Hexagonal lattices with three-point interactions

Hervé Le Dret, Annie Raoult

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Abstract

We characterize the macroscopic effective mechanical behavior of a graphene sheet modeled by a hexagonal lattice with two- and three-point atomic interactions, using Γ-convergence.

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1 Introduction

We consider a two-dimensional hexagonal atomic network with two- and three-point interactions. Such a network can be used to model the mechanical behavior of a graphene sheet with nearest neighbor atom to atom interaction on the one hand, and torques resulting from three-point interactions on the other hand. We are interested in deriving an equivalent continuum mechanics model for the deformations of the sheet by means of a homogenization procedure when the rest lengths of the bonds go to 0, using Γ-convergence techniques, since we work with an energy minimization formulation. The electronic properties of graphene are out of the scope of this article.

There is a comprehensive body of work on the homogenization of discrete networks, see for instance [1, 2, 4, 6, 7, 18], mostly in the context of two-point interactions, either short or long range, with polynomial growth energies. Our previous work on hexagonal networks was also concerned with only two-point, nearest neighbor interactions with polynomial growth, see [14]. There are relatively few works dealing with three-point interactions, let us mention [3, 8, 10, 15] in this direction, or nonpolynomial growth, see [4, 18], which do not seem to apply to our problem.

The two-point interactions we consider are composed of two terms, an elastic term as in [14], and a Lennard-Jones type term. The Lennard-Jones type energy is a phenomenological term which is supposed to model quantum repulsion between neighboring atoms. Since it tends to $+\infty$ when the distance between two bonded

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atoms goes to 0, its presence precludes any polynomial growth assumption. The addition of an elastic term is compatible with physical behavior around the ground state, but not necessarily elsewhere. We however add it for coercivity reasons, as is classically done in most of the above-mentioned works.

The three-point interactions correspond to the fact that the three chemical bonds radiating from any given atom in a graphene sheet have a preferred pairwise angle of $\frac{2\pi}{3}$. Deviations from this angle thus result in torques relative to the angle vertex, caused by the deformations of triangles of atoms. Energy densities corresponding to such torques can be found in the material science literature. They penalize deviations from the preferred angle, see *e.g.* [19].

In the same spirit as [6] and many other works in the literature, we rewrite the problem as a sequence of problems in the calculus of variations, indexed by a parameter representing the interatomic distance. We replace the discrete displacements of the atoms in the sheet by continuous piecewise affine functions defined on a domain, which makes it easy to talk about convergence in a Sobolev space setting. As opposed to [14], it is not possible to replace the discrete energies by continuous energies at the onset, because of the three-point interactions which have a slightly non local effect. We therefore use an entirely different approach, following the work of Alicandro-Cicalese, [2], taking in addition advantage of a simplified slicing technique introduced in [12].

We show that the discrete energy minimizers for the energy with Dirichlet boundary conditions weakly converge in a Sobolev space to minimizers of a limit continuous energy, see Proposition 4.2 and Corollary 4.4, when the parameter goes to 0. We also identify the limit energy density via a homogenization formula, see Proposition 4.3.

2 Setting of the problem

In our previous article [14], we considered graphene sheets of arbitrary shape and devoted a lot of effort to properly defining boundary conditions. In order to avoid such technicalities, we consider here a much simpler setup, which we presently introduce. A sheet is a discrete two-dimensional structure that deforms in three-dimensional Euclidean space. We choose an orthonormal basis (e_1, e_2, e_3) of $\mathbb{R}^3$. The scalar product and norm in $\mathbb{R}^3$ are respectively denoted by $\cdot$ and $|\ |$.

The basic hexagonal lattice in $\mathbb{R}^2$ is spanned by the three vectors

$$s_1 = \sqrt{3}e_1, \quad s_2 = \frac{\sqrt{3}}{2}e_1 + \frac{3}{2}e_2 \quad \text{and} \quad p = \frac{1}{3}(s_1 + s_2).$$

In the description we use, the lattice is comprised of two types of nodes: The type 1 nodes, which occupy points $is_1 + js_2$ with $(i, j) \in \mathbb{Z}^2$, and the type 2 nodes, which occupy points $is_1 + js_2 + p$, again with $(i, j) \in \mathbb{Z}^2$, see Figure 1. Associated with this set of nodes are two Delaunay triangulations. The main Delaunay triangulation

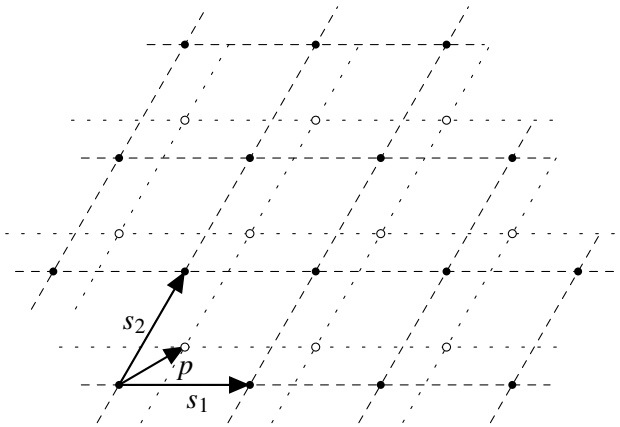

Figure 1: •: type 1 nodes, ◦: type 2 nodes

we use is depicted in Figure 2, its edges are the solid lines and the dashed lines. The alternate one, which we will use less, is depicted in Figure 3.

The chemical bonds between atoms join nearest neighboring type 1 and type 2 nodes. The bonds are represented by the closed segments joining two neighboring nodes, see Figure 2.

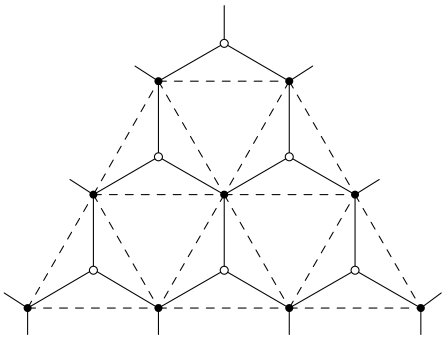

Figure 2: Hexagonal structure, main Delaunay triangulation.

Let now Y be the open parallelogram based on vectors s_1 and s_2. This set will also be used later on as the unit cell of our homogenization procedure. Let us pick a scale factor $L > 0$ and set $\omega = LY$ to be the reference configuration of a family of sheets. Each sheet in the family consists of the global, scale 1, lattice scaled by a factor $\varepsilon = L/n$ where n is an integer, and cropped to ω, see Figure 4, which deforms in $\mathbb{R}^3$. Homogenization will occur in the limit $n \to +\infty$ or equivalently $\varepsilon \to 0$. This setting considerably simplifies boundary condition issues, which we know are tractable in much more general geometric situations as shown in [14].

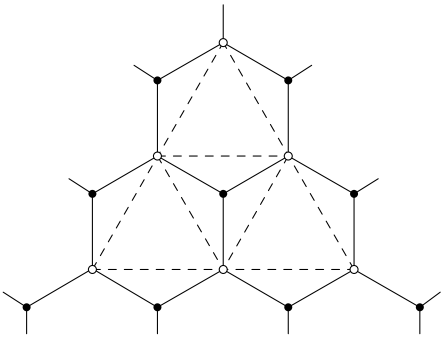

Figure 3: Alternate Delaunay triangulation.

Indeed, we assume here that all type 1 nodes on $\partial\omega$ are submitted to a boundary condition of place defined by a given deformation φ_0 which is at least continuous on $\bar{\omega}$ in order for its node values to make sense. We can also consider the case when the boundary condition of place is enforced only on part of $\partial\omega$.

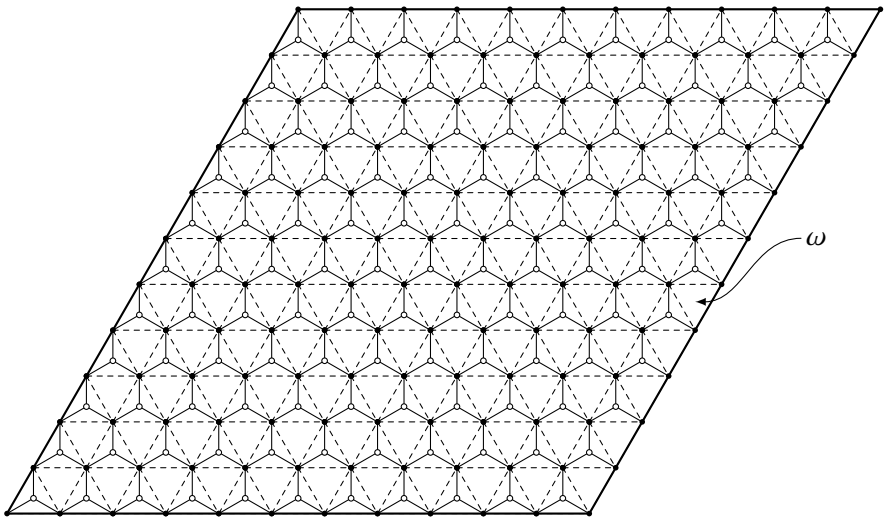

Figure 4: A typical sheet with its main Delaunay triangulation.

Let us now turn to the mechanical side of the model. We first describe the deformations of the sheet in $\mathbb{R}^3$. We will switch between two equivalent points of view depending on whichever is the most convenient at any given point in the proofs.

We denote by $\mathbb{L}$ the $\mathbb{Z}$-lattice generated by s_1 and s_2 and let $\mathbb{L}_* = \mathbb{L} + p$. Basically, a deformation φ^ε is a mapping from $\big(\varepsilon(\mathbb{L} \cup \mathbb{L}_*)\big) \cap \bar{\omega}$ into $\mathbb{R}^3$ that satisfies the boundary condition. This is the discrete point of view. With this discrete point

of view, we associate a continuous point of view by letting the same φ^ε denote the piecewise affine Lagrange interpolate of the nodal values of the former φ^ε on the main Delaunay triangulation of $\bar{\omega}$ depicted in Figure 4. We denote by $A(\varepsilon)$ the set of all such continuous piecewise affine functions, without boundary conditions.

