

# A DERIVATION OF LINEAR ELASTIC ENERGIES FROM PAIR-INTERACTION ATOMISTIC SYSTEMS

ANDREA BRAIDES

Dipartimento di Matematica, Università di Roma 'Tor Vergata'  
via della Ricerca Scientifica, 1 - 00133 Rome, Italy

MARGHERITA SOLCI

DAP, Università di Sassari  
piazza Duomo, 6 - 07041 Alghero, Italy

ENRICO VITALI

Dipartimento di Matematica 'F. Casorati', Università di Pavia  
via Ferrata, 1 - 27100 Pavia, Italy

ABSTRACT. Pair-interaction atomistic energies may give rise, in the framework of the passage from discrete systems to continuous variational problems, to nonlinear energies with genuinely quasiconvex integrands. This phenomenon takes place even for simple harmonic interactions as shown by an example by Friesecke and Theil [19]. On the other hand, a rigorous derivation of linearly elastic energies from energies with quasiconvex integrands can be obtained by  $\Gamma$ -convergence following the method by Dal Maso, Negri and Percivale [14]. We show that the derivation of linear theories by  $\Gamma$ -convergence can be obtained directly from lattice interactions in the regime of small deformations. Our proof relies on a lower bound by comparison with the continuous result, and on a direct Taylor expansion for the upper bound. The computation is carried over for a family of lattice energies comprising interactions on the triangular lattice in dimension two.

**1. Introduction.** In recent years variational tools for the mathematical analysis of energies defined on discrete lattices have been developed, whose main goal is the description of macroscopical properties of systems whose microscopical behaviour is governed, from an 'atomistic' standpoint, by interactions between points of the lattice. This type of problems have been addressed both following the methods of  $\Gamma$ -convergence with in mind the convergence of discrete minimum problems to their continuous counterparts (for a partial review see the recent review paper [6]; see also [9, 5]) and from a more 'pointwise' perspective that, even though not guaranteeing the convergence of minimizers, allows for some more flexibility in the energies treated and is an important step in the actual computation of the  $\Gamma$ -limits and in the applications to problems in Mathematical Physics (see the review paper by Le Bris and Lions [20]) and Computational Material Science (see Blanc, Le Bris and Lions [3]).

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The simplest type of lattice interactions treated by these methods are ‘central’ or pair interactions; that is, those in which the energy between two points of the lattice depends on the difference of the values of some parameter  $u = \{u_i\}$  indexed by the lattice sites (to whom we can associate the meaning of atomic position, spin, displacement, etc.) at the two points  $i$  and  $j$ ; *i.e.*, it has the form

$$E(u) = \sum_{i,j} f_{i,j}(u_i - u_j), \quad (1)$$

where the sum runs over all points in a portion of some lattice contained in some space region. In order to understand the overall properties of such an energy some change of variables must be performed, scaling the original lattice by a small factor  $\varepsilon$ , and correspondingly also scaling the energy (the latter is in general a delicate issue and the precise scaling depends on the growth of the energy densities  $f_{i,j}$  and their decay properties as  $|i - j| \rightarrow +\infty$ ). In this way, after identifying each such scaled functions with piecewise-constant interpolations on finer and finer meshes, the resulting energies (now depending on  $\varepsilon$ ) are identified with a family of functions defined on a common Lebesgue space, and can therefore undergo a  $\Gamma$ -convergence process. Since the terms  $u_i - u_j$  can be interpreted as difference quotients that, after scaling, approximate some gradient  $Du$  as  $\varepsilon \rightarrow 0$ , the limit is actually defined on some Sobolev space. Under the suitable growth and decay assumptions hinted at above, a general compactness result by Alicandro and Cicalese [1] ensures that the limit of such energies is indeed an integral functional of the usual form

$$F(u) = \int_{\Omega} W(x, Du) dx \quad (2)$$

defined on some Sobolev space. However the computation of  $W$  is in general a complex task involving, besides macroscopic homogenization and relaxation due to mesoscopic oscillations, also oscillations at the length scale of the lattice. Such microscopic oscillations can be interpreted as a weak form, or even a failure, of the Cauchy-Born rule as stated by Ericksen [16], which holds when to a macroscopic deformation there corresponds a regular microscopic deformation (see, *e.g.*, Friesecke and Theil [19], and also recent work by Braides and Cicalese [7], and E and Ming [15]). An important subclass of such pair-interaction energies (1) are translation-invariant ones; that is, such that  $f_{i,j} = f_{i-j}$ , and those depending only on nearest neighbours; *i.e.*, such that  $f_{i,j} = 0$  except when  $|i - j|$  is equal to the minimal lattice spacing. Even in such a simplified situation following examples in [1] the resulting integrand  $W = W(Du)$  may be a complex genuinely quasiconvex function.

The simple example that will be the starting point of the analysis in this paper is that of a triangular lattice in  $\mathbb{R}^2$  where the nodes of the lattice can be interpreted as material points linked by harmonic springs; *i.e.*, our parameters  $u_i$  can be interpreted as the position of the points occupying the node  $i$  in the reference lattice, and the overall energy (before scaling) depending on  $u = \{u_i\}$  is simply

$$E(u) = \sum_{i,j} (|u_i - u_j| - 1)^2, \quad (3)$$

where the sum is now taken over all nearest-neighbours in a triangular lattice (see Fig. 1). An additional natural constraint, in the spirit of the work of Friesecke and Theil [19] is to assume that the admissible discrete functions  $u$  are ‘microscopically orientation-preserving’, which in this case can be simply expressed by requiring that the corresponding piecewise-affine interpolations have gradients with positive

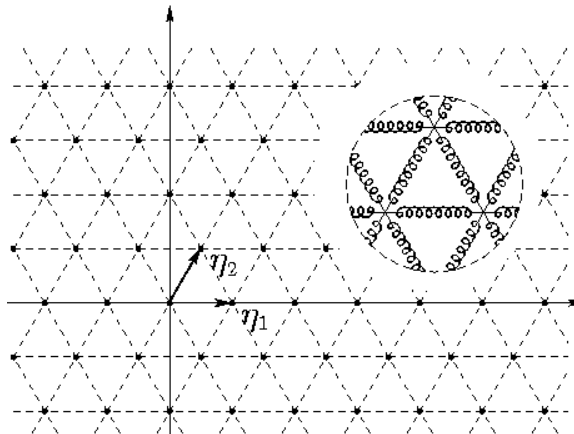


FIGURE 1. A mass-springs system in a two-dimensional triangular lattice

determinant. After normalizing the reference lattice so that  $|i - j| = 1$  on nearest neighbours, in this case an absolute minimizer of this energy is (the discretization of) the identity, and then such are all (discretization of) affine functions with gradients in  $SO(2)$ ; those are all absolute minimizers up to translations. As a result, the set of minimizers of the corresponding continuous energy density  $W$  is precisely  $SO(2)$ , and therefore  $W$  is a (non convex) quasiconvex function as in the nonlinear hyperelastic theories of finite elasticity (see [21, 2]). Note that the positive-determinant constraint cannot be included in the energies of the general compactness result by Alicandro and Cicalese [1]; however this example can be treated by the same methods as in [19]. There, an energy in a two-dimensional square mesh with interactions between nearest and diagonal neighbours is taken into account, with the same quadratic energy densities (3) as above and a determinant constraint. For this energy an accurate analysis is performed of the elastic energy per unit volume as the system size gets large as a function of a macroscopic affine deformation prescribed on the boundary, whose asymptotic behaviour gives  $W$ . As remarked by Friesecke and Theil, the form of the limit is due to the geometrically non-linear nature of the energy  $E$ , despite the fact that the integrands are quadratic functions. Note that in dimension two the choice of the triangular lattice is particularly natural since it can be shown to be the (local) equilibrium state for some classes of interatomic potentials (for a recent discussion on the subject we refer to the paper by Theil [22]).

