.3) of a deformation  $u_\epsilon : \epsilon\mathbb{Z}^2 \cap \Omega \rightarrow \mathbb{R}^2$ , takes then the form:

$$E_\epsilon(u_\epsilon) = \sum_{i,j=1}^2 \sum_{\alpha \in R_\epsilon^{(-1)^j e_i}(\Omega)} \epsilon^2 \left| \frac{|u_\epsilon(\alpha + (-1)^j \epsilon e_i) - u_\epsilon(\alpha)|}{\epsilon |A(\alpha) e_i|} - 1 \right|^2.$$

Let  $U_\epsilon \subset \Omega$  be the union of those (open) cells in the lattice  $\epsilon\mathbb{Z}^2$ , which have non-empty intersection with the set  $\Omega_{\sqrt{2}\epsilon}$ . We consider the standard triangulation  $\mathcal{T}_{\epsilon, 2}$  of the lattice  $\epsilon\mathbb{Z}^2$ , as in (1.4), and we identify the discrete map  $u_\epsilon$  with the unique continuous function on  $U_\epsilon$ , affine on all the triangles in  $\mathcal{T}_{\epsilon, 2} \cap U_\epsilon$ , and matching with  $u_\epsilon$  at each node.

Define the function  $W : \mathbb{R}^{2 \times 2} \rightarrow \mathbb{R}$ :

$$W([M_{ij}]_{i,j=1..2}) = \sum_{j=1}^2 \left( \left( \sum_{i=1}^2 |M_{ij}|^2 \right)^{1/2} - 1 \right)^2 \quad \forall M \in \mathbb{R}^{2 \times 2}.$$

We easily see that for every  $\alpha \in \epsilon\mathbb{Z}^2 \cap U_\epsilon$ :

$$\begin{aligned} & \epsilon^2 \left( \left| \frac{|u_\epsilon(\alpha + \epsilon e_1) - u_\epsilon(\alpha)|}{\epsilon|A(\alpha)e_1|} - 1 \right|^2 + \left| \frac{|u_\epsilon(\alpha + \epsilon(e_1 + e_2)) - u_\epsilon(\alpha + \epsilon e_1)|}{\epsilon|A(\alpha + \epsilon e_1)e_2|} - 1 \right|^2 \right) \\ &= 2 \int_{T_\alpha^{(1,2)}} W(\nabla u_\epsilon(x)\lambda_\epsilon(x)) \, dx, \end{aligned}$$

where  $\lambda_\epsilon : U_\epsilon \rightarrow \mathbb{R}^{2 \times 2}$  is a piecewise constant matrix field, given by:

$$\begin{aligned} \forall x \in T_\alpha^{(1,2)} \cap U_\epsilon, & \quad \lambda_\epsilon(x) = \text{diag} \{ |A(\alpha)e_1|^{-1}, |A(\alpha + \epsilon e_1)e_2|^{-1} \} \\ \forall x \in T_\alpha^{(2,1)} \cap U_\epsilon, & \quad \lambda_\epsilon(x) = \text{diag} \{ |A(\alpha + \epsilon e_2)e_1|^{-1}, |A(\alpha)e_2|^{-1} \} \end{aligned}$$

while we recall that  $T_\alpha^{(1,2)} = \text{conv}\{\alpha, \alpha + \epsilon e_1, \alpha + \epsilon(e_1 + e_2)\}$  and  $T_\alpha^{(2,1)} = \text{conv}\{\alpha, \alpha + \epsilon e_2, \alpha + \epsilon(e_1 + e_2)\}$ . Similarly, we get:

$$\begin{aligned} & \epsilon^2 \left( \left| \frac{|u_\epsilon(\alpha + \epsilon e_2) - u_\epsilon(\alpha)|}{\epsilon|A(\alpha)e_2|} - 1 \right|^2 + \left| \frac{|u_\epsilon(\alpha + \epsilon(e_1 + e_2)) - u_\epsilon(\alpha + \epsilon e_2)|}{\epsilon|A(\alpha + \epsilon e_2)e_1|} - 1 \right|^2 \right) \\ &= 2 \int_{T_\alpha^{(2,1)}} W(\nabla u_\epsilon(x)\lambda_\epsilon(x)) \, dx. \end{aligned}$$

For the interactions in the opposite directions:  $-e_1$  and  $-e_2$ , we obtain:

$$\begin{aligned} & \epsilon^2 \left( \left| \frac{|u_\epsilon(\alpha + \epsilon e_1) - u_\epsilon(\alpha + \epsilon(e_1 + e_2))|}{\epsilon|A(\alpha + \epsilon(e_1 + e_2))e_2|} - 1 \right|^2 + \left| \frac{|u_\epsilon(\alpha) - u_\epsilon(\alpha + \epsilon e_1)|}{\epsilon|A(\alpha + \epsilon e_1)e_1|} - 1 \right|^2 \right) \\ &= 2 \int_{T_\alpha^{(1,2)}} W(\nabla u_\epsilon(x)\bar{\lambda}_\epsilon(x)) \, dx, \end{aligned}$$

and:

$$\begin{aligned} & \epsilon^2 \left( \left| \frac{|u_\epsilon(\alpha + \epsilon e_2) - u_\epsilon(\alpha + \epsilon(e_1 + e_2))|}{\epsilon|A(\alpha + \epsilon(e_1 + e_2))e_1|} - 1 \right|^2 + \left| \frac{|u_\epsilon(\alpha) - u_\epsilon(\alpha + \epsilon e_2)|}{\epsilon|A(\alpha + \epsilon e_2)e_2|} - 1 \right|^2 \right) \\ &= 2 \int_{T_\alpha^{(2,1)}} W(\nabla u_\epsilon(x)\bar{\lambda}_\epsilon(x)) \, dx, \end{aligned}$$

where  $\bar{\lambda}_\epsilon : U_\epsilon \rightarrow \mathbb{R}^{2 \times 2}$  is given by:

$$\begin{aligned} \forall x \in T_\alpha^{(1,2)} \cap U_\epsilon, & \quad \bar{\lambda}_\epsilon(x) = \text{diag} \{ |A(\alpha + \epsilon e_1)e_1|^{-1}, |A(\alpha + \epsilon(e_1 + e_2))e_2|^{-1} \} \\ \forall x \in T_\alpha^{(2,1)} \cap U_\epsilon, & \quad \bar{\lambda}_\epsilon(x) = \text{diag} \{ |A(\alpha + \epsilon(e_1 + e_2))e_1|^{-1}, |A(\alpha + \epsilon e_2)e_2|^{-1} \} \end{aligned}$$

Summing over all 2-simplices and noting that each interaction was counted twice, we obtain:

$$(2.1) \quad 0 \leq E_\epsilon(u_\epsilon) - I_{\epsilon,1}(u_\epsilon) \leq \sum_{i,j=1}^2 \sum_{\alpha \in R_\epsilon^{(-1)^j e_i}(\overline{\Omega \setminus U_\epsilon})} \epsilon^2 \left| \frac{|u_\epsilon(\alpha + \epsilon(-1)^j \epsilon e_i) - u_\epsilon(\alpha)|}{\epsilon|A(\alpha)e_i|} - 1 \right|^2,$$

where:

$$(2.2) \quad I_{\epsilon,1}(u_\epsilon) = \int_{U_\epsilon} \left( W(\nabla u_\epsilon(x)\lambda_\epsilon(x)) + W(\nabla u_\epsilon(x)\bar{\lambda}_\epsilon(x)) \right) \, dx.$$

**2.2. Case 2: nearest-neighbour interactions in  $\mathbb{R}^n$ .** Let now  $\Omega \subset \mathbb{R}^n$ , and assume that  $\psi(1) = 1$  and  $\psi(|\xi|) = 0$  for  $|\xi| \geq \sqrt{n}$ . For small  $\epsilon > 0$ , define  $U_\epsilon \subset \Omega$  as the union of all cells in  $\epsilon\mathbb{Z}^n$ , with the standard triangulation  $\mathcal{T}_{\epsilon,n}$ , that have nonempty intersection with  $\Omega_{\epsilon\sqrt{n}}$ . As in Case 1, we identify the given discrete deformation  $u_\epsilon : \epsilon\mathbb{Z}^n \cap \Omega \rightarrow \mathbb{R}^n$  with its unique extension to the continuous function on  $U_\epsilon$ , affine on all of the  $n$ -dimensional simplices in  $\mathcal{T}_{\epsilon,n} \cap U_\epsilon$ .