The function φ^ε thus defined is in $H^1(\omega;\mathbb{R}^3)$, and we can freely take its gradient in the distributional sense, which is piecewise constant, $M_{3,2}$-valued, where $M_{3,2}$ denotes the space of 3×2 matrices. The boundary condition reads

$$\varphi^\varepsilon(x) = \varphi_0^\varepsilon(x) \text{ for all } x \text{ belonging to } \partial\omega, \tag{1}$$

where φ_0^ε denotes the piecewise affine Lagrange interpolate of $\varphi_{0|\partial\omega}$ on the nodes located on $\partial\omega$. Note that φ_0^ε is also the trace on $\partial\omega$ of the piecewise Lagrange interpolate $\Pi^\varepsilon\varphi_0$ of φ_0 on the main Delaunay triangulation. We will make additional regularity assumptions on φ_0 in section 4.

We now describe the energy of the sheet. Let us be given a global numbering of the bonds b_k contained in $\bar{\omega}$. Each bond b_k links a type 1 node n_{k1} and a type 2 node n_{k2}. We let $\varphi^\varepsilon(b_k) = \varphi^\varepsilon(n_{k2}) - \varphi^\varepsilon(n_{k1})$. This particular choice of orientation is not important, but it needs to be consistent over the whole sheet.

We consider that there are several contributions to the energy. First, as in [14], there is a two-point elastic contribution for each bond b_k of the form

$$B_k^\varepsilon(\varphi^\varepsilon) = \varepsilon^2\kappa_1(\varepsilon^{-1}|\varphi^\varepsilon(b_k)| - 1)^2, \tag{2}$$

where $\kappa_1 > 0$ is a stiffness parameter, ε is the natural length of the bond and $|\varphi^\varepsilon(b_k)|$ is its deformed length. The ε^2 scaling factor is the right one to obtain a finite nonzero limit energy (without rescaling). Then there is a two-point, Lennard-Jones type contribution of the form

$$R_k^\varepsilon(\varphi^\varepsilon) = \varepsilon^2 r(\varepsilon^{-1}|\varphi^\varepsilon(b_k)|), \tag{3}$$

where $r\colon \mathbb{R}_+ \to \bar{\mathbb{R}}_+$ is a Lennard-Jones type potential, *i.e.*, a continuous function such that $r(0) = +\infty$, r is decreasing on $[0,1]$, $r(1) = 0$, r is nondecreasing on $[1,+\infty[$, and $r(\ell) \to c$ when $\ell \to +\infty$ for some constant $c \geq 0$. The sum of these two terms forms an energy for each bond that is minimum at the natural length ε. This energy is infinitely repulsive when the deformed length of a bond goes to 0 and tends to $+\infty$ when the deformed length of a bond goes to $+\infty$. While the former behavior is desirable from the atomistic modeling point of view, the latter one is more debatable, because interatomic forces should tend to 0 when the interatomic distance tends to $+\infty$. It is mostly there for coercivity reasons. We refer to [4] for work in which such coercivity assumptions are not made.

Finally, and this is the second main aspect of our purpose here, there is a three-point potential that penalizes deviations from $\frac{2\pi}{3}$ of the angle between pairs of bonds radiating out of each node. The specific form of this moment potential is not very important, but it is clear that it must be discontinuous when the deformed length of one of the bonds goes to 0 and the angle in question becomes undefined.

For definiteness, for any such pair of bonds $\{b_k, b_l\}$ with $|\varphi^\varepsilon(b_k)|\,|\varphi^\varepsilon(b_l)| > 0$, we choose

$$M^\varepsilon_{kl}(\varphi^\varepsilon) = \varepsilon^2\kappa_2\Big(\frac{\varphi^\varepsilon(b_k)\cdot\varphi^\varepsilon(b_l)}{|\varphi^\varepsilon(b_k)|\,|\varphi^\varepsilon(b_l)|} + \frac{1}{2}\Big)^2, \tag{4}$$

where $\kappa_2 > 0$ is another stiffness coefficient, see [16, 19] where similar energies are used and for experimental values of the constants.

The total stored energy of the sheet under deformation is thus the sum of all the above terms when no bond is of zero deformed length,

$$I^\varepsilon(\varphi^\varepsilon, \bar\omega) = \sum_k \big(B^\varepsilon_k(\varphi^\varepsilon) + R^\varepsilon_k(\varphi^\varepsilon)\big) + \sum_{k,l} M^\varepsilon_{kl}(\varphi^\varepsilon) \tag{5}$$

the first summation index k running through all the bonds in $\bar\omega$ and the second $\{k, l\}$ through all pairs of bonds in $\bar\omega$ sharing one node, and

$$I^\varepsilon(\varphi^\varepsilon, \bar\omega) = +\infty \tag{6}$$

when at least one bond has zero deformed length. This energy is clearly frame indifferent.

Let us remark that it is easy to abstract the properties of the above energies that play an effective role in the ensuing convergence analysis, and to write down a more general result with more general energy densities. We however chose to keep the above specific forms because they correspond to classical modeling hypotheses.

To complete the description of the mechanical setting, we impose external dead loading forces on all nodes in the sheet. We are thus given a function $f\colon \bar\omega \to \mathbb{R}^3$, which we assume to be continuous and independent of ε, such that the external force acting on a node is $\varepsilon^2 f(x)$, where x is the location of the node in question in the reference configuration. The corresponding energy term reads

$$F^\varepsilon(\varphi^\varepsilon) = \varepsilon^2\Big(\sum_{0\le i,j\le n} f\big(\varepsilon(is_1+js_2)\big)\cdot\varphi^\varepsilon\big(\varepsilon(is_1+js_2)\big) + \sum_{0\le i,j\le n-1} f\big(\varepsilon(is_1+js_2+p)\big)\cdot\varphi^\varepsilon\big(\varepsilon(is_1+js_2+p)\big)\Big).$$

We consequently end up with a total energy for the sheet which is the difference $I^\varepsilon(\cdot,\bar\omega) - F^\varepsilon(\cdot)$ of the total stored energy and the above force term. For any given ε, the deformed configuration of the sheet at equilibrium minimizes the total energy among all possible deformations φ^ε satisfying condition (1). The existence of such minimizers is obvious because the discontinuity of the three-point interaction potential is counterbalanced by the singularity of the Lennard-Jones term, and the elastic term plus boundary condition provides coercivity.

3 Convergence without boundary conditions

Let us first give some background on Γ-convergence and integral representation results. We follow essentially the same strategy as that of [1, 2, 6, 7], which is

to appropriately restrict the stored energy to arbitrary open subsets of ω in order to define a sequence of functionals on the Cartesian product of a function space X (in our case $X = L^2(\omega;\mathbb{R}^3)$) with the set $\mathcal{O}$ of the open subsets of ω. The Γ-limit of this sequence is thus roughly speaking also defined on the same Cartesian product. Buttazzo-Dal Maso's integral representation theorem in then used in order to identify the Γ-limit as a functional of the calculus of variations. For the reader's convenience, let us briefly go over the definitions and results.

Let X be a metric space. We consider a sequence of functionals $I^\varepsilon : X \times \mathcal{O} \to \bar{\mathbb{R}} = \mathbb{R} \cup \{+\infty\}$. The lower and upper Γ-limits are respectively defined by

$$I'(\psi, U) = \Gamma\text{-}\liminf_{\varepsilon\to 0} I^\varepsilon(\psi, U) = \inf_{\psi^\varepsilon \to \psi \text{ in } X} \liminf_{\varepsilon\to 0} I^\varepsilon(\psi^\varepsilon, U)$$

and

$$I''(\psi, U) = \Gamma\text{-}\limsup_{\varepsilon\to 0} I^\varepsilon(\psi, U) = \inf_{\psi^\varepsilon \to \psi \text{ in } X} \limsup_{\varepsilon\to 0} I^\varepsilon(\psi^\varepsilon, U).$$

When $I'(\cdot, U) = I''(\cdot, U) = I(\cdot, U)$, the sequence is said to Γ-converge (on U) for the topology of X to $\Gamma\text{-}\lim_{\varepsilon\to 0} I^\varepsilon(\cdot, U) = I(\cdot, U)$. It is well-known that if the minimizers of the sequence of functionals remain in a compact subset of X, then their limit points are minimizers of the Γ-limit. The concept of Γ-convergence is thus perfectly suited to the asymptotic study of sequences of problems in the calculus of variations.

We next state Buttazzo-Dal Maso's integral representation theorem in a simplified setting that is sufficient for our purposes here, see [5, 9].

Theorem 3.1 *Let $I : H^1(\omega;\mathbb{R}^3) \times \mathcal{O} \to \mathbb{R}$, bounded below and such that*
i) for all $\psi \in H^1(\omega;\mathbb{R}^3)$, the mapping $U \mapsto I(\psi, U)$ is the restriction of a Borel measure to $\mathcal{O}$,
ii) there exists a constant C such that for all $\psi \in H^1(\omega;\mathbb{R}^3)$ and all $U \in \mathcal{O}$, $I(\psi, U) \le C \int_U (1 + |\nabla\psi|^2)\, dx$,
iii) I is local, i.e.*, $I(\psi_1, U) = I(\psi_2, U)$ whenever $\psi_1 = \psi_2$ a.e. on U,*
iv) for all $\psi \in H^1(\omega;\mathbb{R}^3)$, $U \in \mathcal{O}$ and $a \in \mathbb{R}^3$, $I(\psi + a, U) = I(\psi, U)$,
v) for all $U \in \mathcal{O}$, the mapping $\psi \mapsto I(\psi, U)$ is sequentially weakly lower semicontinuous on $H^1(\omega;\mathbb{R}^3)$.