In the variational framework outlined above, in this paper we describe how the same simple atomistic model as above giving a nonlinear hyperelastic limit energy can lead under a different scaling to the standard linearized (two-dimensional) theory of elasticity. Within the theory of Continuum Mechanics, a classical mathematical derivation of the linearized model can be obtained by computing the Fréchet derivative (in suitable Sobolev spaces) of the non-linear operator which enters the standard differential displacement-traction problem (see, *e.g.*, Ciarlet [12]). A different path, more adapted to a variational setting, has been recently followed by Dal Maso, Negri and Percivale [14] looking at the minimum problems for the energies rather than at the differential equation: let  $W$  be the stored energy density

(as a function of the deformation gradient) of a homogeneous, isotropic, hyper-elastic material; if we assume that the reference configuration is a natural state (*i.e.*, stress-free), then a perturbation  $\delta u$  (with fixed  $u$ ) of the identity deformation yields a function  $\delta \mapsto W(I + \delta \nabla u)$  whose asymptotic expansion as  $\delta \rightarrow 0$  has a quadratic principal part. Clearly the functionals  $W$  and  $W/\delta^2$  are equivalent, as far as minimum problems of the total energy are concerned. A rigorous analysis by  $\Gamma$ -convergence of the rescaled energies  $\delta^{-2} \int W(I + \delta \nabla u) dx$  as  $\delta \rightarrow 0$  is performed in [14], ensuring the convergence for the related minimum through compactness properties. We stress that the result is highly non-trivial, requiring in particular, for a given deformation, a fine estimate of the global deviation from being a rotation, in terms of the local deviation (see the geometric rigidity result of Friesecke, James and Müller [17, 18]). In the limit the classical linearized theory is recovered.

Formally linking the two approaches above we may therefore argue that we may obtain some energies of linearized elasticity directly starting from energies of the form (before scaling)

$$E_\delta(v) = E(I + \delta v) = \sum_{i,j} (|(i - j) + \delta(v_i - v_j)| - 1)^2. \quad (4)$$

Note however that in principle such a derivation is only formal since the result in [19] is not a complete  $\Gamma$ -limit, so that we have to combine the asymptotic expansion of the energy around the equilibrium position with the large-scale analysis of discrete two-dimensional lattice energies. In this way we directly derive a linear elastic energy from the discrete model, combining the classical approach of Cauchy with the modern notation of  $\Gamma$ -convergence. We explicitly consider nearest-neighbour interactions on the triangular lattice. Our analysis is also carried over to more general lattices and higher dimensions. It however relies on the validity of the Cauchy-Born rule for minimizers, which is not always the case even for simple square lattices with next-to-nearest interactions, as shown in [19]. In the same way our hypotheses rule out the possibility of microscopic oscillations due to a homogenization process as described by Braides and Francfort [8], or to a random choice of the elastic constants of the harmonic springs in the spirit of the work by Braides and Piatnitski [11], or to stochastic lattices as those considered by Blanc, Le Bris and Lions [4], which may be interesting and non trivial extensions of our result. Moreover, as a technical issue, it must be mentioned that our method also relies on the possibility of regrouping the interactions so that to each such group there corresponds a  $n$ -simplex in  $\mathbb{R}^n$  (which trivially holds for the triangular lattice, upon ‘splitting’ each interaction in two). This limitation of our method prevents us to treat all general lattices in  $\mathbb{R}^n$ , and we hope it will be overcome in future work. Finally, we mention that our results, in analogy with the one-dimensional renormalization-group analysis by Braides, Lew and Ortiz [10], suggests that some of the scalings that we consider but with Lennard-Jones potentials in place of the harmonic interactions should give in the limit some Griffith-type fracture energy, with the bulk part obtained as in the harmonic case, while the determination of the fracture energy density seems an interesting and difficult problem.

**2. Discrete elastic energies. Perturbation of an equilibrium position.** In this section we first introduce a two-dimensional model that can be easily pictured

as in Fig. 1, and then extend the notation of this example to a more general  $n$ -dimensional framework.

*A two-dimensional model.*

Let  $\eta_1 = (1, 0)$  and  $\eta_2 = (\cos(\pi/3), \sin(\pi/3))$ , and  $L = \mathbb{Z}[\eta_1, \eta_2]$  be the lattice on  $\mathbb{Z}^2$  generated by  $\eta_1, \eta_2$ . For any  $\varepsilon > 0$  we set  $L_\varepsilon = \varepsilon L$ . Fix a smooth bounded open subset  $\Omega$  of  $\mathbb{R}^2$ ; we interpret  $\Omega_\varepsilon := \Omega \cap L_\varepsilon$  as a sample of a two-dimensional triangular lattice of particles interacting via interatomic potentials; these are assumed to bind pairs of particles in positions  $x$  and  $x + \varepsilon\xi$ , with  $x \in L_\varepsilon$  and  $\xi$  varying in the set  $P = \{e^{ik\pi/3} : k = 0, \dots, 5\}$ , where we identify  $\mathbb{R}^2$  and  $\mathbb{C}$ .

We consider the simple case where the particles have equal mass and are linked by harmonic springs (see Fig. 1). If  $\varepsilon a$  and  $K$  are the equilibrium length and elastic constant, respectively, of the spring between  $x$  and  $x + \varepsilon\xi$ , the energy corresponding to a deformation  $\varphi$  is  $K(|\varphi(x + \varepsilon\xi) - \varphi(x)| - \varepsilon a)^2/2$ ; in terms of the displacement  $u = \varphi - id$ , this can be expressed as:

$$\frac{1}{2}K\varepsilon^2 \left( \left| \xi + \frac{u(x + \varepsilon\xi) - u(x)}{\varepsilon} \right| - a \right)^2.$$

In order to express the total energy it is convenient to introduce the following notation: for  $\varepsilon > 0$  if  $B$  is a bounded subset of  $\mathbb{R}^2$  then we define the corresponding set of lattice points

$$B(\varepsilon) = \{x \in L_\varepsilon : \text{there exists } y \in B \cap L_\varepsilon \text{ such that } x \in y + \varepsilon P\}.$$

Note that we have  $x + \varepsilon\xi \in B(\varepsilon)$  for all  $x \in B \cap L_\varepsilon$  and  $\xi \in P$ . Given a function  $u : B(\varepsilon) \rightarrow \mathbb{R}^2$  and  $x \in B \cap L_\varepsilon$  we set:

$$D_\varepsilon^\xi u(x) = \frac{u(x + \varepsilon\xi) - u(x)}{\varepsilon} \quad (5)$$

and

$$D_\varepsilon u(x) = \{D_\varepsilon^\xi u(x) : \xi \in P\}. \quad (6)$$

Thus, if we assume the elastic constants and the equilibrium lengths independent of  $x$  (as it is rather natural in such a periodic setting) we have the following discrete energy (where  $n = 2$ ):

$$E_\varepsilon(u, B) = \sum_{x \in L_\varepsilon \cap B} \varepsilon^n \phi(D_\varepsilon u(x)), \quad (7)$$

with ( $K_\xi$  and  $a_\xi$  are fixed positive constants)

$$\phi(D_\varepsilon u(x)) = \sum_{\xi \in P} \frac{1}{4} K_\xi \left( \left| \xi + D_\varepsilon^\xi u(x) \right| - a_\xi \right)^2, \quad (8)$$

Note the additional factor  $1/2$ , due to the fact that the same contribution is shared both by  $x$  and  $x + \varepsilon\xi$ .