We also have  $W : \mathbb{R}^{n \times n} \rightarrow \mathbb{R}$ :

$$(2.3) \quad W([M_{ij}]_{i,j:1..n}) = \sum_{i=1}^n \left( \left( \sum_{i=1}^n |M_{ij}|^2 \right)^{1/2} - 1 \right)^2 \quad \forall M \in \mathbb{R}^{n \times n}.$$

Note that for any permutation  $\pi \in S_n$  one has:

$$\begin{aligned} & \epsilon^n \sum_{j=0}^{n-1} \left| \frac{|u_\epsilon(\alpha + \epsilon \sum_{i=1}^{j+1} e_{\pi(i)}) - u_\epsilon(\alpha + \epsilon \sum_{i=1}^j e_{\pi(i)})|}{\epsilon |A(\alpha + \epsilon \sum_{i=1}^j e_{\pi(i)}) e_{\pi(j+1)}|} - 1 \right|^2 \\ &= n! \int_{T_\alpha^\pi} W(\nabla u_\epsilon(x) \lambda_\epsilon(x)) \, dx, \end{aligned}$$

where the piecewise constant matrix field  $\lambda_\epsilon$  is given by:

$$(2.4) \quad \forall x \in T_\alpha^\pi \cap U_\epsilon, \quad \lambda_\epsilon(x) = \text{diag} \left\{ |A(\alpha + \epsilon \sum_{i=1}^{\pi^{-1}(j)-1} e_{\pi(i)}) e_j|^{-1} \right\}_{j=1}^n.$$

To include the interactions in  $\{-e_j\}$  directions, as before, we write:

$$\begin{aligned} & \epsilon^n \sum_{j=0}^{n-1} \left| \frac{|u_\epsilon(\alpha + \epsilon \sum_{i=1}^j e_{\pi(i)}) - u_\epsilon(\alpha + \epsilon \sum_{i=1}^{j+1} e_{\pi(i)})|}{\epsilon |A(\alpha + \epsilon \sum_{i=1}^{j+1} e_{\pi(i)}) e_{\pi(j+1)}|} - 1 \right|^2 \\ &= n! \int_{T_\alpha^\pi} W(\nabla u_\epsilon(x) \bar{\lambda}_\epsilon(x)) \, dx, \end{aligned}$$

where:

$$(2.5) \quad \forall x \in T_\alpha^\pi \cap U_\epsilon, \quad \bar{\lambda}_\epsilon(x) = \text{diag} \left\{ |A(\alpha + \epsilon \sum_{i=1}^{\pi^{-1}(j)} e_{\pi(i)}) e_j|^{-1} \right\}_{j=1}^n.$$

Summing over all of the  $n$ -simplices, and noting that each one-length interaction is counted  $n!$  times, we obtain:

$$(2.6) \quad 0 \leq E_\epsilon(u_\epsilon) - I_{\epsilon,1}(u_\epsilon) \leq \sum_{|\xi|=1} \sum_{\alpha \in R_\epsilon^\xi(\bar{\Omega} \setminus U_\epsilon)} \epsilon^n \left| \frac{|u_\epsilon(\alpha + \epsilon \xi) - u_\epsilon(\alpha)|}{\epsilon |A(\alpha) \xi|} - 1 \right|^2,$$

where  $I_{\epsilon,1}$  is given by the same formula as in (2.2), with  $\lambda_\epsilon$  and  $\bar{\lambda}_\epsilon$  defined as in (2.4), (2.5).

**2.3. Case 3: next-to-nearest-neighbour interactions in  $\mathbb{R}^2$ .** Let us assume now again that  $\Omega \subset \mathbb{R}^2$ , and that  $\psi(\sqrt{2}) = 1$  and  $\psi(|\xi|) = 0$  for  $|\xi| \geq \sqrt{3}$  and  $|\xi| \leq 1$ . Our goal now is to obtain a similar representation and bound to (2.1)–(2.2) for the discrete energy corresponding to the next-to-nearest-neighbour interactions of length  $\sqrt{2}$ . The canonical lattice  $\epsilon\mathbb{Z}^2$  is now mapped onto the lattice  $\epsilon B\mathbb{Z}^2$ , where:

$$B = \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}.$$

We will also need to work with the translated lattice  $\epsilon(e_1 + B\mathbb{Z}^2)$ . Let  $U_{\epsilon, \sqrt{2}}^0 \subset \Omega$  be the union of all open cells in the lattice  $\epsilon B\mathbb{Z}^2$  which have nonempty intersection with  $\Omega_{2\epsilon}$ . Define  $u_{\epsilon, \sqrt{2}}^0$  to be the unique continuous function on  $U_{\epsilon, \sqrt{2}}^0$ , affine on the triangles of the induced triangulation  $B\mathcal{T}_{\epsilon, 2} \cap U_{\epsilon, \sqrt{2}}^0$ , matching with the original deformation  $u_\epsilon$  at each node of the lattice  $\epsilon B\mathbb{Z}^2 \cap U_{\epsilon, \sqrt{2}}^0$ . Likewise, by  $U_{\epsilon, \sqrt{2}}^1 \subset \Omega$  we call the union of cells in the lattice  $\epsilon(e_1 + B\mathbb{Z}^2)$  which have nonempty intersection with  $\Omega_{2\epsilon}$ , while  $u_{\epsilon, \sqrt{2}}^1$  is the matching continuous piecewise affine (on triangles in  $\epsilon e_1 + B\mathcal{T}_{\epsilon, 2}$ ) extension of  $u_\epsilon$ .

Denoting  $\xi_1 = Be_1$  and  $\xi_2 = Be_2$  we obtain, as before:

$$\begin{aligned} \epsilon^2 \left( \left| \frac{|u_\epsilon(B(\alpha + \epsilon e_1)) - u_\epsilon(B\alpha)|}{\epsilon |A(B\alpha)\xi_1|} - 1 \right|^2 + \left| \frac{|u_\epsilon(B(\alpha + \epsilon(e_1 + e_2))) - u_\epsilon(B(\alpha + \epsilon e_1))|}{\epsilon |A(B(\alpha + \epsilon e_1))\xi_2|} - 1 \right|^2 \right) \\ = \frac{2}{|\det B|} \int_{BT_\alpha^{(1,2)}} W(\nabla u_{\epsilon, \sqrt{2}}^0(x) \lambda_{\epsilon, \sqrt{2}}^0(x)) \, dx, \end{aligned}$$

where  $\lambda_{\epsilon, \sqrt{2}}^0 : U_{\epsilon, \sqrt{2}}^0 \rightarrow \mathbb{R}^{2 \times 2}$  is given by:

$$\begin{aligned} \forall x \in BT_\alpha^{(1,2)} \cap U_{\epsilon, \sqrt{2}}^1 \quad \lambda_{\epsilon, \sqrt{2}}^0(x) &= \sqrt{2} B \operatorname{diag} \{ |A(B\alpha)\xi_1|^{-1}, |A(B(\alpha + \epsilon e_1))\xi_2|^{-1} \} \\ \forall x \in BT_\alpha^{(2,1)} \cap U_{\epsilon, \sqrt{2}}^1 \quad \lambda_{\epsilon, \sqrt{2}}^0(x) &= \sqrt{2} B \operatorname{diag} \{ |A(B(\alpha + \epsilon e_2))\xi_1|^{-1}, |A(B\alpha)\xi_2|^{-1} \}. \end{aligned}$$

Interactions in the opposite directions  $-\xi_i$ , yield the integrals:

$$\frac{2}{|\det B|} \int_{BT_\alpha^{1,2}} W(\nabla u_{\epsilon, \sqrt{2}}^0(x) \bar{\lambda}_{\epsilon, \sqrt{2}}^0(x)) \, dx,$$

where now  $\bar{\lambda}_{\epsilon, \sqrt{2}}^0 : U_{\epsilon, \sqrt{2}}^1 \rightarrow \mathbb{R}^{2 \times 2}$  satisfies:

$$\begin{aligned} \forall x \in BT_\alpha^{(1,2)} \cap U_{\epsilon, \sqrt{2}}^1 \\ \bar{\lambda}_{\epsilon, \sqrt{2}}^0(x) &= \sqrt{2} B \operatorname{diag} \{ |A(B(\alpha + \epsilon e_1))\xi_1|^{-1}, |A(B(\alpha + \epsilon(e_1 + e_2)))\xi_2|^{-1} \}, \\ \forall x \in BT_\alpha^{(2,1)} \cap U_{\epsilon, \sqrt{2}}^1 \\ \bar{\lambda}_{\epsilon, \sqrt{2}}^0(x) &= \sqrt{2} B \operatorname{diag} \{ |A(B(\alpha + \epsilon(e_1 + e_2)))\xi_1|^{-1}, |A(B(\alpha + \epsilon e_2))\xi_2|^{-1} \}. \end{aligned}$$

Similarly, we obtain the integral representations on the triangulation  $\epsilon e_1 + B\mathcal{T}_{\epsilon, 2}$  of the set  $U_{\epsilon, \sqrt{2}}^1$ :

$$\int W(\nabla u_{\epsilon, \sqrt{2}}^1(x) \lambda_{\epsilon, \sqrt{2}}^1(x)) \, dx \quad \text{and} \quad \int W(\nabla u_{\epsilon, \sqrt{2}}^1(x) \lambda_{\epsilon, \sqrt{2}}^1(x)) \, dx,$$

with the piecewise affine functions:

$$\begin{aligned}
\forall x \in (\epsilon e_1 + BT_\alpha^{(1,2)}) \cap U_{\epsilon, \sqrt{2}}^1 & \\
\lambda_{\epsilon, \sqrt{2}}^1(x) &= \sqrt{2}B \operatorname{diag} \{ |A(\epsilon e_1 + B\alpha)\xi_1|^{-1}, |A(\epsilon e_1 + B(\alpha + \epsilon e_1))\xi_2|^{-1} \} \\
\forall x \in (\epsilon e_1 + BT_\alpha^{(2,1)}) \cap U_{\epsilon, \sqrt{2}}^1 & \\
\lambda_{\epsilon, \sqrt{2}}^1(x) &= \sqrt{2}B \operatorname{diag} \{ |A(\epsilon e_1 + B(\alpha + \epsilon e_2))\xi_1|^{-1}, |A(\epsilon e_1 + B\alpha)\xi_2|^{-1} \} \\
\forall x \in (\epsilon e_1 + BT_\alpha^{(1,2)}) \cap U_{\epsilon, \sqrt{2}}^1 & \\
\bar{\lambda}_{\epsilon, \sqrt{2}}^1(x) &= \sqrt{2}B \operatorname{diag} \{ |A(\epsilon e_1 + B(\alpha + \epsilon e_1))\xi_1|^{-1}, |A(\epsilon e_1 + B(\alpha + \epsilon(e_1 + e_2)))\xi_2|^{-1} \} \\
\forall x \in (\epsilon e_1 + BT_\alpha^{(2,1)}) \cap U_{\epsilon, \sqrt{2}}^2 & \\
\bar{\lambda}_{\epsilon, \sqrt{2}}^1(x) &= \sqrt{2}B \operatorname{diag} \{ |A(\epsilon e_1 + B(\alpha + \epsilon(e_1 + e_2)))\xi_1|^{-1}, |A(\epsilon e_1 + B(\alpha + \epsilon e_2))\xi_2|^{-1} \}
\end{aligned}$$