Then there exists a Carathéodory function $W : \omega \times M_{3,2} \to \mathbb{R}$ bounded below satisfying $W(x, F) \le C(1 + |F|^2)$ such that

$$I(\psi, U) = \int_U W(x, \nabla\psi(x))\, dx \tag{7}$$

for all $\psi \in H^1(\omega;\mathbb{R}^3)$ and $U \in \mathcal{O}$.

If in addition,
vi) for all affine ψ, $I(\psi, B) = I(\psi, B')$ where B and B' are any two balls of the same radius included in ω, then W does not depend on x.

The main part of the work is to obtain condition i) by means of the De Giorgi-Letta criterion, namely by showing that the mapping $U \mapsto I(\psi, U)$ is increasing, additive and inner regular, see [5].

In section 4, we reintroduce the boundary condition in the Γ-limit process and show that the result is unchanged. We also add the external force terms. Once this is done, we obtain a homogenization formula that identifies the limit density W.

We need to restrict the stored energy of the sheet to arbitrary open subsets U of ω. Each pair of bonds $\{b_k, b_l\}$ sharing one common node determines a closed triangle t_{kl} either of the main Delaunay triangulation or of the alternate Delaunay triangulation, see Figure 5.

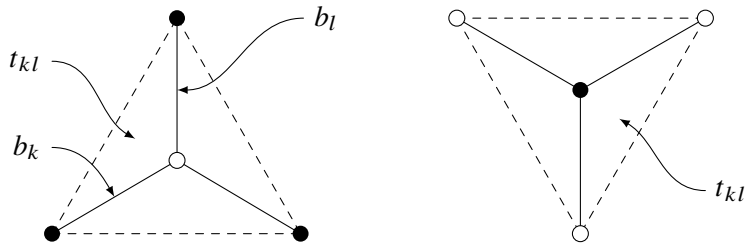

Figure 5: Bonds and associated triangles.

We let $T_m(U)$ (resp. $T_a(U)$) denote the subset of closed triangles of the main (resp. alternate) Delaunay triangulation that are contained in U. A bond will be counted in the energy restricted to U if it belongs to one of the triangles of $T_m(U)$ and an angle will be counted if it belongs to a triangle of $T_m(U)$ or $T_a(U)$. We thus define I^ε on $L^2(\omega;\mathbb{R}^3)\times\mathfrak{O}$ by

$$I^\varepsilon(\varphi^\varepsilon, U) = \sum_{b_k \subset t \in T_m(U)} \left(B_k^\varepsilon(\varphi^\varepsilon) + R_k^\varepsilon(\varphi^\varepsilon)\right) + \sum_{t_{kl} \in T_m(U)\cup T_a(U)} M_{kl}^\varepsilon(\varphi^\varepsilon), \quad (8)$$

if $\varphi^\varepsilon \in A(\varepsilon)$ and $I^\varepsilon(\varphi^\varepsilon, U) = +\infty$ if $\varphi^\varepsilon \in L^2(\omega;\mathbb{R}^3) \setminus A(\varepsilon)$. Note that for any element φ^ε of $A(\varepsilon)$ such that at least one bond involved has zero deformed length, we also have $I^\varepsilon(\varphi^\varepsilon, U) = +\infty$, due to the Lennard-Jones energy term. Thus the energy is not bounded from above even on $A(\varepsilon)$. Let us stress that it is important to stay clear of ∂U, which can be very irregular, in defining $I^\varepsilon(\cdot, U)$ for an arbitrary open set U.

We are primarily interested in $I^\varepsilon(\cdot,\bar\omega)$, which is not equal to $I^\varepsilon(\cdot,\omega)$ since the energy in ω does not take into account bonds that touch $\partial\omega$. Obviously, $I^\varepsilon(\cdot,\omega) \le I^\varepsilon(\cdot,\bar\omega)$.

We first note an equicoercivity result. We call empty triangle of the main Delaunay triangulation any such triangle that does not contain any bond. A union of triangles of the main Delaunay triangulation is called admissible if every empty triangle in the union is adjacent to at least two triangles of the form t_{kl} that also belong to the union.

Lemma 3.2 *There exists a constant $C > 0$ independent of ε such that for all $\psi \in A(\varepsilon)$ and all admissible unions T of triangles and all open subsets U such that $T \subset U$,*

$$I^\varepsilon(\psi, U) \geq C\big(\|\nabla\psi\|^2_{L^2(T)} - |T|\big).$$

Proof. The difficulty is that the equilateral triangles in the triangulation do not contain any bond. However, the energy is larger than the one considered in [14], it is thus enough to adapt the argument of Proposition 2 therein to the slightly different piecewise affine interpolation that we are presently using. The admissibility is used to recover coercivity over the empty triangles in the union considered. □

Corollary 3.3 *If $I'(\psi, \omega) < +\infty$ or $I''(\psi, \omega) < +\infty$, then $\psi \in H^1(\omega; \mathbb{R}^3)$.*

Proof. We use Lemma 3.2 to show that there exists a constant C such that for all open subsets $\omega' \Subset \omega$, we have $\psi \in H^1(\omega'; \mathbb{R}^3)$ with $\|\psi\|_{H^1(\omega')} \leq C$. This implies the result. □

We next show an essential technical lemma implying that it is possible to keep all neighboring nodes uniformly separated while locally lowering the stored energy.

Lemma 3.4 *There exists $0 < \alpha < 1$ such that for all $\psi \in L^2(\omega; \mathbb{R}^3)$ and $\psi^\varepsilon \in A(\varepsilon)$ such that $\psi^\varepsilon \to \psi$ strongly in $L^2(\omega; \mathbb{R}^3)$ when $\varepsilon \to 0$, we can find $\bar\psi^\varepsilon \in A(\varepsilon)$ such that $\bar\psi^\varepsilon \to \psi$ strongly in $L^2(\omega; \mathbb{R}^3)$, the deformed lengths of all bonds are larger than $\varepsilon\alpha$ and for all $U \in \mathcal{O}$,*

$$I^\varepsilon(\bar\psi^\varepsilon, U) \leq I^\varepsilon(\psi^\varepsilon, U).$$

Proof. The idea is to move apart neighboring nodes that are too close to each other in a given deformation ψ^ε, while locally controlling the energy. We only modify the positions of type 2 nodes, keeping type 1 nodes unchanged. Let us take $0 < \alpha < 1$ to be chosen later on. We examine each type 2 node in ω in turn. If the three bonds attached to this node are of deformed length larger than $\varepsilon\alpha$, we do not do anything. If on the other hand, one of the three bonds has deformed length strictly smaller than $\varepsilon\alpha$, then we modify ψ^ε at the type 2 node. Let us see how more precisely.

Without loss of generality, we can assume that the three bonds attached to the type 2 node are b_1, b_2 and b_3, with $|\psi^\varepsilon(b_1)| < \varepsilon\alpha$. We denote by A_i, $i = 1, 2, 3$, the position in $\mathbb{R}^3$ of the three type 1 nodes belonging to b_i and by P the position of the type 2 node, so that $|A_1P| < \varepsilon\alpha$. There are three cases.

Case 1: $|A_2P| \geq \varepsilon\alpha$ and $|A_3P| \geq \varepsilon\alpha$. We pick a straight line passing through P and orthogonal to A_2P and A_3P. As $|A_1P| < \varepsilon$, this straight line intersects the sphere centered at A_1 and of radius ε at two points. We let $\bar P$ denote one of these points closest to P and set $|P\bar P| = \beta$, with $0 < \beta \leq \varepsilon$, see Figure 6. By construction, $|A_1\bar P| = \varepsilon$, $|A_2\bar P| > |A_2P| \geq \varepsilon\alpha$ and $|A_3\bar P| > |A_3P| \geq \varepsilon\alpha$. This operation only modifies the lengths of the three bonds linked to P, the three angles around P and at

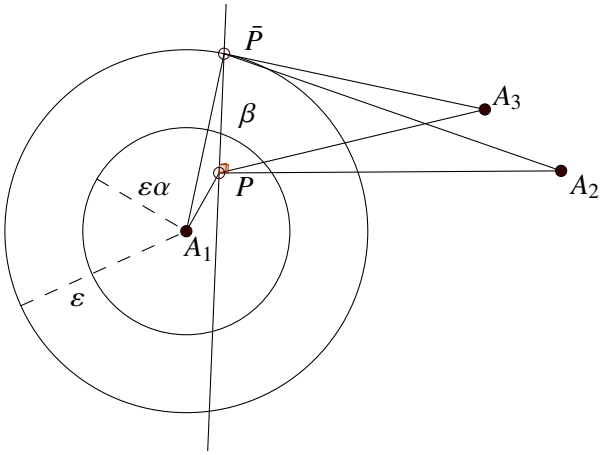

Figure 6: Construction of the modified deformation, case 1.

most two angles around each A_i. It does not affect any other length or angle taken into account in the energy. We need to show that α can be chosen in such a way that the energy decreases.

If $|A_1P| = 0$, there is nothing to prove. Let us thus assume that $|A_1P| > 0$. We only consider the case when there are nine angles, which is the generic case. The argument should make clear that the other cases can be worked out as well. We denote by B_i (resp. $\bar{B}_i$) and R_i (resp. $\bar{R}_i$), $i = 1, 2, 3$, the elastic and Lennard-Jones energies of the three bonds before (resp. after) modification, and by M_j (resp. $\bar{M}_j$), $j = 1, \dots, 9$, the moment energies before (resp. after) modification. The corresponding energies are

$$E = \sum_{i=1}^{3}(B_i + R_i) + \sum_{j=1}^{9} M_j$$
$$\bar{E} = \sum_{i=1}^{3}(\bar{B}_i + \bar{R}_i) + \sum_{j=1}^{9} \bar{M}_j.$$

Let us consider each term. For $i = 2, 3$, let $\ell_i = |A_iP|$ and $\bar{\ell}_i = |A_i\bar{P}|$. By construction, $\bar{\ell}_i^2 = \ell_i^2 + \beta^2$ so that

$$\bar{B}_i - B_i = \kappa_1\Big((\bar{\ell}_i - \varepsilon)^2 - (\ell_i - \varepsilon)^2\Big) = \kappa_1(\beta^2 - 2\varepsilon(\bar{\ell}_i - \ell_i)) \le \kappa_1\beta^2 \le \kappa_1\varepsilon^2,$$

since $\beta \le \varepsilon$.