The factor  $\varepsilon^n$  will also appear in the  $n$ -dimensional version of the energy, since a suitable scaling is needed to get a non-trivial  $\Gamma$ -limit.

**Remark 1.** With in mind to perform an asymptotic analysis around an equilibrium position, we point out that the assumption  $K_\xi = 1$  and  $a_\xi = 1$  for every  $\xi$  implies that the reference configuration (*i.e.*, the null displacement) is stress-free, in the sense that the energy density  $\phi$  is stationary with respect to any affine perturbation. This can be easily checked directly (see, however, (10)). Note that, in this case,  $E_\varepsilon(0, B) = 0$  for any  $B$ .

An  $n$ -dimensional model.

The argument we will follow in the proof of the asymptotic analysis referred to in the previous remark relies on a piecewise-affine extension of the discrete displacements  $u$  on each triangle, in such a way to recast the problem in an integral form. A straightforward  $n$ -dimensional generalization for which the same argument could work may be obtained by a suitable triangulation in  $n$ -simplices. Clearly, natural models such as the body-centered cubic or the hexagonal closed-packed crystal structure do not fall in this framework, and would require a different strategy.

Let  $\mathcal{T}$  be any given triangulation of  $\mathbb{R}^n$  by  $n$ -simplices. Let  $L$  be the set of nodes of  $\mathcal{T}$ , and

$$\mathcal{T}_\varepsilon := \varepsilon\mathcal{T} = \{\varepsilon T : T \in \mathcal{T}\}, \quad L_\varepsilon := \varepsilon L.$$

We say that two nodes  $x, y \in L_\varepsilon$  are *contiguous* if there exists an element  $T \in \mathcal{T}_\varepsilon$  which has both  $x$  and  $y$  as vertices. Clearly the set

$$P(x) := \{\xi \in \mathbb{R}^n : x \text{ and } x + \varepsilon\xi \text{ are contiguous}\}$$

is independent of  $\varepsilon$ .

On the line of the two-dimensional case, we would like to assume a harmonic spring between each pair of contiguous nodes; in order to have some control on the different kind of possible interactions, we restrict to the case of a *structured triangulation*  $\mathcal{T}$ , assuming that

$$P(x) \text{ is independent of } x. \tag{A}$$

Let us denote such a set by  $P$ . Clearly, the two-dimensional model above satisfies this condition. In a three-dimensional setting we can consider, for instance, the so-called Kuhn triangulation, whose set of nodes is simply  $\varepsilon\mathbb{Z}^3$ , and each cube is suitably decomposed in six tetrahedral elements (see Fig. 2). Here  $P = \pm(P_1 \cup P_2 \cup P_3)$ , where

$$\begin{aligned} P_1 &= \{e_i : i = 1, 2, 3\}, & P_2 &= \{e_i + e_j : 1 \leq i < j \leq 3\}, \\ P_3 &= \{e_1 + e_2 + e_3\}. \end{aligned} \tag{9}$$

Condition (A) leads to consider, for a given displacement  $u: B(\varepsilon) \rightarrow \mathbb{R}^n$  for a set  $B \subseteq \mathbb{R}^n$ , the same energy introduced in (7) and (8), where  $D_\varepsilon^\xi u(x)$  and  $D_\varepsilon u(x)$  are defined as in (5) and (6).

**Remark 2.** In order to pass to a continuum model, it is convenient to identify functions on  $L_\varepsilon$  with their extensions by affine interpolation on the elements of  $\mathcal{T}_\varepsilon$ . As noted above, this is made possible by the simplicial form of the finite elements considered.

From the mechanical point of view it is natural to confine the attention to a class  $\mathcal{A}_\varepsilon$  of displacements satisfying an *orientation-preserving condition*. We say that a displacement  $u: B(\varepsilon) \rightarrow \mathbb{R}^n$  is *admissible*, or that  $u \in \mathcal{A}_\varepsilon$ , if for any element  $T$  in  $\mathcal{T}_\varepsilon$  (whose vertices are in  $B(\varepsilon)$ ) the determinant of the gradient (of the affine extension) of  $u$  is positive on  $T$ .

In the sequel we will deal with prescribed boundary values, where for an open set  $B$  the discrete boundary is given by

$$\partial B(\varepsilon) = \{x \in B(\varepsilon) : x + \varepsilon P \not\subseteq B\}.$$

Let  $\Omega \subseteq \mathbb{R}^n$  and  $M \in M^{n \times n}$  ( $n \times n$  real matrix) be given; we denote by  $\mathcal{A}_\varepsilon^M$  the set of the functions in  $\mathcal{A}_\varepsilon$  which take the value  $Mx$  on the boundary of  $\Omega$ , in the

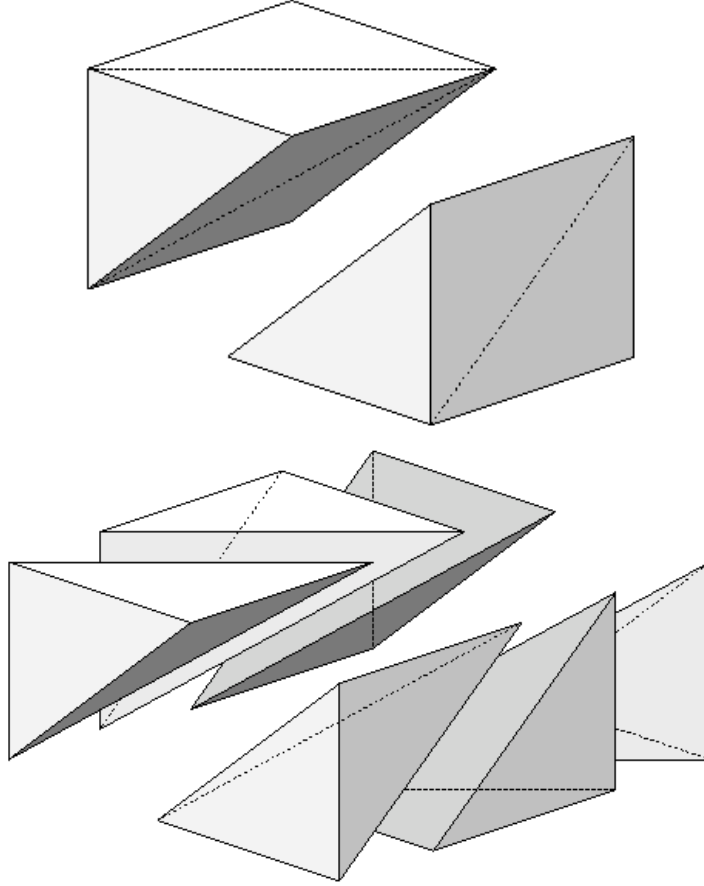


FIGURE 2. Kuhn decomposition of a cube in tetrahedral elements

sense that:

$$u(y) = My \quad \text{if } y \in \partial\Omega(\varepsilon);$$

moreover, we set  $\mathring{\Omega}_\varepsilon = \{x \in \Omega_\varepsilon : x + \varepsilon P \subseteq \Omega_\varepsilon\}$ .