Consequently:

$$\begin{aligned}
(2.7) \quad & 0 \leq E_\epsilon(u_\epsilon) - I_{\epsilon, \sqrt{2}}(u_\epsilon) \\
& \leq \sum_{i,j=1}^2 \sum_{\alpha \in R_\epsilon^{(-1)^j \xi_i}(\bar{\Omega} \setminus \Omega_{2\epsilon})} \epsilon^2 \left| \frac{|u_\epsilon(\alpha + \epsilon(-1)^j \xi_i) - u_\epsilon(\alpha)|}{\epsilon |A(\alpha)\xi_i|} - 1 \right|^2,
\end{aligned}$$

where:

$$\begin{aligned}
I_{\epsilon, \sqrt{2}}(u_\epsilon) &= \frac{1}{2} \int_{U_{\epsilon, \sqrt{2}}^0} \left( W(\nabla u_{\epsilon, \sqrt{2}}^0(x) \lambda_{\epsilon, \sqrt{2}}^0(x)) + W(\nabla u_{\epsilon, \sqrt{2}}^1(x) \bar{\lambda}_{\epsilon, \sqrt{2}}^1(x)) \right) dx \\
&+ \frac{1}{2} \int_{U_{\epsilon, \sqrt{2}}^1} \left( W(\nabla u_{\epsilon, \sqrt{2}}^1(x) \lambda_{\epsilon, \sqrt{2}}^1(x)) + W(\nabla u_{\epsilon, \sqrt{2}}^1(x) \bar{\lambda}_{\epsilon, \sqrt{2}}^1(x)) \right) dx.
\end{aligned}$$

### 3. INTEGRAL REPRESENTATION OF DISCRETE ENERGIES (1.3) - THE GENERAL CASE

**Lemma 3.1.** *Let  $\xi = (\xi^1, \dots, \xi^n) \in \mathbb{Z}^n \setminus \{0\}$ . Let  $k$  denote the number of non-zero coordinates in  $\xi$ , and denote:  $\xi^{i_1}, \dots, \xi^{i_k} \neq 0$  with  $i_1 < i_2 \dots < i_k$ , while  $\xi^{j_1} = \dots = \xi^{j_{n-k}} = 0$  with  $j_1 < j_2 \dots < j_{n-k}$ . Fix  $\bar{s} \in \{1 \dots k\}$  and define  $n$  vectors  $\xi_1, \dots, \xi_n \in \mathbb{Z}^n$  by the following algorithm:*

$$\begin{aligned}
\xi_1 &= \xi \\
\forall p = 2, \dots, k - \bar{s} + 1 & \quad \xi_p^{i_{\bar{s}-1+p}} = -\xi^{i_{\bar{s}-1+p}}, \quad \text{and} \quad \xi_p^i = \xi^i \quad \text{for all other indices } i \\
\forall p = k - \bar{s} + 2, \dots, k & \quad \xi_p^{i_{\bar{s}-1+p-k}} = -\xi^{i_{\bar{s}-1+p-k}}, \quad \text{and} \quad \xi_p^i = \xi^i \quad \text{for all other indices } i \\
\forall p = k + 1, \dots, n & \quad \xi_p^{i_{\bar{s}}} = 0, \quad \xi_p^{j_{p-k}} = \xi^{i_{\bar{s}}}, \quad \text{and} \quad \xi_p^i = \xi^i \quad \text{for all other indices } i.
\end{aligned}$$

(In other words, given  $\xi$  and fixing one of its nonzero coordinates  $i_{\bar{s}}$ , we first change sign of all its nonzero coordinates but  $\xi^{i_{\bar{s}}}$ , in the cyclic order, starting from  $\xi^{i_{\bar{s}}}$ : this gives  $k$  vectors  $\xi_p$ . Then we permute the  $\xi^{i_{\bar{s}}}$  coordinate with all the zero coordinates: this gives the remaining  $n - k$  coordinates).

Then the  $n$ -tuple of vectors  $\xi_1, \dots, \xi_n$  is linearly independent.



*Proof.* Without loss of generality, we may assume that  $i_p = p$  for all  $p = 1, \dots, k$  and  $\bar{s} = 1$ .

Consider first the case when  $k = n$ , i.e. when all coordinates of the vector  $\xi$  are nonzero. Then the matrix  $B = [\xi_1, \dots, \xi_n]$  is similar to the following matrix:

$$\tilde{B} = \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & -1 & 1 & \cdots & 1 \\ 1 & 1 & -1 & \cdots & 1 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 1 & 1 & 1 & \cdots & -1 \end{bmatrix},$$

by the basic operations of dividing each row by  $|\xi^i|$ . The matrix  $\tilde{B}$  above has nonzero determinant, which proves the claim.

Assume now that  $k \neq n$ , i.e. the last  $n - k > 0$  coordinates of  $\xi$  are zero. Then, the  $k \times k$  principal minor of the matrix  $B = [\xi_1, \dots, \xi_n]$  is invertible, as in the first case above. The minor consisting of  $n - k$  last rows and  $k$  first columns of  $B$  equals zero, hence  $B$  is invertible if and only if its minor  $B_0$  consisting of  $n - k$  last rows and  $n - k$  last columns is invertible. But  $B_0 = \xi^{i_{\bar{s}}} \text{Id}_{n-k}$  and hence the lemma is achieved.  $\blacksquare$

**3.1. Case 4: interactions of a given length  $|\xi_0| \neq 0$  in  $\mathbb{R}^n$ .** Assume now that  $\Omega \subset \mathbb{R}^n$  and let  $\psi(|\xi_0|) = 1$  and  $\psi(|\xi|) = 0$  for  $\|\xi| - |\xi_0|\| > s$ , and a small  $s > 0$ . Consider the following set of unordered  $n$ -tuples, which we assume to be nonempty:

$$(3.1) \quad S_{|\xi_0|} = \left\{ \zeta = \{\zeta^1, \dots, \zeta^n\} \subset \mathbb{Z}, |\zeta|^2 = |\xi_0|^2 \right\}.$$

Fix  $\zeta \in S_{|\xi_0|}$  and let  $N_\zeta$  be the set of all distinct signed permutations without repetitions of the coordinates of  $\zeta$ , i.e.:

$$(3.2) \quad N_\zeta = \left\{ (\pm \zeta^{\pi(1)}, \pm \zeta^{\pi(2)}, \dots, \pm \zeta^{\pi(n)}); \pi \in S_n \right\}.$$

Clearly:  $|N_\zeta| = 2^k \frac{n!}{k_1! \dots k_n!}$ , where  $k_1, \dots, k_n$  denote the numbers of repetitions of distinct coordinates in  $\zeta$ , and  $k$  is the number of non-zero coordinates in  $\zeta$ .

For each  $\xi \in N_\zeta$  and each of its  $k$  non-zero entries  $\xi^{i_{\bar{s}}}$  we define the set of linearly independent vectors  $\xi_1, \dots, \xi_n$  using the algorithm described in Lemma 3.1. We call  $K_\zeta$  the set of all matrices  $B = [\xi_1, \dots, \xi_n]$  obtained by this procedure; it corresponds to the set of lattices  $\epsilon B \mathbb{Z}^n$  whose edges have lengths  $\epsilon |\xi_0|$ . Note that:

$$|K_\zeta| = k |N_\zeta| = 2^k k \frac{n!}{k_1! \dots k_n!}.$$

**Lemma 3.2.** *Let  $\zeta \in S_{|\xi_0|}$  have  $k$  non-zero entries. Then every vector  $\xi \in N_\zeta$  is included in exactly  $nk$  lattices  $B$ , as described above.*

*Proof.* Firstly, the number of lattices where  $\xi$  is one of the first  $k$  columns of  $B$ , equals  $k^2$  ( $k$  possible columns and  $k$  choices of a non-zero entry  $\xi^{i_{\bar{s}}}$ ). Secondly, the number of lattices where  $\xi$  is one of the last  $n - k$  columns, equals  $(n - k)k$  (given by  $n - k$  possible columns and  $k$  choices of a non-zero entry which defines the first vector in  $B$ ). We hence obtain  $nk$  total number of lattices, as claimed.  $\blacksquare$

**Remark 3.3.** The total number of vectors (with repetitions) which are columns of lattices in the set  $K_\zeta$ , equals  $|K_\zeta|n = nk|N_\zeta|$ . This is consistent with Lemma 3.2, as each vector in  $N_\zeta$  is repeated  $nk$  times.