Similarly, $\frac{\bar{\ell}_i}{\varepsilon} \ge \frac{\ell_i}{\varepsilon} \ge \alpha$, so that $r\big(\frac{\bar{\ell}_i}{\varepsilon}\big) \le r\big(\frac{\ell_i}{\varepsilon}\big) + c$, due to the properties of the function r. Consequently,

$$\bar{R}_i - R_i = \varepsilon^2\left(r\left(\frac{\bar{\ell}_i}{\varepsilon}\right) - r\left(\frac{\ell_i}{\varepsilon}\right)\right) \le c\varepsilon^2.$$

Each moment term is bounded by $\frac{9}{4}\kappa_2\varepsilon^2$, therefore

$$\sum_{j=1}^{9}(\bar{M}_j - M_j) \leq \frac{81}{2}\kappa_2\varepsilon^2.$$

By construction, $\bar{B}_1 = \bar{R}_1 = 0$. Letting $C = 2(\kappa_1 + c) + \frac{81}{2}\kappa_2$, we thus have

$$\bar{E} - E \leq -B_1 - R_1 + C\varepsilon^2 \leq -R_1 + C\varepsilon^2 = \Big(- r\Big(\frac{|A_1P|}{\varepsilon}\Big) + C\Big)\varepsilon^2,$$

where we recall that $|A_1P| < \varepsilon\alpha$. We now choose $\alpha < 1$ such that $r(\alpha) > C$, which is possible since $r(\alpha) \to +\infty$ when $\alpha \to 0^+$, so that $\bar{E} < E$.

Case 2: $|A_2P| < \varepsilon\alpha$ and $|A_3P| \geq \varepsilon\alpha$. We can only consider the case when both $|A_1P|$ and $|A_2P|$ are nonzero. We may assume that $\alpha < \frac{1}{4}$, so that $|A_1A_2| < \frac{\varepsilon}{2}$. The sphere of radius ε centered at A_1 intersects the plane orthogonal to the third bond and passing through P on a circle of radius less than ε. We pick a point $\bar{P}$ on this circle closest to P. We thus have $|P\bar{P}| \leq \varepsilon$, $|A_1\bar{P}| = \varepsilon$ and $|A_3P|^2 \leq |A_3\bar{P}|^2 \leq |A_3P|^2 + \varepsilon^2$. By the triangle inequality, we moreover see that $\varepsilon\alpha \leq |A_2\bar{P}| \leq \varepsilon(\alpha + 1)$. The same kind of calculations on the energies as in Case 1 then allow us to obtain an appropriate value of α.

Case 3: $|A_2P| < \varepsilon\alpha$ and $|A_3P| < \varepsilon\alpha$. In this case, we take a plane containing the three points A_i. We take $\bar{P}$ at distance ε of the plane on the orthogonal to the plane passing through P. It follows that $\varepsilon \leq |A_i\bar{P}| \leq \sqrt{2}\varepsilon$ for all i. This provides a third value of α, which we retain if it smaller than the previous one.

The procedure ends when all type 2 nodes have been processed. We thus have a new deformation $\bar{\psi}^\varepsilon$ that globally diminishes the energy. It also does so for local energies for any open set U. Indeed, the new deformation is obtained via a local construction, and when a type 2 node is taken into account in a local energy, there are a priori less bonds and angles attached to it involved than in the global energy, so it is easier to decrease the energy.

It remains to show that $\bar{\psi}^\varepsilon$ still tends to ψ strongly in $L^2(\omega;\mathbb{R}^3)$. This is quite obvious since by construction, $\|\bar{\psi}^\varepsilon - \psi^\varepsilon\|_{L^\infty} \leq 2\varepsilon$. □

We now establish several properties of the Γ-limsup and Γ-liminf of the sequence I^ε.

Proposition 3.5 *There exists a constant C such that for all $\psi \in H^1(\omega;\mathbb{R}^3)$ and $U \in \mathcal{O}$, we have*

$$I''(\psi, U) \leq C\big(\|\nabla\psi\|^2_{L^2(U)} + |U|\big). \tag{9}$$

Proof. We first take $\psi \in C^\infty(\bar{\omega};\mathbb{R}^3)$ and denote by $\Pi^\varepsilon\psi \in A(\varepsilon)$ the piecewise affine Lagrange interpolate of ψ on the main Delaunay triangulation. We consider the corresponding modified deformation $\overline{\Pi^\varepsilon\psi}$ of Lemma 3.4. By construction, we have $\overline{\Pi^\varepsilon\psi} \to \psi$ in $L^2(\omega)$ strong.

Let U be an open subset of ω and b_k be a bond included in a triangle of $T_m(U)$. We choose one of the at most two possible triangles, t_k. Let $\bar{B}_k^\varepsilon$ and $\bar{R}_k^\varepsilon$ denote the elastic and Lennard-Jones energies of bond b_k. By Lemma 3.4, $|\bar{R}_k^\varepsilon| \le C\varepsilon^2 \le C|t_k|$. Moreover, we have

$$\bar{B}_k^\varepsilon \le C\varepsilon^2\Big(\Big|\nabla\Big(\overline{\Pi^\varepsilon\psi}_{|t_k}\Big)\Big|^2 + 1\Big) \le C\int_{t_k}\Big(\Big|\nabla\Big(\overline{\Pi^\varepsilon\psi(x)}\Big)\Big|^2 + 1\Big)\,dx.$$

When we add up the contributions of all the bonds, any such triangle is counted at most twice, thus

$$\begin{aligned}\sum_{b_k\subset t\in T_m(U)}(\bar{B}_k^\varepsilon + \bar{R}_k^\varepsilon) &\le C\int_{\bigcup T_m(U)}\Big(\Big|\nabla\Big(\overline{\Pi^\varepsilon\psi(x)}\Big)\Big|^2 + 1\Big)\,dx\\ &\le C\Big(\int_{\bigcup T_m(U)}\Big|\nabla\Big(\overline{\Pi^\varepsilon\psi(x)}\Big)\Big|^2\,dx + |U|\Big),\end{aligned}$$

since all the triangles are included in U. Here and in the sequel, we denote $\bigcup T_m(U) = \bigcup_{t\in T_m(U)} t$, for brevity. Likewise, each angle taken into account belongs to exactly one triangle, so that

$$\sum_{t_{kl}\in T_m(U)\cup T_a(U)}\bar{M}_{kl}^\varepsilon \le C\int_{\bigcup(T_m(U)\cup T_a(U))}dx \le C|U|.$$

Consequently,

$$I^\varepsilon(\overline{\Pi^\varepsilon\psi}, U) \le C\Big(\int_{\bigcup T_m(U)}\Big|\nabla\Big(\overline{\Pi^\varepsilon\psi}(x)\Big)\Big|^2\,dx + |U|\Big).$$

By construction, $\overline{\Pi^\varepsilon\psi} = \Pi^\varepsilon\psi + \delta^\varepsilon$ with $\|\nabla\delta^\varepsilon\|_{L^\infty} \le C$. Therefore

$$I^\varepsilon(\overline{\Pi^\varepsilon\psi}, U) \le C\Big(\int_{\bigcup T_m(U)}\Big|\nabla\Big(\Pi^\varepsilon\psi(x)\Big)\Big|^2\,dx + |U|\Big).$$

By classical finite element theory, we know that there exists a constant C independent of ψ such that, for any union T of triangles t_{kl},

$$\|\nabla\psi - \nabla\Pi^\varepsilon\psi\|_{L^2(T)} \le C\varepsilon\|\psi\|_{H^2(T)} \le C\varepsilon\|\psi\|_{H^2(\omega)},$$

hence

$$\begin{aligned}I^\varepsilon(\overline{\Pi^\varepsilon\psi}, U) &\le C\Big(\int_{\bigcup T_m(U)}\Big|\nabla\psi(x)\Big)\Big|^2\,dx + |U|\Big) + C\varepsilon^2\|\psi\|^2_{H^2(\omega)}\\ &\le C\Big(\int_U\Big|\nabla\psi(x)\Big)\Big|^2\,dx + |U|\Big) + C\varepsilon^2\|\psi\|^2_{H^2(\omega)}.\end{aligned}$$

We now let ε tend to 0 and obtain

$$I''(\psi, U) \le \limsup I^\varepsilon(\overline{\Pi^\varepsilon\psi}, U) \le C\Big(\int_U\Big|\nabla\psi(x)\Big)\Big|^2\,dx + |U|\Big).$$

We conclude by density of $C^\infty(\bar{\omega})$ in $H^1(\omega)$ and lower-semicontinuity of $I''(\cdot, U)$ in $L^2(\omega)$. □

Proposition 3.6 *The* Γ- lim sup *and* Γ- lim inf *are increasing set functions,* i.e.*, for all* $\psi \in L^2(\omega;\mathbb{R}^3)$ *and* $U, V \in \mathcal{O}$ *with* $U \subset V$*,*

$$I'(\psi, U) \leq I'(\psi, V) \text{ and } I''(\psi, U) \leq I''(\psi, V). \tag{10}$$

Proof. Clear. □

We next show that both Γ- lim sup and Γ- lim inf are inner regular. We begin with a technical lemma pertaining to the convergence of piecewise affine interpolates.