*Perturbation of an equilibrium position.*

Following the line sketched in the Introduction, we now consider perturbations of an equilibrium position, say the reference configuration (*i.e.*, the null displacement). More precisely, we require that for every  $A \in M^{n \times n}$  with positive determinant the function  $\delta \mapsto \phi(\delta A)$  is stationary in  $\delta = 0$ , where, with a slight abuse of notation with respect to (8),  $\phi$  is defined, for every  $M \in M^{n \times n}$ , by:

$$\phi(M) = \sum_{\xi \in P} \frac{1}{4} K_\xi \left( |\xi + M\xi| - a_\xi \right)^2.$$

This condition can be equivalently stated as the stationarity of

$$\delta \mapsto E_\varepsilon(\delta u_A, B) = \sum_{x \in B \cap L_\varepsilon} \phi_\varepsilon(\delta A)$$

in  $\delta = 0$  for any  $B$ , where  $u_A$  denotes the affine map  $x \mapsto Ax$ .

The equilibrium condition amounts to:

$$\sum_{\xi \in P} K_\xi \left(1 - \frac{a_\xi}{|\xi|}\right) \xi^T A \xi = 0, \quad \text{for every } A \in M^{n \times n} \text{ with } \det A > 0. \quad (10)$$

In the two-dimensional model, as mentioned in Remark 1, under the assumption of the independence of  $K_\xi$  and  $a_\xi$  on  $\xi$ , condition (10) amounts to requiring that the equilibrium length has value 1. In particular, the equilibrium condition is trivially satisfied if  $a_\xi = |\xi|$  for every  $\xi \in P$ . In such a case  $\phi(0) = 0$ .

Let us now consider the three-dimensional model referred to in (9); it is a rather natural assumption that the bonds in  $P_1$  (as well as those in  $P_2$ ) share the same elastic constants, say  $K_1$  and  $a_1$  ( $K_2$  and  $a_2$  respectively); likewise, we denote the elastic constants for  $e_1 + e_2 + e_3$  ( $P_3$ ) by  $K_3$  and  $a_3$ .

Then the equilibrium condition (10) for the reference configuration adds up to requiring that for every  $n \times n$  matrix  $A = (a_{ij})$  with  $\det A > 0$ :

$$\begin{aligned} K_1(1 - a_1) \sum_{\xi \in P_1} \xi^T A \xi + K_2(1 - a_2/\sqrt{2}) \sum_{\xi \in P_2} \xi^T A \xi \\ + K_3(1 - a_3/\sqrt{3}) \xi_3^T A \xi_3 = 0, \end{aligned}$$

where  $\xi_3 = e_1 + e_2 + e_3$ . The explicit computation gives:

$$\begin{aligned} [K_1(1 - a_1) + 2K_2(1 - a_2/\sqrt{2}) + K_3(1 - a_3/\sqrt{3})] \operatorname{tr} A \\ + [K_2(1 - a_2/\sqrt{2}) + K_3(1 - a_3/\sqrt{3})] \sum_{i \neq j} a_{ij} = 0. \end{aligned}$$

By the arbitrariness of  $A$  we conclude that:

$$\begin{cases} K_1(1 - a_1) + 2K_2(1 - a_2/\sqrt{2}) + K_3(1 - a_3/\sqrt{3}) = 0 \\ K_2(1 - a_2/\sqrt{2}) + K_3(1 - a_3/\sqrt{3}) = 0. \end{cases}$$

An obvious solution is  $a_1 = 1$ ,  $a_2 = \sqrt{2}$ ,  $a_3 = \sqrt{3}$ .

Let us now examine the second-order term in the expansion of  $\delta \mapsto \phi(\delta A)$  with respect to  $\delta \rightarrow 0^+$ . An elementary computation shows that:

$$\frac{d^2}{d\delta^2} \phi(\delta A) \Big|_{\delta=0} = \frac{1}{2} \sum_{\xi \in P} K_\xi \left[ \left(1 - \frac{a_\xi}{|\xi|}\right) |A\xi|^2 + \frac{a_\xi}{|\xi|^3} (\xi^T A \xi)^2 \right];$$

applying the equilibrium condition (10) with respect to  $A^T A$ , the part corresponding to the first term in the square brackets vanishes, and we get:

$$\frac{d^2}{d\delta^2} \phi(\delta A) \Big|_{\delta=0} = \frac{1}{2} \sum_{\xi \in P} K_\xi \frac{a_\xi}{|\xi|^3} (\xi^T A \xi)^2.$$

We conclude that:

$$\phi(\delta A) = \phi(0) + \frac{1}{2} \gamma(A) \delta^2 + \sigma_A(\delta), \quad (11)$$

where  $\sigma_A(\delta) = O(\delta^3)$  and

$$\gamma(A) = \frac{1}{2} \sum_{\xi \in P} K_\xi \frac{a_\xi}{|\xi|^3} (\xi^T A \xi)^2. \quad (12)$$

It is immediately seen that  $\delta \mapsto \delta^{-3} \sigma_A(\delta)$  is bounded in a neighbourhood of 0, uniformly with respect to  $A$ , when  $A$  varies in a bounded subset of  $M^{n \times n}$ .



**Remark 3.** For every  $\xi \in P$  let  $\varphi^\xi(A)$  be the single interaction corresponding to the direction  $\xi$  for an affine *deformation* with gradient  $F$ , *i.e.*

$$\varphi^\xi(F) = \frac{1}{2} K_\xi (|F\xi| - a_\xi)^2.$$

We point out that under the particular stationarity assumption that  $a_\xi = |\xi|$  for every  $\xi \in P$ , we have the following expansion:

$$\varphi^\xi(I + \delta A) = \frac{1}{2} \frac{K_\xi}{|\xi|^2} (\xi^T A \xi)^2 \delta^2 + \sigma_A(\delta),$$

The Taylor expansion of  $\phi$  allows the following expression for the energy  $E_\varepsilon$ :

$$\frac{1}{\delta^2} \left( E_\varepsilon(\delta u_A, B) - E_\varepsilon(0, B) \right) = \frac{1}{2} C |B| \gamma(A) + o_\delta(1), \quad (13)$$

where

$$C = \lim_{\varepsilon \rightarrow 0^+} \frac{\varepsilon^n \#(B \cap L_\varepsilon)}{|B|}$$

is independent of  $B$  and can be explicitly computed from the geometry of  $\mathcal{T}$  (see the next section). Clearly this estimate holds also after additions of constants to  $u_A$ . In the next section we will see that a corresponding asymptotic analysis holds in terms of  $\Gamma$ -convergence.