We now construct the integral representation of the discrete energy in the presently studied Case 4. Fix  $B \in K_\zeta$  as above, and define  $U_{\epsilon,|\xi_0|}^{0,B} \subset \Omega$  to be the union of all open cells in  $\epsilon B\mathbb{Z}^n$  that have nonempty intersection with  $\Omega_{\epsilon\sqrt{n}|\xi_0|}$ . We identify the discrete deformation  $u_\epsilon$  with its unique continuous extension  $u_{\epsilon,|\xi_0|}^{0,B}$  on  $U_{\epsilon,|\xi_0|}^{0,B}$ , affine on all the simplices of the induced triangulation  $\epsilon B\mathcal{T}_{\epsilon,n}$ . Following the same observations as in the particular cases before, we obtain, for any  $\pi \in S(n)$ :

$$\begin{aligned} \epsilon^n \sum_{j=0}^{n-1} \left| \frac{|u_\epsilon(B(\alpha + \epsilon \sum_{i=1}^{j+1} e_{\pi(i)})) - u_\epsilon(B(\alpha + \epsilon \sum_{i=1}^j e_{\pi(i)}))|}{\epsilon |A(B(\alpha + \epsilon \sum_{i=1}^j e_{\pi(i)})e_{\pi(j+1)})|} - 1 \right|^2 \\ = \frac{n!}{|\det B|} \int_{BT_\alpha^\pi} W(\nabla u_{\epsilon,|\xi_0|}^{0,B}(x) \lambda_{\epsilon,|\xi_0|}^{0,B}(x)) \, dx, \end{aligned}$$

where  $W$  is as in (2.3), and:

$$\begin{aligned} \forall x \in BT_\alpha^\pi \cap U_{\epsilon,|\xi_0|}^{0,B} \\ \lambda_{\epsilon,|\xi_0|}^{0,B}(x) = |\xi_0| B \operatorname{diag} \left\{ |A(B(\alpha + \epsilon \sum_{i=1}^{\pi^{-1}(j)-1} e_{\pi(i)})) B e_j|^{-1} \right\}_{j=1}^n. \end{aligned}$$

In order to take into account all of the interactions of length  $|\xi_0|$ , we need to consider translations of the lattice  $\epsilon B\mathbb{Z}^n$ . Define:

$$(3.3) \quad V_B = \epsilon \mathbb{Z}^n \cap \left( \left( \operatorname{Int}(\epsilon BC_n) \cup \bigcup_{i=1}^n \epsilon B \{ (x_1 \dots x_n) \in C_n; x_i = 1 \} \right) \setminus \epsilon BV_n \right),$$

where  $V_n$  is the set of vertices of the unit cube  $C_n$ . For every  $\tau \in V_B$ , define  $U_{\epsilon,|\xi_0|}^{\tau,B} \subset \Omega$  to be the union of all cells in  $\tau + \epsilon B\mathbb{Z}^n$  that have nonempty intersection with  $\Omega_{\epsilon\sqrt{n}|\xi_0|}$ . We extend the discrete deformation  $u_\epsilon$  to the continuous function  $u_{\epsilon,|\xi_0|}^{\tau,B}$  on  $U_{\epsilon,|\xi_0|}^{\tau,B}$ , affine on all the simplices of the induced triangulation  $\tau + B\mathcal{T}_{\epsilon,n}$ . We then have:

$$\begin{aligned} \epsilon^n \sum_{j=0}^{n-1} \left| \frac{|u_\epsilon(\tau + B(\alpha + \epsilon \sum_{i=1}^{j+1} e_{\pi(i)})) - u_\epsilon(\tau + B(\alpha + \epsilon \sum_{i=1}^j e_{\pi(i)}))|}{\epsilon |A(\tau + B(\alpha + \epsilon \sum_{i=1}^j e_{\pi(i)})e_{\pi(j+1)})|} - 1 \right|^2 \\ = \frac{n!}{|\det B|} \int_{\tau + BT_\alpha^\pi} W(\nabla u_{\epsilon,|\xi_0|}^{\tau,B}(x) \lambda_{\epsilon,|\xi_0|}^{\tau,B}(x)) \, dx, \end{aligned}$$

where:

$$\begin{aligned} \forall x \in (\tau + BT_\alpha^\pi) \cap U_{\epsilon,|\xi_0|}^{\tau,B} \\ \lambda_{\epsilon,|\xi_0|}^{\tau,B}(x) = |\xi_0| B \operatorname{diag} \left\{ |A(\tau + B(\alpha + \epsilon \sum_{i=1}^{\pi^{-1}(j)-1} e_{\pi(i)})) B e_j|^{-1} \right\}_{j=1}^n. \end{aligned}$$

Summing now over all simplices in the triangulations, we obtain the functional:

$$(3.4) \quad I_{\epsilon,|\xi_0|}(u_\epsilon) = \sum_{\zeta \in S_{|\xi_0|}} \frac{1}{n!(nk)} \sum_{B \in K_\zeta} \frac{n!}{|\det B|} \sum_{\tau \in \{0\} \cup V_B} \int_{U_{\epsilon,|\xi_0|}^{\tau,B}} W(\nabla u_{\epsilon,|\xi_0|}^{\tau,B}(x) \lambda_{\epsilon,|\xi_0|}^{\tau,B}(x)) \, dx,$$

and the bound:

$$(3.5) \quad \begin{aligned} 0 &\leq E_\epsilon(u_\epsilon) - I_{\epsilon,|\xi_0|}(u_\epsilon) \\ &\leq \sum_{\xi \in \mathbb{Z}^n, |\xi|=|\xi_0|} \sum_{\alpha \in R_\epsilon^\xi(\Omega \setminus \Omega_{\epsilon\sqrt{n}|\xi_0|})} \epsilon^n \left| \frac{|u_\epsilon(\alpha + \epsilon\xi) - u_\epsilon(\alpha)|}{\epsilon|A(\alpha)\xi|} - 1 \right|^2. \end{aligned}$$

In (3.4),  $k$  is the number of non-zero entries in the vector  $\zeta$ , while the factor  $n!$  in the first denominator is due to the fact that every edge in a given lattice is shared by  $n!$  simplices in  $\mathcal{T}_{\epsilon,n}$ .

**3.2. Case 5: the general case of finite range interactions in  $\mathbb{R}^n$ .** Reasoning as in the previously considered specific cases, we get:

$$(3.6) \quad 0 \leq E_\epsilon(u_\epsilon) - I_\epsilon(u_\epsilon) \leq \sum_{\xi \in \mathbb{Z}^n, 1 \leq |\xi| \leq M} \sum_{\alpha \in R_\epsilon^\xi(\Omega \setminus \Omega_{\epsilon\sqrt{n}M})} \epsilon^n \psi(|\xi|) \left| \frac{|u_\epsilon(\alpha + \epsilon\xi) - u_\epsilon(\alpha)|}{\epsilon|A(\alpha)\xi|} - 1 \right|^2,$$

where:

$$(3.7) \quad I_\epsilon = \sum_{1 \leq |\xi_0| \leq M} \psi(|\xi_0|) I_{\epsilon,|\xi_0|}.$$

#### 4. BOUNDS ON THE VARIATIONAL LIMITS OF THE LATTICE ENERGIES

Consider the following family of energies:

$$F_\epsilon : L^2(\Omega, \mathbb{R}^n) \rightarrow \overline{\mathbb{R}}, \quad F_\epsilon(u) = \begin{cases} E_\epsilon(u|_{\epsilon\mathbb{Z}^n \cap \Omega}) & \text{if } u \in \mathcal{C}(\Omega) \text{ is affine on } \mathcal{T}_{\epsilon,n} \cap \Omega \\ +\infty & \text{otherwise.} \end{cases}$$

By Theorem 7.3, the sequence  $F_\epsilon$  has a subsequence (which we do not relabel)  $\Gamma$ -converging to some lsc functional  $\mathcal{F} : L^2(\Omega, \mathbb{R}^n) \rightarrow \overline{\mathbb{R}}$ . Our goal is to identify the limiting energy  $\mathcal{F}$  in its exact form, whenever possible, or find its lower and upper bounds. This will be accomplished in Theorem 4.4, and in the next section.

We first state some easy preliminary results regarding the quasiconvexification  $QW$  and the piecewise affine extensions  $u_{\epsilon,|\xi_0|}^{\tau,B}$  of the discrete deformations  $u_\epsilon$ .