Lemma 3.7 *Let* $\psi \in L^2(\omega;\mathbb{R}^3)$ *such that* $\psi_{|U} \in H^1(U;\mathbb{R}^3)$ *and* $\psi^\varepsilon \in A(\varepsilon)$ *a sequence such that* $\psi^\varepsilon \to \psi$ *strongly in* $L^2(\omega;\mathbb{R}^3)$ *and* $\nabla\psi^\varepsilon$ *is bounded in* $L^2(U)$*. Then, for any smooth function* θ *with support in* U*,* $\Pi^\varepsilon(\theta\psi^\varepsilon) \to \theta\psi$ *strongly in* $L^2(\omega;\mathbb{R}^3)$*.*

Proof. It suffices to show that $\Pi^\varepsilon(\theta\psi^\varepsilon) - \theta\psi^\varepsilon$ tends to 0 in $L^2(\omega;\mathbb{R}^3)$. For ε small enough, this function is identically 0 in any triangle not included in U. We thus just need to see what happens on any triangle $t \subset U$. Let S_i, $i = 1, 2, 3$ be the vertices of this triangle and λ_i the associated barycentric coordinates. For all $x \in t$, we can write

$$\begin{aligned}\big(\Pi^\varepsilon(\theta\psi^\varepsilon) - \theta\psi^\varepsilon\big)(x) &= \sum_{i=1}^{3} \lambda_i(x)\theta(S_i)\psi^\varepsilon(S_i) - \theta(x)\psi^\varepsilon(x)\\ &= \sum_{i=1}^{3} \lambda_i(x)\big((\theta(S_i) - \theta(x))\psi^\varepsilon(S_i) + \theta(x)(\psi^\varepsilon(S_i) - \psi^\varepsilon(x)\big).\end{aligned}$$

We thus have for all $x \in t$,

$$\big|\big(\Pi^\varepsilon(\theta\psi^\varepsilon) - \theta\psi^\varepsilon\big)(x)\big|^2 \leq C\varepsilon^2\Big(\sum_{i=1}^{3} |\psi^\varepsilon(S_i)|^2 + |\nabla\psi^\varepsilon(x)|^2\Big).$$

Indeed, ψ^ε is affine on t. Now it is fairly clear that

$$\varepsilon^2\Big(\sum_{i=1}^{3} |\psi^\varepsilon(S_i)|^2 \leq C\int_t |\psi^\varepsilon(x)|^2\,dx$$

for the same reason, see [14]. Consequently,

$$\int_t \big|\big(\Pi^\varepsilon(\theta\psi^\varepsilon) - \theta\psi^\varepsilon\big)(x)\big|^2\,dx \leq C\varepsilon^2\int_t \big(|\psi^\varepsilon(x)|^2 + |\nabla\psi^\varepsilon(x)|^2\big)\,dx,$$

and the result follows by summing over all such triangles t. □

Proposition 3.8 *For all* $U \in \mathcal{O}$ *and* $\psi \in H^1(\omega;\mathbb{R}^3)$*, we have*

$$I'(\psi, U) = \sup_{U' \Subset U} I'(\psi, U') \text{ and } I''(\psi, U) = \sup_{U' \Subset U} I''(\psi, U'). \tag{11}$$

Proof. Let us take U and ψ. We treat the case of the Γ-limsup. We have already seen that the Γ-limsup is an increasing set function, so that $I''(\psi, U') \leq I''(\psi, U)$ for all open sets U' compactly included in U. We thus just need to find a sequence of open sets U' that achieves this upper bound.

Actually we will prove that for all $U' \Subset U$ and $U'' \Subset U'$, we have

$$I''(\psi, U) \leq I''(\psi, U') + I''(\psi, U \setminus \bar{U}'') \tag{12}$$

and the conclusion will follow by taking $U'_m = \{x \in U; d(x, \complement U) > 1/m\}$, $U''_m = \{x \in U; d(x, \complement U) > 2/m\}$ and by letting $m \to +\infty$ and appealing to estimate (9).

Let us thus take U' and U'' as above. There exist two sequences $\psi_1^\varepsilon, \psi_2^\varepsilon \in A(\varepsilon)$ such that $\psi_1^\varepsilon, \psi_2^\varepsilon \to \psi$ in $L^2(\omega; \mathbb{R}^3)$ strong, and

$$I^\varepsilon(\psi_1^\varepsilon, U') \to I''(\psi, U') \text{ and } I^\varepsilon(\psi_2^\varepsilon, U \setminus \bar{U}'') \to I''(\psi, U \setminus \bar{U}''). \tag{13}$$

By Lemma 3.4, we may assume that no bond has deformed length smaller than $\varepsilon\alpha$ by both sequences so that $\overline{\psi_1^\varepsilon} = \psi_1^\varepsilon$ and $\overline{\psi_2^\varepsilon} = \psi_2^\varepsilon$.

We need to patch the two sequences together by a slicing argument. The standard slicing argument involves a number of slices that goes to infinity. We use here a variant thereof introduced in [12] that only involves a small fixed number of slices. For $s \geq 0$, let $U'_s = \{x \in U'; d(x, \complement U') > s\}$. The open slices will be sets of the form $U'_{is} \setminus \bar{U}'_{(i+1)s}$, $i = 0, 1, \ldots, 4$. We take $s > 0$ small enough so that the five slices are all compactly included in $U' \setminus \bar{U}''$.

Let us take a smooth cut-off function θ_s such that $\theta_s = 1$ on U'_{3s}, $\theta_s = 0$ on $\omega \setminus U'_{2s}$, $|\nabla\theta_s| \leq \frac{C}{s}$. We define

$$\psi_s^\varepsilon = \overline{\Pi^\varepsilon\big(\theta_s\psi_1^\varepsilon + (1-\theta_s)\psi_2^\varepsilon\big)}.$$

By construction, $\psi_s^\varepsilon \in A(\varepsilon)$ is such that $\psi_s^\varepsilon \to \psi$ in $L^2(\omega; \mathbb{R}^3)$ strong when $\varepsilon \to 0$ by Lemmas 3.4 and 3.7, and no bond has deformed length smaller than $\varepsilon\alpha$.

The energy of ψ_s^ε in U takes into account the bonds attached to triangles t_{kl} of the main Delaunay triangulation that are included in U and the angles attached to triangles t_{kl} of both Delaunay triangulations also included in U. If such a triangle intersects the closure of one slice, *i.e.*, $t_{kl} \cap \big(\bar{U}'_{is} \setminus U'_{(i+1)s}\big) \neq \emptyset$, we claim that t_{kl} intersects at most three slices for ε small enough (indeed, in the sequel, we will let $\varepsilon \to 0$ first). Let $x_0 \in t_{kl} \cap \big(\bar{U}'_{is} \setminus U'_{(i+1)s}\big)$. Let us take $\varepsilon < \frac{s}{\sqrt{3}}$. Since $\operatorname{diam} t_{kl} = \sqrt{3}\varepsilon$, for any $x \in t_{kl}$, we have

$$d(x, \complement U') \leq d(x, x_0) + d(x_0, \complement U') \leq \sqrt{3}\varepsilon + (i+1)s < (i+2)s.$$

Therefore, $x \notin U'_{(i+2)s}$. Similarly, for any $x \in t_{kl}$,

$$d(x, \complement U') \geq d(x_0, \complement U') - d(x, x_0) \geq is - \sqrt{3}\varepsilon > (i-1)s.$$

Therefore, $x \notin U'_{(i-2)s} \setminus \bar{U}'_{(i-1)s}$. It follows that t_{kl} intersects at most the slices $U'_{js} \setminus \bar{U}'_{(j+1)s}$ for $j = i-1, i$ and $i+1$.

There are three possible cases for any given triangle t_{kl}:

Case 1: $t_{kl} \subset U'_{3s}$. In this case, $\psi_s^\varepsilon = \psi_1^\varepsilon$ on t_{kl}, since $\overline{\psi_1^\varepsilon} = \psi_1^\varepsilon$, and the corresponding terms add up to $I^\varepsilon(\psi_1^\varepsilon, U'_{3s})$. We note that $I^\varepsilon(\psi_1^\varepsilon, U'_{3s}) \le I^\varepsilon(\psi_1^\varepsilon, U')$.

Case 2: $t_{kl} \subset U \setminus \bar{U}'_{2s}$. In this case, for the same reason, $\psi_s^\varepsilon = \psi_2^\varepsilon$ on t_{kl} and the corresponding terms add up to $I^\varepsilon(\psi_2^\varepsilon, U \setminus \bar{U}'_{2s})$. We note that $I^\varepsilon(\psi_2^\varepsilon, U \setminus \bar{U}'_{2s}) \le I^\varepsilon(\psi_2^\varepsilon, U \setminus \bar{U}'')$.

Case 3: $t_{kl} \cap \big(\bar{U}'_{2s} \setminus U'_{3s}\big) \neq \emptyset$. By the remark above, the sum of all terms corresponding to this case is smaller than $I^\varepsilon(\psi_s^\varepsilon, U'_s \setminus \bar{U}'_{4s})$.

We thus see that

$$I^\varepsilon(\psi_s^\varepsilon, U) \le I^\varepsilon(\psi_1^\varepsilon, U') + I^\varepsilon(\psi_2^\varepsilon, U \setminus \bar{U}'') + I^\varepsilon(\psi_s^\varepsilon, U'_s \setminus \bar{U}'_{4s}).$$

As in the proof of Proposition 3.5, we have

$$I^\varepsilon(\psi_s^\varepsilon, U'_s \setminus \bar{U}'_{4s}) \le C \int_{T_s^\varepsilon} \Big(\Big| \nabla \big(\Pi^\varepsilon \big(\theta_s \psi_1^\varepsilon + (1-\theta_s)\psi_2^\varepsilon \big) \big) \Big|^2 + 1 \Big)\, dx,$$

where T_s^ε denotes the union of triangles t_{kl} included in $U'_s \setminus \bar{U}'_{4s}$.