**Remark 4.** Here we make some comments on the limit density  $\gamma$ . First, we note that, since  $\xi^T A \xi = \xi^T \frac{A + A^T}{2} \xi$ , the function  $\gamma(A)$  turns out to be a quadratic form in the symmetric part  $(A + A^T)/2$  of  $A$ . Clearly, we can rewrite  $\gamma(A)$  as:

$$\gamma(A) = \sum_{i,j,h,k=1}^n m_{ijhk} a_{ij} a_{hk},$$

where  $\mathbb{M} = (m_{ijhk})$  is the fourth-order symmetric tensor defined by:

$$\mathbb{M} = \sum_{\xi \in P} \frac{K_\xi a_\xi}{2|\xi|^3} \xi \otimes \xi \otimes \xi \otimes \xi.$$

This defines a linear symmetric operator on the space  $M_{sym}^{n \times n}$  of  $n \times n$  symmetric matrices by setting:

$$(\mathbb{M}A)_{ij} = \sum_{h,k=1}^n m_{ijhk} a_{hk}.$$

In the three-dimensional setting of the Kuhn decomposition a direct computation yields the existence of two simple eigenvalues  $\lambda_1, \lambda_2$  satisfying the equation:

$$\lambda^2 - [K_1 + 3(K_2 + K_3)]\lambda + K_1 K_2 + 2K_1 K_3 + K_2 K_3 = 0,$$

and two double eigenvalues  $\lambda_3, \lambda_4$  which solve the equation:

$$2\lambda^2 - (2K_1 + 3K_2)\lambda + 2K_1 K_2 = 0.$$

In case  $K_1 = K_2 = K_3 =: K$  we get the values:

$$\lambda_{1,2} = K(7 \pm \sqrt{33})/2, \quad \lambda_3 = K/2, \quad \lambda_4 = 2K.$$

For the two-dimensional model introduced in the previous section the result appears more meaningful; by a direct computation we obtain that for a symmetric matrix  $A$ :

$$\gamma(A) = \mu|A^D|^2 + \frac{\kappa}{2}\left|\frac{1}{2}(\text{tr } A)I\right|^2, \quad \text{with } \mu = 3/4 \text{ and } \kappa = 3,$$

where  $A^D = A - \frac{1}{2}(\text{tr } A)I$  denotes the deviatoric part of  $A$ . This energy corresponds to a material with a Poisson ratio  $\nu = 5/13 \sim 0.38$ .

#### Further models.

The mechanical setting we deal with in the two-dimensional case appears as the simplest case for the asymptotic analysis near an equilibrium position as the mesh size tends to zero. Other relevant choices for the interatomic potentials and the lattice can be made. If  $L = \mathbb{Z}[\eta_1, \eta_2]$  denotes the lattice generated on  $\mathbb{Z}$  by two linearly independent unit vectors  $\eta_1, \eta_2$ , and, as above,  $L_\varepsilon = \varepsilon L$ , we can assume that the atomic bonds relate particles in positions  $x \in L_\varepsilon$  and  $x + \varepsilon\xi \in L_\varepsilon$  whenever  $\xi$  varies in a fixed finite subset  $P \subseteq L$ , with  $-P = P$ . For instance, in this framework we find the case of a square lattice generated by  $e_1$  and  $e_2$ , with interactions between nearest and next-to-nearest (*i.e.*, diagonally connected) neighbours: here  $P = \pm\{e_1, e_2, e_1 \pm e_2\}$ .

In this setting it is meaningful to consider different elasticity parameters  $K_1, a_1$  and  $K_2, a_2$  for nearest and next-to-nearest (diagonal) interactions respectively. The energy functional is the same as in (7), with

$$\begin{aligned} \phi(D_\varepsilon u(x)) &= \frac{1}{4} \sum_{\xi \in \pm\{e_1, e_2\}} K_1(|\xi + D_\varepsilon^\xi u(x)| - a_1)^2 \\ &\quad + \frac{1}{4} \sum_{\xi \in \pm\{e_1 \pm e_2\}} K_2(|\xi + D_\varepsilon^\xi u(x)| - a_2)^2. \end{aligned}$$

The equilibrium condition amounts to  $K_1(1 - a_1)\text{tr } A + 2K_2(1 - a_2/\sqrt{2})\text{tr } A = 0$  for every  $A$ ; *i.e.*,  $K_1 a_1 + \sqrt{2}K_2 a_2 = K_1 + 2K_2$ . This is nothing but the condition that, in the class of cubic deformations  $\varphi(x) = rx$  ( $r \geq 0$ ), the value  $r = 1$  is the minimum of the unscaled cell energy:

$$2[K_1(r - a_1)^2 + K_2(\sqrt{2}r - a_2)^2].$$

Moreover, the expansion in (13) holds with

$$\gamma(A) = \frac{1}{2}K_1 a_1 \sum_{\xi \in \pm\{e_1, e_2\}} (\xi^T A \xi)^2 + \frac{1}{2}K_2 a_2 \sum_{\xi \in \pm\{e_1 \pm e_2\}} (\xi^T A \xi)^2.$$

A direct computation yields, for every symmetric matrix  $A = (a_{ij})$ :

$$\gamma(A) = K_1 a_1 (a_{11}^2 + a_{22}^2) + K_2 a_2 [(\text{tr } A)^2 + 4a_{12}^2].$$

Additional analyses can be found in the paper by Friesecke and Theil [19].

We may generalize the computations above to more complex lattices. In the three-dimensional case we may for instance examine interactions in the body-centered cubic lattice, that may be parameterized as  $\mathbb{Z}^3 \cup (\mathbb{Z}^3 + (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}))$ , given by

$$P = \pm\left\{e_1, e_2, e_3, \frac{1}{2}(e_1 + e_2 + e_3), \frac{1}{2}(e_1 - e_2 + e_3), \frac{1}{2}(e_1 + e_2 - e_3), \frac{1}{2}(e_1 - e_2 - e_3)\right\}.$$

Under the assumptions that the interactions in the directions  $\pm e_i$  share the same constants  $K_1, a_1$  and those in the remaining directions the constants  $K_2, a_2$  we have

$$\gamma(A) = K_1 a_1 \sum_{i=1}^3 a_{ii}^2 + \frac{2}{3\sqrt{3}} K_2 a_2 [(\operatorname{tr} A)^2 + 4 \sum_{i < j} a_{i,j}^2],$$

with the equilibrium condition (10).

**3. Asymptotic analysis in terms of  $\Gamma$ -convergence.** For the sake of simplicity we restrict to the case where the triangulation  $\mathcal{T}_\varepsilon$  satisfies, in addition to condition (A) above, the following assumption:

$$\mathcal{T}_\varepsilon \text{ consists of simplices of the same volume.} \tag{B}$$

Clearly, the models considered in the previous sections when  $n = 2$  or  $n = 3$  (see Figures 1 and 2) fall within this setting. If we denote the volume of a single element in  $\mathcal{T}_1 = \mathcal{T}$  by  $\tau$ , then

$$\tau = \sqrt{3}/4 \quad (n = 2); \quad \tau = 1/6 \quad (n = 3).$$

In view of the structure of the triangulation we can select a finite number of elements in  $\mathcal{T}_1$ , say  $T_1, T_2, \dots, T_l$ , in such a way that each other simplex in  $\mathcal{T}_1$  coincides, up to a translation, with one of them. For instance, in the case of Fig. 2 we can choose the six tetrahedra which decompose the unit cube. If a simplex  $T \in \mathcal{T}_\varepsilon$  coincides, up to a translation, with  $\varepsilon T_i$  for some  $i$ , we will write  $T \sim T_i$ . The assumption on  $\mathcal{T}_1$  implies that there exist  $n$  independent directions along which  $\chi^i$  is periodic; let  $Y$  be the minimal periodicity cell. Then the constant  $C$  in (13) is given by  $C = 1/|Y|$ .