**Lemma 4.1.** *The quasiconvexification  $QW : \mathbb{R}^{n \times n} \rightarrow \mathbb{R}$  of  $W$  in (2.3), is a convex function, and:*

$$(4.1) \quad QW(M) = \sum_{i=1..n; |Me_i| > 1} (|Me_i| - 1)^2 \quad \forall M \in \mathbb{R}^{n \times n}.$$

*Proof.* By Theorem 6.12 and Theorem 5.3 in [10] (see Theorem 7.4) we note that:

$$QW(M) = \sum_{i=1}^n Q(|Me_i| - 1)^2.$$

and that the convexification: and the quasiconvexification  $Qf$  of the function  $f : \mathbb{R}^n \rightarrow \mathbb{R}$  given by  $f(\xi) = (|\xi| - 1)^2$  coincide with each other. The claim follows by checking directly that:

$$Cf(\xi) = \begin{cases} 0 & \text{if } |\xi| \leq 1 \\ (|\xi| - 1)^2 & \text{if } |\xi| > 1. \end{cases}$$

■

**Lemma 4.2.** *For every  $u \in W^{1,2}(\Omega, \mathbb{R}^n)$ , and every mesh-size sequence  $\epsilon \rightarrow 0$ , there exists a subsequence  $\epsilon$  (which we do not relabel) and a sequence  $u_\epsilon \in W_0^{1,2}(\mathbb{R}^n, \mathbb{R}^n)$  of continuous piecewise affine on the triangulation in  $\mathcal{T}_{\epsilon,n}$  functions, such that:*

$$\begin{aligned} \forall 1 \leq |\xi_0| \leq M \quad \forall \zeta \in S_{|\xi_0|} \quad \forall B \in K_\zeta \quad \forall \tau \in \{0\} \cup V_B \\ u = \lim_{\epsilon \rightarrow 0} u_{\epsilon,|\xi_0|}^{\tau,B} \quad \text{in } W^{1,2}(\Omega, \mathbb{R}^n). \end{aligned}$$

*Proof.* Approximate  $u$  by  $u_k \in C_0^\infty(\mathbb{R}^n, \mathbb{R}^n)$ , so that  $u_k \rightarrow u$  in  $W^{1,2}(\Omega, \mathbb{R}^n)$ . Fix  $|\xi_0| \leq M$ ,  $\zeta \in S_{|\xi_0|}$ ,  $B \in K_\zeta$  and  $\tau \in V_B$ . Then, by the fundamental estimate of finite elements [9], the  $\mathbb{P}_1$ -interpolation  $u_{\epsilon,k}$  of  $u_k$  on  $\mathcal{T}_{\epsilon,n}$ , i.e. the continuous function affine on the simplices in  $\mathcal{T}_{\epsilon,n}$  which coincides with  $u_k$  on  $\epsilon\mathbb{Z}^n$ , satisfies:

$$\|u_{\epsilon,k} - u_k\|_{W^{1,2}(\Omega)} \leq \frac{1}{k} \quad \forall \epsilon \leq \epsilon_k.$$

Likewise, because the set of all involved quantities  $|\xi_0|, \zeta, B, \tau$  is finite, it follows that:

$$\|(u_{\epsilon,k})_{\epsilon,|\xi_0|}^{\tau,B} - u_k\|_{W^{1,2}(\Omega)} \leq \frac{1}{k}$$

if only  $\epsilon \leq \epsilon_k$  is sufficiently small. We set  $u_\epsilon := u_{\epsilon,k}$  which satisfies the claim of the Lemma.  $\blacksquare$

We now observe a compactness property of  $E_\epsilon$ , which together with the  $\Gamma$ -convergence of  $F_\epsilon$  to  $\mathcal{F}$ , implies convergence of the minimizers of  $E_\epsilon$  to the minimizers of  $\mathcal{F}$  (see Theorem 7.2).

**Lemma 4.3.** *Assume that  $E_\epsilon(u_\epsilon) \leq C$ , for some sequence of discrete deformations  $u_\epsilon : \epsilon\mathbb{Z}^n \cap \Omega \rightarrow \mathbb{R}^n$ , which we identify with  $u_\epsilon \in \mathcal{C}(\Omega)$  that are piecewise affine on  $\mathcal{T}_{\epsilon,n} \cap \Omega$  and agree with the discrete  $u_\epsilon$  at each node of the lattice. Then there exist constants  $c_\epsilon \in \mathbb{R}^n$  such that  $u_\epsilon - c_\epsilon$  converges (up to a subsequence) in  $L^2(\Omega, \mathbb{R}^n)$  to some  $u \in W^{1,2}(\Omega, \mathbb{R}^n)$ .*

*Proof.* Observe that for every  $|\xi_0|, \tau, B$  as in (3.7), (3.4), and every  $\epsilon \leq \epsilon_0$ :

$$(4.2) \quad \int_{U_{\epsilon,|\xi_0|}^{\tau,B}} W(\nabla u_{\epsilon,|\xi_0|}^{\tau,B}(x) \lambda_{\epsilon,|\xi_0|}^{\tau,B}(x)) \, dx \leq C.$$

Thus in particular, for some  $\xi_0 \in \mathbb{Z}^n$  such that  $\psi(|\xi_0|) \neq 0$ , and for every  $\eta > 0$ :

$$\|\nabla u_{\epsilon,|\xi_0|}^{0,B}\|_{L^2(\Omega_\eta)} \leq C.$$

if only  $\epsilon \leq \epsilon_0$  is small enough. Fix  $\eta > 0$ . The above bound implies that  $\nabla u_{\epsilon,|\xi_0|}^{0,B}$  converges weakly (up to a subsequence) in  $L^2(\Omega_\eta)$ , which by means of the Poincaré inequality yields weak convergence of  $u_{\epsilon,|\xi_0|}^{0,B} - c_\epsilon$  in  $W^{1,2}(\Omega_\eta)$ . We now observe that:

$$\|u_{\epsilon,|\xi_0|}^{0,B} - u_\epsilon\|_{L^2(\Omega_\eta)} \leq C\epsilon|\xi_0| \|u_\epsilon\|_{W^{1,2}(\Omega_\eta)},$$

because  $u_{\epsilon,|\xi_0|}^{\tau,B}$  is a  $\mathbb{P}_1$  interpolation of  $u_\epsilon$  on the lattice  $\epsilon B\mathbb{Z}^n \cap \Omega_\eta$ , allowing to use the classical finite element error estimate in [9, Theorem 3.1.6]. This ends the proof.  $\blacksquare$

**Theorem 4.4.** *We have:*

$$(4.3) \quad \forall u \in W^{1,2}(\Omega, \mathbb{R}^n) \quad I_Q(u) \leq \mathcal{F}(u) \leq I(u),$$

where:

$$(4.4) \quad \begin{aligned} I_Q(u) &= \sum_{1 \leq |\xi_0| \leq M} \sum_{\zeta \in S_{|\xi_0|}, B \in K_\zeta} \psi(|\xi_0|) \frac{(1 + |V_B|)}{(nk) |\det B|} \int_{\Omega} QW(\nabla u(x)) \lambda_{|\xi_0|}^B(x) \, dx, \\ I(u) &= \sum_{1 \leq |\xi_0| \leq M} \sum_{\zeta \in S_{|\xi_0|}, B \in K_\zeta} \psi(|\xi_0|) \frac{(1 + |V_B|)}{(nk) |\det B|} \int_{\Omega} W(\nabla u(x)) \lambda_{|\xi_0|}^B(x) \, dx, \end{aligned}$$

and where  $\lambda_{|\xi_0|}^B(x)$  is given by:

$$(4.5) \quad \lambda_{|\xi_0|}^B(x) = |\xi_0| B \operatorname{diag} \{ |A(x) B e_j|^{-1} \}_{j=1}^n.$$

*Proof. 1.* Let  $u \in W^{1,2}(\Omega, \mathbb{R}^n)$  and consider the approximating sequence  $u_\epsilon$  as in Lemma 4.2. Directly from the definition of  $\Gamma$ -convergence (see (7.1)), we obtain:

$$(4.6) \quad \mathcal{F}(u) \leq \liminf_{\epsilon \rightarrow 0} F_\epsilon(u_\epsilon) = \liminf_{\epsilon \rightarrow 0} E_\epsilon(u_\epsilon).$$

Further, in view of the boundedness of  $\psi$ , and of the sequence  $\|\nabla u_\epsilon\|_{L^2(\Omega)}$ , (3.6) implies:

$$(4.7) \quad \begin{aligned} 0 \leq E_\epsilon(u_\epsilon) - I_\epsilon(u_\epsilon) &\leq C \sum_{\xi \in \mathbb{Z}^n, 1 \leq |\xi| \leq M} \sum_{\alpha \in R_\epsilon^\xi(\Omega \setminus \Omega_{\epsilon\sqrt{n}M})} \epsilon^n \left( \left| \frac{u_\epsilon(\alpha + \epsilon\xi) - u_\epsilon(\alpha)}{\epsilon|\xi|} \right|^2 + 1 \right) \\ &\leq C \left( \|\nabla u_\epsilon\|_{L^2(\Omega \setminus \Omega_{\epsilon\sqrt{n}M})}^2 + |\Omega \setminus \Omega_{\epsilon\sqrt{n}M}| \right) \rightarrow 0 \quad \text{as } \epsilon \rightarrow 0. \end{aligned}$$

Indeed, the third inequality in (4.7) can be proven by the same argument as in the proof of Lemma 4.2. Alternatively, a direct proof can be obtained as follows. Since  $u_\epsilon$  is piecewise affine, we have:

$$\left| \frac{u_\epsilon(\alpha + \epsilon\xi) - u_\epsilon(\alpha)}{\epsilon|\xi|} \right|^2 = \left| \int_0^1 \langle \nabla u_\epsilon(\alpha + t\epsilon\xi), \frac{\xi}{|\xi|} \rangle \, dt \right|^2 \leq \int_0^1 q_\epsilon(\alpha + t\epsilon\xi)^2 \, dt,$$

where  $q_\epsilon(p) = \sup_i \langle \nabla u_\epsilon(p), v_i \rangle$  when  $p$  is an interior point of a face of the triangulation  $\mathcal{T}_{\epsilon,n}$  spanned by unit vectors  $v_1, \dots, v_k$  (here  $0 \leq k \leq n$ ). Note that:

$$q_\epsilon(p)^2 \leq \frac{n!}{\epsilon^n} \int_T |\nabla u_\epsilon|^2 \quad \forall p \in T \in \mathcal{T}_{\epsilon,n}.$$

We hence obtain:

$$\begin{aligned} \forall 1 \leq |\xi| \leq M \quad &\sum_{\alpha \in R_\epsilon^\xi(\Omega \setminus \Omega_{\epsilon\sqrt{n}M})} \epsilon^n \left| \frac{u_\epsilon(\alpha + \epsilon\xi) - u_\epsilon(\alpha)}{\epsilon|\xi|} \right|^2 \leq \int_0^1 \sum_{\alpha \in R_\epsilon^\xi(\Omega \setminus \Omega_{\epsilon\sqrt{n}M})} \epsilon^n q_\epsilon(\alpha + \epsilon\xi)^2 \, dt \\ &\leq C \int_0^1 \left( \sum_\alpha \int_T |\nabla u_\epsilon|^2 \right) \, dt \leq C \int_0^1 \|\nabla u_\epsilon\|_{L^2(\Omega \setminus \Omega_{\epsilon\sqrt{n}M})}^2 \, dt = \|\nabla u_\epsilon\|_{L^2(\Omega \setminus \Omega_{\epsilon\sqrt{n}M})}^2, \end{aligned}$$

which achieves (4.7).