Now it follows from the same argument as in Lemma 4.4 of [14] with a slightly different piecewise affine Lagrange interpolation that

$$\begin{aligned} \int_{T_s^\varepsilon} \Big| \nabla \Big(\Pi^\varepsilon \big(\theta_s \psi_1^\varepsilon + (1-\theta_s)\psi_2^\varepsilon \big) \Big) \Big|^2 \, dx & \\ &= \int_{T_s^\varepsilon} \Big| \nabla \Big(\psi_2^\varepsilon + \Pi^\varepsilon \big(\theta_s (\psi_1^\varepsilon - \psi_2^\varepsilon) \big) \Big) \Big|^2 \, dx \\ &\le C \int_{U'_s \setminus \bar{U}'_{4s}} \Big(|\nabla \psi_1^\varepsilon|^2 + |\nabla \psi_2^\varepsilon|^2 + \frac{1}{s^2} |\psi_1^\varepsilon - \psi_2^\varepsilon|^2 \Big) \mathbf{1}_{T_s^\varepsilon} \, dx. \end{aligned}$$

We first let $\varepsilon \to 0$. The sequence $\big(|\nabla \psi_1^\varepsilon|^2 + |\nabla \psi_2^\varepsilon|^2 + 1 \big) \mathbf{1}_{T_s^\varepsilon}$ is bounded in $L^1(U' \setminus \bar{U}'')$, by coercivity of Lemma 3.2. Therefore, up to a further subsequence, it weakly-$*$ converges to a finite Radon measure ν on $U' \setminus \bar{U}''$, and we have

$$\begin{aligned} \limsup_{\varepsilon \to 0} \int_{U'_s \setminus \bar{U}'_{4s}} & \big(|\nabla \psi_1^\varepsilon|^2 + |\nabla \psi_2^\varepsilon|^2 + 1 \big) \mathbf{1}_{T_s^\varepsilon} \, dx \\ & \le \nu\big(\overline{U'_s \setminus \bar{U}'_{4s}} \big) = \nu\big(\overline{U'_s} \setminus U'_{4s} \big) \le \nu(U' \setminus U'_{4s}). \end{aligned}$$

Therefore, since

$$\int_{U'_s \setminus \bar{U}'_{4s}} |\psi_1^\varepsilon - \psi_2^\varepsilon|^2 \mathbf{1}_{T_s^\varepsilon} \, dx \le \int_{U'_s \setminus \bar{U}'_{4s}} |\psi_1^\varepsilon - \psi_2^\varepsilon|^2 \, dx \to 0$$

when $\varepsilon \to 0$, it follows that

$$I''(\psi, U) \le \limsup_{\varepsilon \to 0} I^\varepsilon(\psi_s^\varepsilon, U) \le I''(\psi, U') + I''(\psi, U \setminus \bar{U}'') + C\nu(U' \setminus U'_{4s}).$$

We now take a decreasing sequence $s \to 0$ and obtain estimate (12).

The argument is exactly the same for the Γ-liminf. □

At this point, we can extract a subsequence, still denoted ε such that $I^\varepsilon(\cdot, U)$ is Γ-convergent for all open sets $U \in \mathcal{O}$ and all $\psi \in H^1(\omega; \mathbb{R}^3)$, by appealing to Theorem 10.3 of [5], *i.e.*,

$$I'(\psi, U) = I''(\psi, U) = I(\psi, U).$$

Let us now show that the Γ-limit I is superadditive.

Proposition 3.9 *Let $U, V \in \mathcal{O}$ be such that $U \cap V = \emptyset$. For all $\psi \in L^2(\omega; \mathbb{R}^3)$, we have*

$$I(\psi, U \cup V) \geq I(\psi, U) + I(\psi, V). \tag{14}$$

Proof. Indeed, for any ψ^ε we clearly have $I^\varepsilon(\psi^\varepsilon, U \cup V) \geq I^\varepsilon(\psi^\varepsilon, U) + I^\varepsilon(\psi^\varepsilon, V)$, hence the result by passing to the inferior limit. □

We now turn to subadditivity.

Proposition 3.10 *Let $U, V \in \mathcal{O}$. For all $\psi \in L^2(\omega; \mathbb{R}^3)$, we have*

$$I(\psi, U \cup V) \leq I(\psi, U) + I(\psi, V). \tag{15}$$

Proof. It suffices to consider the case when $I(\psi, U) < +\infty$ and $I(\psi, V) < +\infty$. By the inner regularity of Proposition 3.8, it is also enough to prove that

$$I(\psi, U' \cup V') \leq I(\psi, U) + I(\psi, V),$$

for all $U' \Subset U$ and $V' \Subset V$. Again, there exist two sequences $\psi_1^\varepsilon, \psi_2^\varepsilon \in A(\varepsilon)$ both converging to ψ in $L^2(\omega; \mathbb{R}^3)$ strong and

$$I^\varepsilon(\psi_1^\varepsilon, U) \to I(\psi, U) \text{ and } I^\varepsilon(\psi_2^\varepsilon, V) \to I(\psi, V).$$

Again by Lemma 3.4, we may assume that no bond has deformed length smaller than $\varepsilon\alpha$ by both sequences.

The argument is basically the same as in Proposition 3.8 and we just sketch it, see also [2]. We define slices in U' and associated cut-off functions θ_s which are loosely speaking equal to 1 inside the innermost slice and to 0 on $V \setminus U'$. As before, we set

$$\psi_s^\varepsilon = \overline{\Pi^\varepsilon\big(\theta_s \psi_1^\varepsilon + (1 - \theta_s)\psi_2^\varepsilon\big)}.$$

and check that the slicing argument proceeds to its end. □

We can now apply the De Giorgi-Letta criterion, see Theorem 10.2 in [5].

Proposition 3.11 *For all $\psi \in H^1(\omega; \mathbb{R}^3)$, the mapping $U \mapsto I(\psi, U)$ is the restriction of a Borel measure to $\mathcal{O}$.*

Proof. Indeed, this set function is increasing, subadditive by Proposition 3.10, superadditive by Proposition 3.9, and inner regular by Proposition 3.8. □

In view of applying Buttazzo-Dal Maso's representation theorem, we still need one ingredient.

Proposition 3.12 *Let $\psi_1, \psi_2 \in H^1(\omega;\mathbb{R}^3)$. If $\psi_1 = \psi_2$ on $U \in \mathcal{O}$, then we have*

$$I(\psi_1, U) = I(\psi_2, U). \tag{16}$$

Proof. By inner regularity, it is enough to consider the case $U \Subset \omega$. Let us thus be given two sequences ψ_1^ε and ψ_2^ε in $A(\varepsilon)$, with $\psi_\alpha^\varepsilon \to \psi_\alpha$, $\alpha = 1, 2$, strongly in $L^2(\omega;\mathbb{R}^3)$ and

$$I^\varepsilon(\psi_1^\varepsilon, U) \to I(\psi_1, U) \text{ and } I^\varepsilon(\psi_2^\varepsilon, U) \to I(\psi_2, U).$$

We use again the same slicing argument. Let $U' \Subset U$ and place slices between U' and U with associated cut-off functions θ_s. As before, we set

$$\psi_s^\varepsilon = \overline{\Pi^\varepsilon\big(\theta_s\psi_1^\varepsilon + (1-\theta_s)\psi_2^\varepsilon\big)}.$$

Since $\psi_1 = \psi_2$ in ω, we have $\psi_s^\varepsilon \to \psi_2$ strongly in $L^2(\omega;\mathbb{R}^3)$ by Lemmas 3.4 and 3.7 again, so that

$$I(\psi_2, U) \le \liminf_{\varepsilon\to 0} I^\varepsilon(\psi_s^\varepsilon, U).$$

On the other hand,

$$I^\varepsilon(\psi_s^\varepsilon, U) \le I^\varepsilon(\psi_1^\varepsilon, U') + D^\varepsilon \le I^\varepsilon(\psi_1^\varepsilon, U) + D^\varepsilon,$$

and the usual slicing argument shows that the inferior limit of the remainder terms D^ε can be made as small as we want. Therefore,

$$I(\psi_2, U) \le I(\psi_1, U),$$

from which the conclusion follows. □

Proposition 3.13 *There exists a Carathéodory function $W : \omega\times M_{3,2} \to \mathbb{R}$ bounded below, satisfying $W(x,F) \le C(1+|F|^2)$, such that*

$$I(\psi, U) = \int_U W(x, \nabla\psi(x))\,dx \tag{17}$$

for all $\psi \in H^1(\omega;\mathbb{R}^3)$ and $U \in \mathcal{O}$.

Proof. We apply the first part of Buttazzo-Dal Maso's integral representation theorem 3.1. We have seen that conditions i), ii) and iii) are satisfied. Condition iv) obviously holds true. Condition v) is also quite clear since if $\psi^m \rightharpoonup \psi$ weakly in $H^1(\omega;\mathbb{R}^3)$, then $\psi^m \to \psi$ strongly in $L^2(\omega;\mathbb{R}^3)$, and the sequential lower semicontinuity follows from the general properties of Γ-convergence. □

Proposition 3.14 *The function W is independent of x.*

Proof. We apply the last part of Buttazzo-Dal Maso's theorem, namely condition v). Let us be given $\rho > 0$ and x_1, x_2 such that $B(x_i, \rho) \subset \omega$, $i = 1, 2$. Let us take any gradient g and let $\psi(x) = gx$. We thus have a sequence $\psi_2^\varepsilon \in A(\varepsilon)$ such that $\psi_2^\varepsilon \to \psi$ strongly in $L^2(\omega; \mathbb{R}^3)$ and $I^\varepsilon(\psi_2^\varepsilon, B(x_2, \rho)) \to I(\psi, B(x_2, \rho))$. Let T_2^ε denote the set of full triangles included in $B(x_2, \rho)$. We look for the same pattern of triangles that has the maximum number of triangles included in $B(x_1, \rho)$. This is possible since there is only a finite number of such patterns. We let T_1^ε denote the corresponding set of translated triangles, by a vector τ^ε.