In the sequel we will require that  $a_\xi = |\xi|$  for every  $\xi \in P$ : this is a strong form of stationarity of the null displacement and implies (10). Moreover, it turns out that  $\phi(0) = 0$ .

Let  $\Omega$  be a fixed bounded open subset of  $\mathbb{R}^n$  with Lipschitz boundary. For any  $\varepsilon, \delta > 0$ ,  $u \in \mathcal{A}_\varepsilon^M$ , and  $B \subseteq \Omega$ , accordingly to (13) we define

$$G_{\varepsilon, \delta}(u, B) = \frac{1}{\delta^2} E_\varepsilon(\delta u, B). \tag{14}$$

Let us now state the two main results, which will be proved below.

**Theorem 3.1** (compactness). *Let  $(\varepsilon_j)$  and  $(\delta_j)$  be positive infinitesimal sequences, and for every  $j \in \mathbb{N}$  let  $u_j$  be a function in  $\mathcal{A}_{\varepsilon_j}^M$ . Let the triangulations  $\mathcal{T}_{\varepsilon_j}$  satisfy conditions (A) and (B). Assume that  $a_\xi = |\xi|$  for every  $\xi \in P$ .*

*If  $(G_{\varepsilon_j, \delta_j}(u_j, \Omega))$  is bounded, then  $(u_j)$ , extended to piecewise-affine functions as in Remark 2, is bounded in  $H^1(\Omega; \mathbb{R}^n)$ .*

It is now convenient to extend the definition of  $G_{\varepsilon, \delta}$  with the value  $+\infty$  on  $H^1(\Omega; \mathbb{R}^n) \setminus \mathcal{A}_\varepsilon^M$ . In the framework of  $\Gamma$ -convergence (see for instance [5, 6] and [13] for the general theory), the previous theorem implies that the functions in the domain of the  $\Gamma$ -limit of any sequence  $(G_{\varepsilon_j, \delta_j})$ , with respect to the  $L^1$ -convergence or equivalently the weak  $H^1$ -convergence, belong to  $H^1(\Omega; \mathbb{R}^n)$ . Moreover they also have trace  $Mx$  on  $\partial\Omega$  since the elements of  $\mathcal{A}_\varepsilon^M$  coincide with that affine function in a neighbourhood of  $\partial\Omega$ .

For every  $u \in H^1(\Omega; \mathbb{R}^n)$  let us set

$$G(u, \Omega) = \frac{1}{2|Y|} \int_{\Omega} \gamma(\nabla u) \, dx, \tag{15}$$

where  $\gamma$  is given by (12). We point out that if  $n = 2$  and we consider the triangular lattice in Fig. 1, then  $k = 6$  and the explicit form of  $\gamma$  previously computed yields

$$\begin{aligned} G(u, \Omega) &= \frac{\sqrt{3}}{4} \int_{\Omega} \left( |\mathcal{E}(u)^D|^2 + \frac{1}{2} (\operatorname{div} u)^2 \right) dx \\ &= \frac{\sqrt{3}}{4} \int_{\Omega} \left( |\mathcal{E}(u)|^2 - \frac{1}{2} (\operatorname{div} u)^2 \right) dx, \end{aligned} \quad (16)$$

where  $\mathcal{E}(u) = \frac{1}{2}(\nabla u + \nabla u^T)$ . A similar computation is easily performed for the Kuhn triangulation.

**Theorem 3.2** ( $\Gamma$ -convergence). *Let  $(\varepsilon_j)$  and  $(\delta_j)$  be positive infinitesimal sequences and let the triangulations  $\mathcal{T}_{\varepsilon_j}$  satisfy conditions (A) and (B). Assume that  $a_{\xi} = |\xi|$  for every  $\xi \in P$ . Then the sequence  $(G_{\varepsilon_j, \delta_j})$  has the functional  $G$  defined in (15) as  $\Gamma$ -limit with respect to the  $L^1$ -convergence or equivalently the weak convergence in  $H^1(\Omega; \mathbb{R}^n)$ .*

**Remark 5.** As a consequence of the equivalence of the  $L^1$ -convergence and the weak  $H^1$ -convergence in the computation of the  $\Gamma$ -limit, we remark that the same result holds if we consider the functions  $u$  extended as piecewise-constant functions, since the difference between such piecewise-constant and piecewise-affine interpolations tends to zero in  $L^1$  in the hypotheses of Theorem 3.1.

We now prove Theorems 3.1 and 3.2.

*Reduction to a continuum setting: compactness and lower bound.*

The proof of Theorem 3.1 will be obtained by estimating from below  $G_{\varepsilon, \delta}(u, \Omega)$  by suitable integral energies of the form  $\delta^{-2} \int W_0(I + \delta \nabla u) dx$ , which are coercive in  $H^1$  by the results in [14].

If  $\xi \in P$  and  $T \in \mathcal{T}_{\varepsilon}$  we will write  $\xi \parallel \partial T$  if there exists an edge of  $T$  which has the same direction as  $\xi$ . Define:

$$P(i) = \{\xi \in P : \xi \parallel \partial T_i\} \quad (i = 1, \dots, l).$$

Then  $P = \cup_i P(i)$ . Note that the sets  $P(i)$  are not pairwise disjoint; if  $\xi \in P$  we denote by  $m(\xi)$  the number of  $T \in \{T_1, \dots, T_l\}$  such that  $\xi \parallel \partial T$ .

Fix  $\varepsilon > 0$ . For any  $u \in \mathcal{A}_{\varepsilon}^M$  (which we consider extended by affine interpolation on the elements of  $\mathcal{T}_{\varepsilon}$ ) we can estimate the discrete energy as follows:

$$E_{\varepsilon}(u, \Omega) \geq \sum_{i=1}^l \sum_{\substack{T \in \mathring{\mathcal{T}}_{\varepsilon} \\ T \sim T_i}} \sum_{\xi \parallel \partial T_i} \frac{1}{m(\xi)} \varphi^{\xi} \left( I + (\nabla u) \Big|_T \right)$$

where  $\mathring{\mathcal{T}}_{\varepsilon}$  stands for the subfamily of the triangles in  $\mathcal{T}_{\varepsilon}$  whose vertices are in  $\mathring{\Omega}_{\varepsilon}$ , and  $\varphi^{\xi}$  is defined in Remark 3.