Consequently, by (4.6), (4.7), we see that:

$$\mathcal{F}(u) \leq \liminf_{\epsilon \rightarrow 0} I_\epsilon(u_\epsilon),$$

so that by Lemma 4.2 and using the dominated convergence theorem, we obtain:

$$(4.8) \quad \mathcal{F}(u) \leq \liminf_{\epsilon \rightarrow 0} \sum_{1 \leq |\xi_0| \leq M} \sum_{\zeta \in S_{|\xi_0|}, B \in K_\zeta} \psi(|\xi_0|) \frac{(1 + |V_B|)}{(nk) |\det B|} \int_{\Omega} W(\nabla u_{\epsilon, |\xi_0|}^{\tau, B}(x) \lambda_{\epsilon, |\xi_0|}^{\tau, B}(x)) \, dx = I(u),$$

in view of the uniform convergence of  $\lambda_{\epsilon, |\xi_0|}^{\tau, B}$  to  $\lambda_{|\xi_0|}^B$  in  $\Omega$ . The proof of the upper bound for  $\mathcal{F}$  in (4.3) is hence accomplished.

**2.** We now show the lower bound in (4.3). Let  $u \in W^{1,2}(\Omega, \mathbb{R}^n)$ ; note that the upper bound proved above yields:  $\mathcal{F}(u) < \infty$ . Therefore,  $u$  has a recovery sequence  $u_\epsilon \in \mathcal{C}(\Omega)$  affine on  $\mathcal{T}_{\epsilon, n} \cap \Omega$ , such that:  $u_\epsilon \rightarrow u$  in  $L^2(\Omega, \mathbb{R}^n)$  and  $E_\epsilon(u_\epsilon) \rightarrow \mathcal{F}(u)$  as  $\epsilon \rightarrow 0$ .

As in the proof of Lemma 4.3, we see that (4.2) holds for every  $|\xi_0|, \tau, B$  as in (3.7), (3.4). Thus, for every  $\eta > 0$  we have:

$$(4.9) \quad \|\nabla u_{\epsilon, |\xi_0|}^{\tau, B}\|_{L^2(\Omega_\eta)} \leq C,$$

for every  $\epsilon \leq \epsilon_0$  is small enough. Fix  $\eta > 0$ . The bound (4.9) implies that every  $\nabla u_{\epsilon, |\xi_0|}^{\tau, B}$  converges weakly (up to a subsequence) in  $L^2(\Omega_\eta)$ . Next, we note that  $u_{\epsilon, |\xi_0|}^{\tau, B}$  converges to  $u$  in  $L^2(\Omega_\eta)$ , which yields that the same convergence is also valid weakly in  $W^{1,2}(\Omega_\eta)$ .

Indeed, by [9, Theorem 3.1.6], we have:

$$\|u_{\epsilon, |\xi_0|}^{\tau, B} - u_\epsilon\|_{L^2(\Omega_\eta)} \leq C\epsilon |\xi_0| \|u_\epsilon\|_{W^{1,2}(\Omega_\eta)},$$

because  $u_{\epsilon, |\xi_0|}^{\tau, B}$  is a  $\mathbb{P}_1$  interpolation of  $u_\epsilon$  on the lattice  $\epsilon B \mathbb{Z}^n \cap \Omega_\eta$ . Consequently, in view of (4.9):

$$\|u_{\epsilon, |\xi_0|}^{\tau, B} - u\|_{L^2(\Omega_\eta)} \leq \|u_{\epsilon, |\xi_0|}^{\tau, B} - u_\epsilon\|_{L^2(\Omega_\eta)} + \|u_\epsilon - u\|_{W^{1,2}(\Omega_\eta)} \leq C\epsilon + \|u_\epsilon - u\|_{W^{1,2}(\Omega_\eta)} \rightarrow 0, \quad \text{as } \epsilon \rightarrow 0.$$

Since  $QW \geq W$ , we further obtain:

$$\begin{aligned} \mathcal{F}(u) &= \lim_{\epsilon \rightarrow 0} F_\epsilon(u_\epsilon) \geq \limsup_{\epsilon \rightarrow 0} I_\epsilon(u_{\epsilon|\Omega_\eta}) \\ &\geq \sum_{1 \leq |\xi_0| \leq M} \sum_{\zeta \in S_{|\xi_0|}} \frac{\psi(|\xi_0|)}{(nk)} \sum_{B \in K_\zeta} \frac{1}{|\det B|} \sum_{\tau \in \{0\} \cup V_{l,B}} \liminf_{\epsilon \rightarrow 0} \int_{\Omega_\eta} QW(\nabla u_{\epsilon, |\xi_0|}^{\tau, B}(x) \lambda_{\epsilon, |\xi_0|}^{\tau, B}(x)) \, dx \\ &\geq \sum_{1 \leq |\xi_0| \leq M} \sum_{\zeta \in S_{|\xi_0|}, B \in K_\zeta} \frac{\psi(|\xi_0|)}{(nk)} \frac{1 + |V_{l,B}|}{|\det B|} \int_{\Omega_\eta} QW(\nabla u(x) \lambda_{|\xi_0|}^B(x)) \, dx = I_Q(u|_{\Omega_\eta}), \end{aligned}$$

where the last inequality above follows by the lower semicontinuity of the functional  $\int_{\Omega} QW(v(x)) \, dx$  with respect to the weak topology of  $L^2(\Omega_\eta, \mathbb{R}^{n \times n})$  (see Theorem 7.5), and by the weak convergence of  $\nabla u_{\epsilon, |\xi_0|}^{\tau, B} \lambda_{\epsilon, |\xi_0|}^{\tau, B}$  to  $\nabla u \lambda_{|\xi_0|}^B$  in  $L^2$ . Since  $\eta > 0$  was arbitrary, the proof is achieved.  $\blacksquare$

**Corollary 4.5.** *We have:  $\mathcal{F}(u) < +\infty$  if and only if  $u \in W^{1,2}(\Omega, \mathbb{R}^n)$ .*

*Proof.* By Theorem 4.4,  $\mathcal{F}$  is finite on all  $W^{1,2}$  deformations. Conversely, let  $u \in L^2(\Omega, \mathbb{R}^n)$  and let  $\mathcal{F}(u) < \infty$ . Then there exists a recovery sequence  $u_\epsilon \in \mathcal{C}(\Omega)$  affine on  $\mathcal{T}_{\epsilon, n} \cap \Omega$ , so that  $u_\epsilon \rightarrow u$  in  $L^2$  and  $F_\epsilon(u_\epsilon)$  is uniformly bounded. This implies (4.2) so in particular  $\|\nabla u_\epsilon\|_{L^2(\Omega)}^2$  is bounded and hence (up to a subsequence)  $u_\epsilon$  converges weakly in  $W^{1,2}(\Omega)$ . Consequently,  $u \in W^{1,2}(\Omega)$ .  $\blacksquare$

**Corollary 4.6.** *Let  $G_0(I)$  denote the sequentially weak lsc envelope of  $I$  in  $W^{1,2}(\Omega, \mathbb{R}^n)$ . Then:*

$$\mathcal{F}(u) \leq G_0(I)(u) \quad \forall u \in W^{1,2}(\Omega, \mathbb{R}^n).$$

*Proof.* The proof is immediate since the  $\Gamma$ -limit  $F$  is sequentially weak lsc in  $W^{1,2}(\Omega, \mathbb{R}^n)$ . ■

## 5. THE CASE OF NEAREST-NEIGHBOUR INTERACTIONS

In this section we improve the result in (4.3) to the exact form of the limiting energy  $\mathcal{F}$ , in the special cases of near and next-to-nearest-neighbour interactions.