We now set $\psi_1^\varepsilon(x) = \psi_2^\varepsilon(x - \tau^\varepsilon)$ at all nodes of T_1^ε, and $\psi_1^\varepsilon(x) = g(x - \tau^\varepsilon)$ at all other nodes. It is fairly clear that $\psi_1^\varepsilon \to \psi - g(x_1 - x_2)$ strongly in $L^2(\omega; \mathbb{R}^3)$ and that $I^\varepsilon(\psi_1^\varepsilon, B(x_1, \rho)) \to I(\psi, B(x_2, \rho))$. Therefore $I(\psi - a, B(x_1, \rho)) \le I(\psi, B(x_2, \rho))$ with $a = g(x_1 - x_2)$, and we conclude by condition iv). □

4 Convergence with boundary conditions and identification of the limit energy

The next step in the proof consists in showing that the limit energy density is not modified when we add a boundary condition of place on $\partial\omega$ defined by a function φ_0 according to equation (1). We define the corresponding energy $I_{\mathrm{bc}}^\varepsilon$ on $L^2(\omega; \mathbb{R}^3)$ by

$$I_{\mathrm{bc}}^\varepsilon(\psi) = \begin{cases} I^\varepsilon(\psi, \bar{\omega}) & \text{if } \psi - \Pi^\varepsilon \varphi_0 \in H_0^1(\omega; \mathbb{R}^3), \\ +\infty & \text{otherwise.} \end{cases}$$

Thus $I_{\mathrm{bc}}^\varepsilon(\psi)$ is finite if and only if ψ is piecewise affine on the main Delaunay triangulation, satisfies the boundary condition of place at the boundary nodes and has no bond of zero deformed length.

Proposition 4.1 *Assume that $\varphi_0 \in H^2(\omega; \mathbb{R}^3)$. Let $\varepsilon \to 0$ be a sequence such that $I^\varepsilon(\cdot, \omega)$ is Γ-convergent. Then $I_{\mathrm{bc}}^\varepsilon$ is Γ-convergent to the functional*

$$I_{\mathrm{bc}}(\psi) = \begin{cases} \int_\omega W(\nabla\psi)\, dx & \text{if } \psi - \varphi_0 \in H_0^1(\omega; \mathbb{R}^3), \\ +\infty & \text{otherwise.} \end{cases} \tag{18}$$

Proof. Since φ_0 belongs to $H^2(\omega; \mathbb{R}^3)$ and the sequence of main Delaunay triangulations is regular in the sense of finite element theory, we have that $\Pi^\varepsilon \varphi_0 \to \varphi_0$ strongly in $H^1(\omega; \mathbb{R}^3)$. It follows that $\gamma\big(\Pi^\varepsilon \varphi_0\big) \to \gamma(\varphi_0)$ strongly in $H^{1/2}(\partial\omega; \mathbb{R}^3)$, where γ denotes the trace mapping.

Let I'_{bc} and I''_{bc} denote the Γ-liminf and Γ-limsup of the sequence $I_{\mathrm{bc}}^\varepsilon$. Let us first note that $I(\cdot, \omega) \le I'_{\mathrm{bc}}$ since $I^\varepsilon(\psi, \omega) \le I_{\mathrm{bc}}^\varepsilon(\psi)$ for all ψ.

We now need to show that $I'_{\mathrm{bc}}(\psi) = +\infty$ for all ψ such that $\psi - \varphi_0 \notin H_0^1(\omega)$ and that $I''_{\mathrm{bc}}(\psi) \le I(\psi, \omega)$ for all ψ such that $\psi - \varphi_0 \in H_0^1(\omega)$.

If we assume that $I'_{\mathrm{bc}}(\psi) < +\infty$, then there exists a sequence ψ^ε such that $\psi^\varepsilon \to \psi$ in $L^2(\omega;\mathbb{R}^3)$ and $I^\varepsilon_{\mathrm{bc}}(\psi^\varepsilon) \leq C < +\infty$ for some C. By Lemma 3.2, it follows that $\nabla\psi^\varepsilon$ is bounded in $L^2(\omega; M_{3,2})$, thus that $\psi \in H^1(\omega;\mathbb{R}^3)$ and $\psi^\varepsilon \rightharpoonup \psi$ weakly in $H^1(\omega;\mathbb{R}^3)$. Consequently, $\gamma(\psi^\varepsilon) \rightharpoonup \gamma(\psi)$ weakly in $H^{1/2}(\partial\omega;\mathbb{R}^3)$. Since $\gamma(\psi^\varepsilon) = \Pi^\varepsilon\varphi_{0|\partial\omega}$, it follows that $\psi - \varphi_0 \in H^1_0(\omega;\mathbb{R}^3)$.

Let us thus turn to the upper bound for the Γ-limsup when $\psi - \varphi_0 \in H^1_0(\omega;\mathbb{R}^3)$. We first consider the case when $\psi \in H^2(\omega;\mathbb{R}^3)$. Then, by the same token as for φ_0, $\Pi^\varepsilon\psi \to \psi$ in $H^1(\omega;\mathbb{R}^3)$, and since the boundary values of the interpolate only depend on the values it takes on the type 1 nodes of $\partial\omega$, $\Pi^\varepsilon\psi$ satisfies the discrete boundary condition as well.

Let ψ^ε be a sequence such that $\psi^\varepsilon \to \psi$ in $L^2(\omega;\mathbb{R}^3)$ and $I^\varepsilon(\psi^\varepsilon,\omega) \to I(\psi,\omega)$. As always, we can assume that $\overline{\psi^\varepsilon} = \psi^\varepsilon$. We use again the slicing argument variant. For $s > 0$ small enough, let $\omega_s = \{x \in \omega;\, d(x, \complement\omega) > s\}$ and θ_s be a smooth cut-off function such that $\theta_s = 1$ on ω_{4s}, $\theta_s = 0$ on $\omega \setminus \omega_{3s}$, $|\nabla\theta_s| \leq \frac{C}{s}$.

We define

$$\psi^\varepsilon_s = \overline{\Pi^\varepsilon\big(\theta_s\psi^\varepsilon + (1-\theta_s)\psi\big)}.$$

Because θ_s is smooth, we have $\psi^\varepsilon_s \to \psi$ in $L^2(\omega;\mathbb{R}^3)$, by Lemmas 3.4 and 3.7 for the first term and due to the fact that $\psi \in H^2(\omega;\mathbb{R}^3)$ for the second term. Moreover, for ε small enough, we have $\psi^\varepsilon_s = \overline{\Pi^\varepsilon\psi}$ in $\omega \setminus \omega_{2s}$. The boundary nodes are all type 1 nodes, thus the modifications of Lemma 3.4 have no effect on the boundary values and ψ^ε_s satisfies the discrete boundary condition of place. Similarly, for ε small enough, we have $\psi^\varepsilon_s = \psi^\varepsilon$ on ω_{5s}.

In terms of energies, we have

$$\begin{aligned} I^\varepsilon(\psi^\varepsilon_s,\bar\omega) &\leq I^\varepsilon(\psi^\varepsilon_s,\omega_{5s}) + I^\varepsilon(\psi^\varepsilon_s,\omega_s \setminus \overline{\omega_{6s}}) + I^\varepsilon(\psi^\varepsilon_s,\bar\omega \setminus \overline{\omega_{2s}}) \\ &= I^\varepsilon(\psi^\varepsilon,\omega_{5s}) + I^\varepsilon(\psi^\varepsilon_s,\omega_s \setminus \overline{\omega_{6s}}) + I^\varepsilon(\overline{\Pi^\varepsilon\psi},\bar\omega \setminus \overline{\omega_{2s}}), \end{aligned}$$

the overlap between the three slices being there to ensure that all contributions to the energy, either bonds or angles, are counted at least once in the right-hand side. Note that the term $I^\varepsilon(\psi^\varepsilon_s,\bar\omega\setminus\overline{\omega_{2s}})$ includes the contribution of the bonds and angles up to $\partial\omega$.

Let us consider each term separately. First of all,

$$I''_{\mathrm{bc}}(\psi) \leq \limsup_{\varepsilon\to 0} I^\varepsilon(\psi^\varepsilon_s,\omega).$$

Secondly,

$$I^\varepsilon(\psi^\varepsilon,\omega_{5s}) \leq I^\varepsilon(\psi^\varepsilon,\omega) \to I(\psi,\omega) \text{ when } \varepsilon \to 0.$$

Thirdly,

$$I^\varepsilon(\overline{\Pi^\varepsilon\psi},\bar\omega\setminus\overline{\omega_{2s}}) \leq C\int_{\omega\setminus\overline{\omega_{2s}}} \big(\big|\nabla\big(\Pi^\varepsilon\psi\big)\big|^2 + 1\big)\,dx \to C\int_{\omega\setminus\overline{\omega_{2s}}} \big(|\nabla\psi|^2+1\big)\,dx,$$

when $\varepsilon \to 0$ by classical finite element error estimates, since $\psi \in H^2(\omega;\mathbb{R}^3)$. Therefore

$$\limsup_{\varepsilon\to 0} I^\varepsilon(\overline{\Pi^\varepsilon\psi},\bar\omega\setminus\overline{\omega_{2s}}) \leq C\mu(\omega\setminus\omega_{6s}),$$

where μ is the finite measure $\mu(A) = \int_A (|\nabla\psi|^2 + 1)\,dx$.

We argue as before for the last term. Indeed, we have

$$I^\varepsilon(\psi_s^\varepsilon, \omega_s \setminus \overline{\omega_{6s}}) \le C \int_{\omega_s \setminus \overline{\omega_{6s}}} \left(|\nabla\psi^\varepsilon|^2 + |\nabla\psi|^2 + 1\right) dx + \frac{C}{s^2} \int_{\omega_s \setminus \overline{\omega_{6s}}} |\psi^\varepsilon - \psi|^2\,dx.$$

The last term in the right-hand side tends to 0 when $\varepsilon \to 0$. The sequence $|\nabla\psi^\varepsilon|^2$ is bounded in $L^1(\omega)$, by coercivity of Lemma 3.2. Therefore, up to a further subsequence, it weakly-$*$ converges to a finite Radon measure ν, and we have

$$\limsup_{\varepsilon\to 0} \int_{\omega_s \setminus \overline{\omega_{6s}}} |\nabla\psi^\varepsilon|^2\,dx \le \nu\big(\overline{\omega_s \setminus \overline{\omega_{6s}}}\big) = \nu\big(\overline{\omega_s} \setminus \omega_{6s}\big) \le \nu(\omega \setminus \omega_{6s}).$$

Finally, putting the above estimates together, we obtain

$$I''_{\rm bc}(\psi) \le I(\psi, \omega) + C\mu(\omega \setminus \omega_{6s}) + \nu(\omega \setminus \omega_{6s}),$$

and the result follows for $\psi \in H^2(\omega; \mathbb{R}^3)$ by letting $s \to 0$.