Let us now introduce the following functions  $W_i: M^{n \times n} \rightarrow \mathbb{R}$  for  $i = 1, \dots, l$

$$W_i(F) = \sum_{\xi \parallel \partial T_i} \frac{1}{m(\xi)} \varphi^{\xi}(F);$$

and set

$$W_0 = \min_{i=1, \dots, l} W_i.$$

Then

$$E_\varepsilon(u, \Omega) \geq \sum_{i=1}^l \sum_{\substack{T \in \mathring{T}_\varepsilon \\ T \sim T_i}} W_i \left( I + (\nabla u) \Big|_T \right) = \sum_{i=1}^l \sum_{\substack{T \in \mathring{T}_\varepsilon \\ T \sim T_i}} \frac{1}{\tau} \int_T W_i(I + \nabla u) \, dx, \quad (17)$$

and also

$$E_\varepsilon(u, \Omega) \geq \sum_{i=1}^l \sum_{\substack{T \in \mathring{T}_\varepsilon \\ T \sim T_i}} \frac{1}{\tau} \int_T W_0(I + \nabla u) \, dx = \frac{1}{\tau} \int_{\bigcup \mathring{T}_\varepsilon} W_0(I + \nabla u) \, dx.$$

Let now  $(\varepsilon_j)$  and  $(\delta_j)$  be positive infinitesimal sequences, and for every  $j \in \mathbb{N}$  let  $u_j$  be a function in  $\mathcal{A}_{\varepsilon_j}^M$  such that  $(G_{\varepsilon_j, \delta_j}(u_j, \Omega))$  is bounded. By the definition of  $W_0$ , and the previous estimate we can easily get

$$\begin{aligned} G_{\varepsilon_j, \delta_j}(u, \Omega) &\geq \frac{1}{\delta_j^2} \left( \int_\Omega W_0(I + \delta \nabla u_j) \, dx - \varepsilon_j c W_0(I + \delta_j M) \right) \\ &\geq \frac{1}{\delta_j^2} \int_\Omega W_0(I + \delta \nabla u_j) \, dx - \varepsilon_j c (1 + |M|)^2, \end{aligned}$$

with  $c$  independent of  $j$ . A simple check guarantees that  $W_0$  vanishes exactly on  $SO(n)$  and satisfies the smoothness and growth assumptions sufficient to apply the results of [14] to  $W$ . In particular, we obtain the boundedness in  $H^1(\Omega; \mathbb{R}^n)$  of the sequence  $(u_j)$  (see [14], Prop. 2.3); hence we immediately get Theorem 3.1.

The proof of the lower bound for the  $\Gamma$ -limit in Theorem 3.2 is obtained by a more careful application of the previous argument and estimating from below  $G_{\varepsilon, \delta}(u, \Omega)$  by suitable integral energies of the form  $\delta^{-2} \int W(x, I + \delta \nabla u) \, dx$ , whose asymptotic behaviour can be deduced from the results in [14].

For any  $i = 1, \dots, l$  let  $\chi^i$  be the characteristic function of the union of the elements  $T \in \mathcal{T}_1$  with  $T \sim T_i$ . Define  $W: \Omega \times M^{n \times n} \rightarrow \mathbb{R}$  as follows

$$W(x, F) = \sum_{i=1}^l \chi^i(x) W_i(F).$$

Then estimate (17) yields:

$$E_{\varepsilon_j}(\delta_j u_j, \Omega) \geq \frac{1}{\tau} \int_{\bigcup \mathring{T}_\varepsilon} W \left( \frac{x}{\varepsilon_j}, I + \delta_j \nabla u_j \right) \, dx. \quad (18)$$

We also have:

$$\int_{\Omega \setminus \bigcup \mathring{T}_\varepsilon} W \left( \frac{x}{\varepsilon_j}, I + \delta_j \nabla u_j \right) \, dx \leq c\varepsilon \sum_{i=1}^l W_i(I + \delta_j M) \quad (19)$$

for a suitable  $c > 0$ .

It is now convenient to express  $W_i$  in terms of the Green-St.Venant tensor  $E = \frac{1}{2}(F^T F - I)$ , as in [14]. Thus  $W_i(F)$  can be written as

$$V_i(E) = \sum_{\xi \parallel \partial T_i} \frac{1}{2m(\xi)} K_\xi \left( \sqrt{|\xi|^2 + 2\xi^T E \xi} - a_\xi \right)^2.$$

With this notation we have:

$$W_i(I + \delta_j \nabla u_j) = V_i(\delta_j \mathcal{E}(u_j) + \delta_j^2 \nabla u_j^T \nabla u_j).$$

Let  $k \in \mathbb{N}$  be fixed. By Lemma 4.2 in [14] there exist an increasing sequence  $(V_i^{k,j})_{j \in \mathbb{N}}$  of convex functions on  $M_{sym}^{n \times n}$  and a positive number  $\mu_i^k$  such that

$$\begin{aligned} V_i(\delta_j E) / \delta_j^2 &\geq V_i^{k,j}(E) \\ V_i^{k,j}(E) &= \frac{1}{2} \left(1 - \frac{1}{k}\right) \partial_E^2 V_i(0)[E, E] \quad \text{if } (\partial_E^2 V_i(0)[E, E])^{1/2} \leq \mu_i^k / \delta_j. \end{aligned}$$

Let  $\tilde{V}_i^{k,j}$  be the Yosida regularization of  $V_i^{k,j}$  with parameter  $\delta_j^{-1/2}$ , *i.e.*

$$\tilde{V}_i^{k,j}(E) = \sup \{ V_i^{k,j}(A) + \delta_j^{-1/2} |E - A| : A \in M_{sym}^{n \times n} \}.$$

Then  $\tilde{V}_i^{k,j}$  has  $\delta_j^{-1/2}$  as a Lipschitz constant and for every  $E$

$$\lim_{j \rightarrow \infty} \tilde{V}_i^{k,j}(E) = \frac{1}{2} \left(1 - \frac{1}{k}\right) \partial_E^2 V_i(0)[E, E].$$

By (18) and (19) and the expansion in Remark 3, for all  $j, k \in \mathbb{N}$  we have:

$$\begin{aligned} G_{\varepsilon_j, \delta_j}(u_j, \Omega) &= \frac{1}{\delta_j^2} E_{\varepsilon_j}(u_j, \Omega) \\ &\geq \frac{1}{\tau} \int_{\Omega} \tilde{V}^{k,j} \left( \frac{x}{\varepsilon_j}, \mathcal{E}(u_j) + \frac{1}{2} \delta_j \nabla u_j^T \nabla u_j \right) dx - c\varepsilon_j \end{aligned}$$

where for every  $E \in M_{sym}^{n \times n}$  we have set

$$\tilde{V}^{k,j}(x, E) = \sum_{i=1}^l \chi^i(x) \tilde{V}_i^{k,j}(E).$$

Since  $j \mapsto V_i^{k,j}(x, E)$  and  $j \mapsto \tilde{V}^{k,j}(x, E)$  are increasing, for every  $j \in \mathbb{N}$  with  $j \geq k$  we have:

$$G_{\varepsilon_j, \delta_j}(u_j, \Omega) \geq \frac{1}{\tau} \int_{\Omega} \tilde{V}^{k,k} \left( \frac{x}{\varepsilon_j}, \mathcal{E}(u_j) + \frac{1}{2} \delta_j \nabla u_j^T \nabla u_j \right) dx - c\varepsilon_j.$$