**Theorem 5.1.** *(Case 1: nearest-neighbour interactions in  $\mathbb{R}^2$ .) Let  $\Omega \subset \mathbb{R}^2$  and let  $\psi(1) = 1$  and  $\psi(|\xi|) = 0$  for all  $|\xi| \geq \sqrt{2}$ . Denote:  $\lambda(x) = \text{diag} \{|A(x)e_1|^{-1}, |A(x)e_2|^{-1}\}$ . Then:*

$$(5.1) \quad \mathcal{F}(u) = \begin{cases} 2 \int_{\Omega} QW(\nabla u(x)\lambda(x)) dx & \text{for } u \in W^{1,2}(\Omega, \mathbb{R}^2) \\ +\infty & \text{for } u \in L^2 \setminus W^{1,2}. \end{cases}$$

*Proof.* From Theorem 4.4 and (2.2), we see that  $I_Q(u) = 2 \int_{\Omega} QW(\nabla u\lambda(x)) dx$  and  $I(u) = 2 \int_{\Omega} W(\nabla u\lambda(x)) dx$ . By Corollary 4.6 it follows that:

$$\mathcal{F}(u) \leq G_0\left(2 \int_{\Omega} W(\nabla u(x)\lambda(x)) dx\right) = 2 \int_{\Omega} QW(\nabla u\lambda(x)) dx.$$

The last equality is a consequence of Theorem 7.6 because the function  $f(x, M) = W(M\lambda(x))$  clearly satisfies the bounds (7.1) and also its quasiconvexification with respect to  $M$  equals:

$$Qf(x, M) = QW(M\lambda(x)).$$

The proof is now complete in view of Corollary 4.5. ■

**Theorem 5.2.** *(Case 2: nearest-neighbour interactions in  $\mathbb{R}^n$ .) Let  $\Omega \subset \mathbb{R}^n$  and let  $\psi(1) = 1$  and  $\psi(|\xi|) = 0$  for  $|\xi| \geq \sqrt{n}$ . Denote:  $\lambda(x) = \text{diag} \{|A(x)e_j|^{-1}\}_{j=1}^n$ . Then, the  $\Gamma$ -limit  $\mathcal{F}$  has the form as in (5.1):*

$$(5.2) \quad \mathcal{F}(u) = \begin{cases} 2 \int_{\Omega} QW(\nabla u(x)\lambda(x)) dx & \text{for } u \in W^{1,2}(\Omega, \mathbb{R}^n) \\ +\infty & \text{for } u \in L^2 \setminus W^{1,2}. \end{cases}$$

*Proof.* The proof follows exactly as in Theorem 5.1, using the representation developed in section 2.2. Alternatively, using the notation and setting of section 3, we see that  $S_1 = \{e_i\}_{i=1}^n$  and:

$$\forall \zeta \in S_1 \quad N_{\zeta} = N = \{e_i, -e_i\}_{i=1}^n, \quad \text{and } K = \bigcup_{\zeta \in S_1} K_{\zeta} = \{B = \pm[e_i, e_{i+1}, \dots, e_{i-1}]\}_{i=1}^n,$$

so that  $|K| = 2n$ . Also, for every  $B \in K$  as above:  $V_B = \emptyset$ ,  $|\det B| = 1$  and  $\lambda_1^B(x) = B \text{diag}\{|A(x)Be_j|^{-1}\}_{j=1}^n$ , i.e.  $\lambda_1^B(x)$  differs from  $\lambda(x)$  only by the order and sign of its columns. Hence:

$$\forall B \in K \quad QW(\nabla u(x)\lambda_1^B(x)) = QW(\nabla u(x)\lambda(x)), \quad W(\nabla u(x)\lambda_1^B(x)) = W(\nabla u(x)\lambda(x))$$

and so:

$$I_Q(u) = \sum_{\zeta \in S_1, B \in K_{\zeta}} \frac{1}{n} \int_{\Omega} QW(\nabla u(x)\lambda_1^B(x)) dx = 2 \int_{\Omega} QW(\nabla u(x)\lambda(x)) dx.$$

Likewise:  $I(u) = 2 \int_{\Omega} W(\nabla u(x)\lambda(x)) \, dx$ . The proof follows now by Corollary 4.6 and Theorem 7.6, as before.  $\blacksquare$

Using the integral representation of section 2.3, we also arrive at:

**Theorem 5.3.** (Case 3: next-to-nearest-neighbour interactions in  $\mathbb{R}^2$ .) Let  $\Omega \subset \mathbb{R}^2$  and assume that  $\psi(\sqrt{2}) = 1$  and  $\psi(|\xi|) = 0$  for all  $|\xi| \geq \sqrt{3}$  and  $|\xi| \leq 1$ . Denote:

$$\lambda_{\sqrt{2}}(x) = \sqrt{2}B \operatorname{diag} \{|A(x)Be_1|^{-1}, |A(x)Be_2|^{-1}\}, \quad B = \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}.$$

Then:

$$\mathcal{F}(u) = \begin{cases} 2 \int_{\Omega} QW(\nabla u(x)\lambda_{\sqrt{2}}(x)) \, dx & \text{for } u \in W^{1,2}(\Omega, \mathbb{R}^2) \\ +\infty & \text{for } u \in L^2 \setminus W^{1,2}. \end{cases}$$

The functionals  $\mathcal{F}$  obtained in Theorems 5.1, 5.2 and 5.3, measure the deficit of a deformation  $u$  from being an orientation preserving (modulo compressive maps, due to the quasiconvexification of the energy density  $W$ ) realisation of the metric  $\bar{G} = (\lambda^{-1})^T(\lambda^{-1})$ . In the next section we compare these functionals with the non-Euclidean energy  $\mathcal{E}$ .

## 6. COMPARISON OF THE VARIATIONAL LIMITS AND THE ENERGY $E$

In this section we assume that  $\Omega$  is an open bounded subset of  $\mathbb{R}^2$ . Our scope is to compare the following integral functionals:

$$\mathcal{F}_1(u) = \int_{\Omega} QW(\nabla u\lambda(x)) \, dx, \quad \mathcal{F}_{\sqrt{2}}(u) = \int_{\Omega} QW(\nabla u\lambda_{\sqrt{2}}(x)) \, dx, \quad \mathcal{E}(u) = \int_{\Omega} \bar{W}(\nabla uA(x)^{-1}) \, dx,$$

where the stored energy density  $\bar{W} : \mathbb{R}^{2 \times 2} \rightarrow \bar{\mathbb{R}}_+$  satisfies (1.2).

**Lemma 6.1.** Assume that  $\min \mathcal{E}(u) = 0$ , so that the prestrain metric  $G$  is realisable by a smooth  $u : \Omega \rightarrow \mathbb{R}^2$  with  $(\nabla u)^T \nabla u = G$ . Then:  $\mathcal{F}_1(u) = 0$ .

*Proof.* Since  $A = \sqrt{G} = \sqrt{(\nabla u)^T \nabla u}$ , it follows that  $A = R\nabla u$ , for some rotation field  $R : \Omega \rightarrow SO(2)$ . Hence,  $|A(x)e_i| = |\nabla u(x)e_i|$ , and so both columns of the matrix:

$$\nabla u(x)\lambda(x) = \begin{bmatrix} \nabla u(x)e_1 & \nabla u(x)e_2 \\ |\nabla u(x)e_1| & |\nabla u(x)e_2| \end{bmatrix}$$

have length 1. The claim follows now by Lemma 4.1.  $\blacksquare$

The following example shows that  $G$  may be realisable, as in Lemma 6.1, but the metric  $\bar{G} = \lambda^{-1,T}\lambda^{-1}$  is still not realisable. The vanishing of the infimum of the derived energy  $\mathcal{F}_1$  is hence due to the quasiconvexification effect in the energy density.

**Example 6.2.** Let  $g : \mathbb{R} \rightarrow (0, +\infty)$  be a smooth function. Consider:

$$G(x_1, x_2) = \begin{bmatrix} 1/2 & 1 \\ 1 & g(x_1) \end{bmatrix}, \quad \bar{G}(x_1, x_2) = \operatorname{diag}\{|A(x_1)e_1|^2, |A(x_1)e_2|^2\} = \begin{bmatrix} 1/2 & 0 \\ 0 & g(x_1) \end{bmatrix},$$

where the formula for  $\bar{G}$  follows from the fact that  $|A(x)e_i|^2 = \langle e_i, A(x)^2 e_i \rangle = \langle e_i, G(x)e_i \rangle$ . We now want to assign  $g$  so that the Gaussian curvatures  $\kappa$  and  $\kappa_1$  of  $G$  and  $\bar{G}$ , satisfy:

$$(6.1) \quad \kappa = 0, \quad \kappa_1 \neq 0.$$



By a direct calculation, we see that:

$$\begin{aligned}\kappa_1 &= \frac{1}{\sqrt{g}} \left( \frac{g'}{\sqrt{g}} \right)' = \frac{-2gg'' + (g')^2}{2g^2} \\ \left(\frac{g}{2} - 1\right)^2 \kappa &= -\frac{1}{2}g''\left(\frac{g}{2} - 1\right) + \frac{1}{8}(g')^2 = \frac{1}{2}g'' + \frac{g^2}{4}\kappa_1.\end{aligned}$$

Hence, (6.1) is equivalent to:

$$(6.2) \quad g > 2, \quad g'' \neq 0, \quad g'' = \frac{(g')^2}{2(g-2)}.$$

Clearly, the second order ODE above has a solution on a sufficiently small interval  $(-\epsilon, \epsilon)$ , for any assigned initial data  $g(0) = g_0 > 2$  and  $g'(0) = g_1 > 0$ . Also, this local solution satisfies all three conditions in (6.2) by continuity, if  $\epsilon > 0$  is small enough.

This completes the example. By rescaling  $\tilde{g}(x_1) = g(\epsilon x_1)$ , we may obtain the metric  $G$  on  $\Omega = (0, 1)^2$ , with the desired properties.

The next example shows that the induced metric  $\bar{G}$  can be realisable even when  $G$  is not. In this case, one trivially has:  $\inf \mathcal{E}(u) > 0$  while  $\min \mathcal{F}_1(u) = 0$ .