To conclude the proof for a general $\psi \in H^1(\omega; \mathbb{R}^3)$, we note that since $\psi - \varphi_0 \in H^1_0(\omega; \mathbb{R}^3)$, there exists a sequence $\phi_m \in \mathcal{D}(\omega; \mathbb{R}^3)$ such that $\varphi_0 + \phi_m \to \psi$ in $H^1(\omega; \mathbb{R}^3)$. Moreover, $\varphi_0 + \phi_m \in H^2(\omega; \mathbb{R}^3)$ and satisfies the boundary condition of place. Thus

$$I''_{\rm bc}(\varphi_0 + \phi_m) \le I(\varphi_0 + \phi_m, \omega) = \int_\omega W(\nabla(\varphi_0 + \phi_m))\,dx.$$

The left-hand side is strongly $L^2(\omega; \mathbb{R}^3)$ lower semicontinuous and the right-hand side is strongly $H^1(\omega; \mathbb{R}^3)$ continuous, so that passing to the limit when $m \to +\infty$, we obtain

$$I''_{\rm bc}(\psi) \le \int_\omega W(\nabla\psi)\,dx = I(\psi, \omega),$$

and the Proposition is proved. □

It is now a simple matter to add the force terms. Let us set $J^\varepsilon : L^2(\omega; \mathbb{R}^3) \to \bar{\mathbb{R}}$,

$$J^\varepsilon(\psi) = I^\varepsilon_{\rm bc}(\psi) - F^\varepsilon(\psi),$$

in the sense that if $\psi \notin A(\varepsilon)$, the second term, which may be undefined, does not count anyway.

Proposition 4.2 *Under the above hypotheses, there exists a sequence $\varepsilon \to 0$ such that the sequence J^ε is Γ-convergent for the strong topology of $L^2(\omega; \mathbb{R}^3)$ and its Γ-limit is given by*

$$J(\psi) = \begin{cases} \int_\omega W(\nabla\psi)\,dx - \frac{4}{3\sqrt{3}} \int_\omega f \cdot \psi\,dx & \text{if } \psi - \varphi_0 \in H^1_0(\omega; \mathbb{R}^3), \\ +\infty & \text{otherwise.} \end{cases} \tag{19}$$

Moreover, the minimizers of J^ε remain in a compact subset of $L^2(\omega; \mathbb{R}^3)$, any limit point of a sequence of minimizers is a minimizer of J and we have

$$\inf_{\psi \in L^2(\omega;\mathbb{R}^3)} J^\varepsilon(\psi) \longrightarrow \inf_{\psi \in L^2(\omega;\mathbb{R}^3)} J(\psi) \text{ when } \varepsilon \to 0. \tag{20}$$

Proof. If a sequence $\psi^\varepsilon \to \psi$ is such that $J^\varepsilon(\psi^\varepsilon) \le C < +\infty$, it follows that ψ^ε is bounded in $H^1(\omega;\mathbb{R}^3)$. The same kind of arguments as those used in the proof of Lemma 3.7 can be used to show that

$$F^\varepsilon(\psi^\varepsilon) \to \frac{4}{3\sqrt{3}} \int_\omega f \cdot \psi \, dx,$$

from which the Γ-convergence result follows.

Of course, we have

$$\inf_{\psi \in L^2(\omega;\mathbb{R}^3)} J^\varepsilon(\psi) \le J^\varepsilon(\overline{\Pi^\varepsilon \varphi_0}) \le C,$$

so that the minimizers are relatively compact in $L^2(\omega;\mathbb{R}^3)$. The convergence of minimizers and minima is then a standard feature of Γ-convergence. □

Let us identify the limit energy density W. For any nonzero integer k, let $A(kY)$ denote the set of continuous piecewise affine functions on the main Delaunay triangulation defined on kY and corresponding to $\varepsilon = 1$. Then for all $\psi \in A(kY)$, we set

$$I_k(\psi) = I^1(\psi, \overline{kY}).$$

Note that I_k includes the contributions of the bonds attached to the boundary of kY and of the angles with vertices on the boundary.

Proposition 4.3 *For all Γ-convergent subsequences and all $g \in M_{3,2}$,*

$$W(g) = \frac{1}{|Y|} \inf_{k \in \mathbb{N}^*} \Big\{ \frac{1}{k^2} \inf_{\substack{\psi \in A(kY) \\ \psi = gx \text{ on } \partial(kY)}} I_k(\psi) \Big\}. \tag{21}$$

Proof. Let us set

$$W_k(g) = \frac{1}{k^2|Y|} \inf_{\substack{\psi \in A(kY) \\ \psi = gx \text{ on } \partial(kY)}} I_k(\psi).$$

We claim that the sequence $W_k(g)$ converges to a limit when $k \to +\infty$, and that this limit is given by $\inf_n W_n(g)$. In order to prove this, we introduce a slightly different energy

$$I_{k,\sharp}(\psi) = \sum_j \big(B_j^1(\psi) + R_j^1(\psi)\big) + \sum_{j,l} M_{jl}^1(\psi) + \sum_l M_{l,\sharp}^1(\psi),$$

where the first three sums are extended over all the bonds in $\overline{kY}$ and angles with three nodes in $\overline{kY}$. The extra terms $M_{l,\sharp}^1(\psi)$ are defined as follows. We add k extra phantom type 2 nodes to the right side of kY and k extra phantom type 2 nodes to the top of kY, see Figure 7, and we extend ψ to these nodes into a function $\psi_\sharp$ such that $x \mapsto \psi_\sharp(x) - gx$ is Y-periodic.

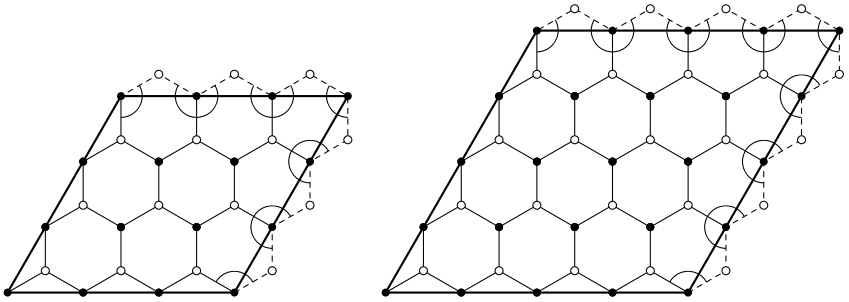

Figure 7: The cells $3Y$ and $4Y$ with added phantom nodes and angles.

Each phantom node gives rise to two extra moment energy terms, $M^1_{l,\sharp}(\psi)$, except for the rightmost node with only one extra moment term, see Figure 7. There is thus a total number of $4k-1$ extra terms in the extended energy.

We now let

$$W_{k,\sharp}(g) = \frac{1}{k^2|Y|} \inf_{\substack{\psi \in A(kY) \\ \psi = gx \text{ on } \partial kY}} I_{k,\sharp}(\psi).$$

This sequence is decreasing for the divisibility order. Indeed, if $k \mid k'$, the periodic repetition of a minimizer for $I_{k,\sharp}$ is a competing function for $I_{k',\sharp}$ (this is the reason for introducing the phantom nodes in the first place). It follows that $W_{k,\sharp}(g) \to \inf_m W_{m,\sharp}(g)$ when $k \to +\infty$.

Now we have for all k and ψ,

$$I_k(\psi) \le I_{k,\sharp}(\psi) = I_k(\psi) + \sum_l M^1_{l,\sharp}(\psi) \le I_k(\psi) + Ck,$$

so that

$$W_k(g) \le W_{k,\sharp}(g) \le W_k(g) + \frac{C}{k},$$

for all g and k. Consequently, $W_k(g) \to \inf_m W_m(g)$.

We now proceed as in [2]. Recall that $\varepsilon = L/n$, $n \ge 1$. Let n' be a sequence such that $I^{\varepsilon'}$ is Γ-convergent, with $\varepsilon' = L/n'$. Since W has quadratic growth and the Γ-limit is weakly lower-semicontinuous on $H^1(\omega;\mathbb{R}^3)$, it follows that W is quasiconvex. In particular,

$$W(g) = \frac{1}{|\omega|} \inf_{\varphi - gx \in H^1_0(\omega;\mathbb{R}^3)} \int_\omega W(\nabla\varphi)\,dx.$$

By Proposition 4.2, we have

$$\inf_{\varphi - gx \in H^1_0(\omega;\mathbb{R}^3)} \int_\omega W(\nabla\varphi)\,dx = \lim_{n' \to +\infty} \Big(\inf_{\psi = gx \text{ on } \partial\omega} I^{\varepsilon'}(\psi) \Big).$$

The change of variables $y = n'x/L$ sends ω onto $n'Y$ and if we define $\widetilde{\psi}(y) = \frac{n'}{L}\psi\big(\frac{Ly}{n'}\big)$, then we have $\widetilde{\psi} = gy$ on $\partial(n'Y)$ and

$$I^{\varepsilon'}(\psi) = \frac{L^2}{(n')^2} I_{n'}(\widetilde{\psi}).$$

It follows from the previous considerations that

$$W(g) = \lim_{n' \to +\infty} W_{n'}(g),$$

and the right-hand side is a subsequence of the total convergent sequence $W_k(g)$.□

Corollary 4.4 *The whole sequence of Proposition 4.2 is* Γ*-convergent.*

Proof. Indeed, Proposition 4.3 shows that the limit of all Γ-convergent subsequences is unique. □

The limit homogenized energy density has symmetry properties.

Proposition 4.5 *The limit energy density W is frame-indifferent and its material symmetry group contains the circular group C_6.*

Proof. See [14]. Actually, as in the previous reference, W is furthermore D_6 right-invariant. □

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