From the Lipschitz property of  $\tilde{V}^{k,k}$  we deduce that

$$\tilde{V}^{k,k} \left( \frac{x}{\varepsilon_j}, \mathcal{E}(u_j) + \frac{1}{2} \delta_j \nabla u_j^T \nabla u_j \right) \geq \tilde{V}^{k,k} \left( \frac{x}{\varepsilon_j}, \mathcal{E}(u_j) \right) - \frac{c}{\delta_j^{1/2}} \delta_j |\nabla u_j^T \nabla u_j|,$$

for a suitable  $c > 0$ . Since  $(u_j)$  is bounded in  $H^1(\Omega; \mathbb{R}^n)$ , we get

$$\liminf_{j \rightarrow \infty} G_{\varepsilon_j, \delta_j}(u_j, \Omega) \geq \frac{1}{\tau} \liminf_{j \rightarrow \infty} \int_{\Omega} \tilde{V}^{k,k} \left( \frac{x}{\varepsilon_j}, \mathcal{E}(u_j) \right) dx.$$

Then, a standard argument in homogenization theory (which can be directly derived from the discrete homogenization results in [1]) gives:

$$\liminf_{j \rightarrow \infty} G_{\varepsilon_j, \delta_j}(u_j, \Omega) \geq \frac{1}{\tau} \int_{\Omega} V_{\text{hom}}^k(\mathcal{E}(u)) dx$$

with

$$V_{\text{hom}}^k(E) = \inf \frac{1}{|Y|} \int_Y \tilde{V}^{k,k}(x, E + \mathcal{E}(u)) dx,$$

where the infimum is taken in the space  $PA_{\#}(Y)$  of all  $u$  piecewise affine on  $Y$ , with underlying mesh  $\mathcal{T}_1$ , with periodic boundary conditions. By taking the supremum for  $k \in \mathbb{N}$  we finally get:

$$\liminf_{j \rightarrow \infty} G_{\varepsilon_j, \delta_j}(u_j, \Omega) \geq \frac{1}{\tau} \int_{\Omega} V_{\text{hom}}(\mathcal{E}(u)) dx$$

where

$$V_{\text{hom}}(E) = \inf_{u \in PA_{\#}(Y)} \frac{1}{|Y|} \int_Y V_0(x, E + \mathcal{E}(u)) \, dx,$$

with

$$V_0(x, E) = \frac{1}{2} \sum_{i=1}^l \chi^i(x) \partial_E^2 V_i(0)[E, E].$$

A direct computation (or a comparison with the expansion in Remark 3) yields that

$$\partial_E^2 V_i(0)[E, E] = \frac{1}{2} \sum_{\xi \parallel \partial T_i} \frac{1}{m(\xi)} \frac{K_\xi}{|\xi|^2} (\xi^T E \xi)^2,$$

for every  $E \in M_{\text{sym}}^{n \times n}$ .

We eventually exploit the structure of the mesh  $\mathcal{T}_1$ ; each simplex in the periodicity cell  $Y$  has its vertices on those of  $Y$ , so that the periodicity condition in  $PA_{\#}(Y)$  is only compatible with constant functions, hence null gradients. Therefore:

$$\begin{aligned} V_{\text{hom}}(E) &= \frac{1}{|Y|} \int_Y V_0(x, E) \, dx = \frac{1}{2} \sum_{i=1}^l \partial_E^2 V_i(0)[E, E] \frac{1}{|Y|} \int_Y \chi^i(x) \, dx \\ &= \frac{\tau}{2|Y|} \sum_{i=1}^l \partial_E^2 V_i(0)[E, E] \\ &= \frac{\tau}{2|Y|} \sum_{i=1}^l \sum_{\xi \parallel \partial T_i} \frac{1}{2} \frac{1}{m(\xi)} \frac{K_\xi}{|\xi|^2} (\xi^T E \xi)^2. \end{aligned}$$

Since each element  $\xi$  of  $P$  is considered  $m(\xi)$  times in the sum, we conclude that:

$$V_{\text{hom}}(E) = \frac{\tau}{2|Y|} \sum_{\xi \in P} \frac{1}{2} \frac{K_\xi}{|\xi|^2} (\xi^T E \xi)^2 = \frac{\tau}{2|Y|} \gamma(E).$$

*Upper bound.*

To complete the proof of Theorem 3.2, we have to show that the lower bound is actually attained; *i.e.*, for every  $u \in H^1(\Omega; \mathbb{R}^n)$  with trace  $Mx$  on  $\partial\Omega$ , there exists a sequence  $(u_j)$  in  $\mathcal{A}_{\varepsilon_j}^M$  such that:

$$u_j \rightharpoonup u \text{ weakly in } H^1(\Omega; \mathbb{R}^n), \quad G_{\varepsilon_j, \delta_j}(u_j, \Omega) \rightarrow G(u, \Omega).$$

Assume first that  $u \in W^{1, \infty}(\Omega; \mathbb{R}^n) \cap C^2(\mathbb{R}^n)$ . In this case we take  $u_j = u$ ; *i.e.*, the recovery sequence is chosen as to be the trace of  $u$  on  $\Omega_{\varepsilon_j}$ . Let  $x \in \Omega_{\varepsilon_j}$  and  $\xi \in P$ . If  $T$  is any of the simplices with an edge parallel to  $\xi$  and with an endpoint in  $x$ , then

$$\begin{aligned} \frac{1}{2} K_\xi (|\xi + \delta_j D_{\varepsilon_j}^\xi u_j(x)| - a_\xi)^2 &= \frac{1}{2} K_\xi \left[ \left| \left( I + \delta_j (\nabla u_j) \Big|_T \right) \xi \right| - a_\xi \right]^2 \\ &= \varphi^\xi \left( I + \delta_j (\nabla u_j) \Big|_T \right). \end{aligned}$$

From the expansion in Remark 3, and taking the equi-boundedness of  $(D_{\varepsilon_j} u_j)_j$  into account, we deduce that:

$$\frac{1}{2\delta_j^2} K_\xi \left( |\xi + \delta_j D_{\varepsilon_j}^\xi u_j(x)| - a_\xi \right)^2 = \frac{1}{2} \frac{K_\xi}{|\xi|^2} \left( \xi^T (\nabla u_j) \Big|_T \xi \right)^2 + o(\delta_j).$$

Since  $(\nabla u_j)|_T$  tends to  $\nabla u(x)$  uniformly in  $x$ , we also have:

$$\frac{1}{2\delta_j^2} K_\xi (|\xi + \delta_j D_{\varepsilon_j}^\xi u_j(x)| - a_\xi)^2 = \frac{1}{2} \frac{K_\xi}{|\xi|^2} (\xi^T \nabla u(x) \xi)^2 + o(1) + o(\delta_j).$$

After summing up we then obtain

$$\lim_{j \rightarrow +\infty} \frac{1}{\delta_j^2} E_{\varepsilon_j}(\delta_j u_{\varepsilon_j}, \Omega) = \frac{1}{2|Y|} \int_{\Omega} \gamma(\nabla u(x)) dx. \quad (20)$$

In the general case  $u \in H^1(\Omega; \mathbb{R}^n)$  we observe that there exists a sequence  $(u_k)$  of Lipschitz and  $C^2$  functions,  $u_k = u_M$  on a neighbourhood of  $\partial\Omega$  and  $u_k \rightarrow u$  strongly in  $H^1(\Omega; \mathbb{R}^n)$ , so that

$$\lim_k \int_{\Omega} \gamma(\nabla u_k) dx = \int_{\Omega} \gamma(\nabla u) dx.$$

Then, we conclude by (20) applied to  $u_k$  and a standard diagonal argument.

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*E-mail address:* braides@mat.uniroma2.it, margherita@uniss.it, enrico.vitali@unipv.it