**Example 6.3.** Let  $w : (0, 1)^2 \rightarrow (0, \frac{\pi}{2})$  be a smooth function such that  $w_{x_1, x_2} \neq 0$ , and define:

$$G(x) = \begin{bmatrix} 1 & \cos w(x) \\ \cos w(x) & 1 \end{bmatrix}, \quad \bar{G}(x) = \text{diag}\{|A(x)e_1|^2, |A(x)e_2|^2\} = \text{Id}_2.$$

Clearly,  $\kappa_1 \neq 0$ . We now compute the Gaussian curvature of  $G$ :

$$\kappa = \frac{1}{\sin^4 w} \left( (-\cos w)w_{x_1}w_{x_2} - (\sin w)w_{x_1, x_2} \right) \sin^2 w + (\sin^2 w)w_{x_2}(\cos w)w_{x_1} = -\frac{w_{x_1, x_2}}{\sin w} \neq 0.$$

The following simple observation establishes the relation between  $\mathcal{F}_1$  and  $\mathcal{F}_{\sqrt{2}}$ .

**Lemma 6.4.** *Let  $\Omega = B(0, 1)$ . Then, we have:*

$$\forall u \in W^{1,2}(\Omega, \mathbb{R}^2) \quad \mathcal{F}_{\sqrt{2}}(u) = \bar{\mathcal{F}}_1(\sqrt{2}u \circ R),$$

where  $\bar{\mathcal{F}}_1$  is defined with respect to the metric  $G_1$  in:

$$G_1(x) = R^T G(Rx)R, \quad R = \frac{1}{\sqrt{2}}B.$$

*Proof.* Note first that  $G_1$  is the pull-back of the metric  $G$  under the rotation  $x \mapsto Rx$ . Thus:

$$\begin{aligned}\mathcal{F}_{\sqrt{2}}(u) &= \int_{\Omega} QW(\nabla u(x)\lambda_{\sqrt{2}}(x)) \, dx \\ &= \int_{\Omega} QW\left(\sqrt{2}\nabla u(Ry)\sqrt{2}R \, \text{diag}\{|A(Ry)Be_1|^{-1}, |A(Ry)Be_2|^{-1}\}\right) \, dy \\ &= \int_{\Omega} QW\left(\nabla(\sqrt{2}u \circ R)(y) \, \text{diag}\{|A(Ry)Re_1|^{-1}, |A(Ry)Re_2|^{-1}\}\right) \, dy \\ &= \int_{\Omega} QW\left(\nabla(\sqrt{2}u \circ R)(y)\bar{\lambda}(y)\right) \, dy = \bar{\mathcal{F}}_1(\sqrt{2}u \circ R),\end{aligned}$$

because  $|\sqrt{G_1(x)}e_i| = |A(Rx)Re_i|$ , which implies:  $\bar{\lambda}(x) = \text{diag}\{|A(Rx)Re_1|^{-1}, |A(Rx)Re_2|^{-1}\}$ . ■

Finally, observe also that if  $\mathcal{F}(u) = \mathcal{F}_1(u) = 0$ , then the length of columns in the matrix  $\nabla u(x)\lambda_{\sqrt{2}}(x)$  equals  $\sqrt{2}$ . Hence  $\mathcal{F}_{\sqrt{2}}(u) \neq 0$ .

## 7. APPENDIX

**7.1.  $\Gamma$ -convergence.** We now recall the definition and some basic properties of  $\Gamma$ -convergence, that will be needed in the sequel.

**Definition 7.1.** Let  $\{I_\epsilon\}, I : X \rightarrow \overline{\mathbb{R}} = \mathbb{R} \cup \{-\infty, \infty\}$  be functionals on a metric space  $X$ . We say that  $I_\epsilon$   $\Gamma$ -converge to  $I$  (as  $\epsilon \rightarrow 0$ ), iff:

- (i) For every  $\{u_\epsilon\}, u \in X$  with  $u_\epsilon \rightarrow u$ , we have:  $I(u) \leq \liminf_{\epsilon \rightarrow 0} I_\epsilon(u_\epsilon)$ .
- (ii) For every  $u \in X$ , there exists a sequence  $u_\epsilon \rightarrow u$  such that  $I(u) = \lim_{\epsilon \rightarrow 0} I_\epsilon(u_\epsilon)$ .

**Theorem 7.2.** [6, Chapter 7] Let  $I_\epsilon, I$  be as in Definition 7.1 and assume that there exists a compact set  $K \subset X$  satisfying:

$$\inf_X I_\epsilon = \inf_K I_\epsilon \quad \forall \epsilon.$$

Then:  $\lim_{\epsilon \rightarrow 0} (\inf_X I_\epsilon) = \min_X I$ , and moreover if  $\{u_\epsilon\}$  is a converging sequence such that:

$$\lim_{\epsilon \rightarrow 0} I_\epsilon(u_\epsilon) = \lim_{\epsilon \rightarrow 0} (\inf_X I_\epsilon),$$

then  $u = \lim u_\epsilon$  is a minimum of  $I$ , i.e.:  $I(u) = \min_X I$ .

**Theorem 7.3.** [6, Chapter 7] Let  $\Omega$  be an open subset of  $\mathbb{R}^n$ . Any sequence of functionals  $I_\epsilon : L^2(\Omega, \mathbb{R}^n) \rightarrow \overline{\mathbb{R}}$  has a subsequence which  $\Gamma$ -converges to some lower semicontinuous functional  $I : L^2(\Omega, \mathbb{R}^n) \rightarrow \overline{\mathbb{R}}$ . Moreover, if every subsequence of  $\{I_\epsilon\}$  has a further subsequence that  $\Gamma$ -converges to (the same limit)  $I$ , then the whole sequence  $I_\epsilon$   $\Gamma$ -converges to  $I$ .

**7.2. Convexity and quasiconvexity.** In this section  $f : \mathbb{R}^{m \times n} \rightarrow \mathbb{R}$  is a function assumed to be Borel measurable, locally bounded and bounded from below. Recall that the convex and quasiconvex envelopes of  $f$ , i.e.  $Cf, Qf : \mathbb{R}^{m \times n} \rightarrow \mathbb{R}$  are defined by:

$$\begin{aligned} Cf(M) &= \sup \{g(M); g : \mathbb{R}^{m \times n} \rightarrow \mathbb{R}, g \text{ convex}, g \leq f\}, \\ Qf(M) &= \sup \{g(M); g : \mathbb{R}^{m \times n} \rightarrow \mathbb{R}, g \text{ quasiconvex}, g \leq f\}. \end{aligned}$$

We say that  $f$  is quasiconvex, if:

$$f(M) \leq \int_D f(M + \nabla \phi(x)) \, dx \quad \forall M \in \mathbb{R}^{m \times n} \quad \forall \phi \in W_0^{1,\infty}(D, \mathbb{R}^m),$$

on every open bounded set  $D \subset \mathbb{R}^n$ .

**Theorem 7.4.** [10, Chapter 6]

- (i) When  $m = 1$  or  $n = 1$  then  $f$  is quasiconvex if and only if  $f$  is convex.
- (ii) For any open bounded  $D \subset \mathbb{R}^n$  there holds:

$$Qf(M) = \inf \left\{ \int_D f(M + \nabla \phi(x)) \, dx; \phi \in W_0^{1,\infty}(D, \mathbb{R}^m) \right\}.$$

- (iii) Assume that, for some  $n_1 + n_2 = n$  we have:

$$f(M) = f_1(M_{n_1}) + f_2(M_{n_2}) \quad \forall M \in \mathbb{R}^{m \times n},$$

where  $M_{n_1}$  stands for the principal minor of  $M$  consisting of its first  $n_1$  columns, while  $M_{n_2}$  is the minor of  $M$  consisting of its  $n_2$  last columns. Assume that  $f_1, f_2$  are Borel measurable and bounded from below. Then:

$$Cf = Cf_1 + Cf_2, \quad Qf = Qf_1 + Qf_2$$

The following classical results explain the role of convexity and quasiconvexity in the integrands of the typical integral functionals.

**Theorem 7.5.** [10] *Let  $\Omega$  be a bounded open set in  $\mathbb{R}^n$  and let  $f : \mathbb{R}^{m \times 1} \rightarrow \mathbb{R}$  be lower semicontinuous (lsc). Then the functional:*

$$I(u) = \int_{\Omega} f(u(x)) \, dx \quad \forall u \in L^2(\Omega, \mathbb{R}^m)$$

*is sequentially lsc with respect to the weak convergence in  $L^2(\Omega, \mathbb{R}^m)$  if and only if  $f$  is convex.*

**Theorem 7.6.** [10, Chapter 9] *Let  $\Omega$  be a bounded open set in  $\mathbb{R}^n$  and let  $f : \Omega \times \mathbb{R}^{m \times n} \rightarrow \mathbb{R}$  be Caratheodory, and satisfying the uniform growth condition:*

$$(7.1) \quad \exists C_1, C_2 > 0 \quad \forall x \in \Omega \quad \forall M \in \mathbb{R}^{m \times n} \quad C_1|M|^2 - C_2 \leq f(x, M) \leq C_2(1 + |M|^2).$$

*Assume that the quasiconvexification  $Qf$  of  $f$  with respect to the variable  $M$ , is also a Caratheodory function. Then for every  $u \in W^{1,2}(\Omega, \mathbb{R}^m)$  there exists a sequence  $\{u_\epsilon\} \in u + W_0^{1,2}(\Omega, \mathbb{R}^m)$  such that, as  $\epsilon \rightarrow 0$ :*

$$u_\epsilon \rightharpoonup u \quad \text{weakly in } W^{1,2} \quad \text{and} \quad \int_{\Omega} f(x, \nabla u_\epsilon(x)) \, dx \rightarrow \int_{\Omega} Qf(x, \nabla u(x)) \, dx.$$

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