A REBO-potential-based model for graphene bending by $\Gamma$-convergence

Cesare Davini$^1$  Antonino Favata$^2$  Roberto Paroni$^3$

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$^1$ Via Parenzo 17, 33100 Udine
cesare.davini@uniud.it

$^2$ Department of Structural and Geotechnical Engineering
Sapienza University of Rome, Rome, Italy
antonino.favata@uniroma1.it

$^3$ DADU
University of Sassari, Alghero (SS), Italy
paroni@uniss.it

Abstract

An atomistic to continuum model for a graphene sheet undergoing bending is presented. Under the assumption that the atomic interactions are governed by a harmonic approximation of the 2nd-generation Brenner REBO (reactive empirical bond-order) potential, involving first, second and third nearest neighbors of any given atom, we determine the variational limit of the energy functionals. It turns out that the $\Gamma$-limit depends on the linearized mean and Gaussian curvatures. If some specific contributions in the atomic interaction are neglected, the variational limit is non-local.

Keywords: Graphene bending, Homogenization, $\Gamma$-convergence, Non-locality

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1 Introduction

Graphene is a two-dimensional carbon allotrope, in the form of a hexagonal lattice whose vertices are occupied by C atoms. It has recently attracted a huge interest of the scientific community, due to its extraordinary mechanical, electrical and thermal conductivity properties [1], that make graphene a candidate for a great variety of technological applications; actually, its potentialities, and those of graphene-based materials, are far from being fully understood, and many studies are carried out in order to develop new technological applications [13]. In particular, understanding the bending behavior of graphene represents a challenge of significant interest because of possible applications in the field of flexible devices.

For the modeling of graphene many different approaches at different scales can be found in the literature, ranging from first principle calculations [14, 18], atomistic calculations [28, 29, 21] and continuum mechanics [27, 6, 19, 23, 22, 25, 24]; furthermore, mixed atomistic formulations with finite elements have been reported for graphene [3, 4]. Both in-plane and bending deformations have been studied in [19] and the out-of-plane bending behavior has been investigated in [23, 22] with the use a special equivalent atomistic-continuum model. In [30], the elastic properties of graphene have been theoretically predicted on taking into account internal lattice relaxation. In [6], by combining continuum elasticity theory and tight-binding atomistic simulations, a constitutive nonlinear stress-strain relation for graphene stretching has been proposed. Atomistic simulations have been employed to investigate the elastic properties of graphene in [21]. Based on the experiments performed in [17], the nonlinear in-plane elastic properties of graphene have been calculated in [26] by means of DFT. A continuum theory of a free-standing graphene monolayer, viewed as a two dimensional 2-lattice, has been proposed in [25, 24], where the shift vector which connects the two simple lattices is considered as an auxiliary variable.

When a continuum picture is pursued, the key point of modeling relies in the connection between the atomistic and the gross description. Frequently, the target continuum model is postulated and that connection is established through a suitable choice of constitutive and geometric parameters.

In this paper, the connection is set within the general framework of homogenization theory. For the case of the out-of-plane deformations of graphene, we determine the variational limit—in the sense of $\Gamma$-convergence—of the discrete energy functionals under a topology that guarantees the convergence of minimizers. Thus, the limit functional describes a continuous two-dimensional medium fully accounting for the bending behavior of a graphene sheet.

Homogenization of graphene has already been studied in [15, 16, 7]. In these works the membranal equations have been deduced, non-linear in [15, 16] and linearized in [7]; moreover, interactions up to the second neighbor have been taken into account.
Our description of the atomic-scale interaction is based on the discrete mechanical model proposed in [10] and exploited in [12, 11, 2, 9, 8], where the results are also obtained for the 2nd-generation Brenner REBO (reactive empirical bond-order) potential, which is largely used in Molecular Dynamics simulations for carbon allotropes. Here, we recall the most relevant features:

(i) interatomic bonds involve first, second and third nearest neighbors of any given atom. In particular, the kinematical variables we consider are bond lengths, bond angles, and dihedral angles; from [5] it results that these latter are of two kinds, that we here term C and Z, as described in Sec. 2.

(ii) graphene does not have a configuration at ease. In particular an angular self-stress is present, and the self-energy associated with the self-stress (sometimes called cohesive energy in the literature) needs to be considered.

Resting on this atomistic energetic description, we here determine the equivalent continuum limit. A pointwise limit has already been determined in [9]; we here prove a compactness result and determine the Γ-limit, which in turn guarantee the convergence of minima and minimizers. The main results we obtain are:

(i) The Γ-limit energy depends on the square of the mean curvature and on the Gaussian curvature; the constitutive coefficients depend on the dihedral contribution and the self-stress.

(ii) If both the self-stress and the C-energy are neglected, the Γ-limit is non-local and depends on a function which is solution of a differential problem.

That graphene could be modeled in the framework of the non-local elasticity has been conjectured in the literature several times. A review of recent research studies on this matter can be found in [20]. Unlike classical continuum models, within the framework of non-local elasticity it is assumed that the stress at a reference point in a body depends not only on the strains at that point, but also on strains at all other points of the body. Since classical model are inefficient to model the mechanical behavior of graphene, and since the description of the atomic bonds leads to consider relatively long interactions, some authors have believed reasonable to postulate a kind of non-locality in the model. As a matter of fact, the connection between atomistic and continuum description has never been mathematically rigorous, and has been limited to fit additional parameters to experiments or atomistic simulations.

The paper is organized as follows. In Sec. 2 we present a description of graphene energetics at atomistic level, as suggested by the 2nd generation Brenner potential. In Sec. 3 we lay down our assumptions and announce the main results. In Sec. 4 we introduce some interpolating functions and determine their limits when the lattice size tends to zero. In Sec. 5 we determine lower bounds of the limit energy and prove a theorem concerning the regularity of the limit function. In Sec. 6 we determine the Γ-limit for the general case and the case when self-stress and C-energy are neglected.
Notation. We use the direct notation. We denote vectors by low-case Roman bold-face letters and scalar fields by low-case Roman or Greek light-face letters. The canonical basis for $\mathbb{R}^3$ is denoted by $\{e_1, e_2, e_3\}$. For a vector $a$ we set $a^\perp = e_3 \wedge a$, the vector $a$ rotated by $\pi/2$ counter-clockwise. For a given scalar field $w$, we denote by $\nabla w$ its gradient and by

$$\partial_a w := \nabla w \cdot \frac{a}{|a|}$$

the derivative in direction $a/|a|$.

2 The bending energy of a graphene sheet

As reference configuration we use the 2–lattice generated by two simple Bravais lattices

$$L_1(\ell) = \{ x \in \mathbb{R}^2 : x = n^1 \ell d_1 + n^2 \ell d_2 \text{ with } (n^1, n^2) \in \mathbb{Z}^2 \},$$
$$L_2(\ell) = \ell p + L_1(\ell),$$

simply shifted with respect to one another by $\ell p$, see Fig. 1. In (1), $\ell$ denotes the lattice size (the reference interatomic distance), while $\ell d_3$ and $\ell p$ respectively are the lattice vectors and the shift vector, with

$$d_1 = \sqrt{3} e_1, \quad d_2 = \frac{\sqrt{3}}{2} e_1 + \frac{3}{2} e_2 \quad \text{and} \quad p = \frac{\sqrt{3}}{2} e_1 + \frac{1}{2} e_2.$$
The sides of the hexagonal cells in Figure 1 stand for the bonds between pairs of next nearest neighbor atoms and are represented by the vectors
\[ p_\alpha = d_\alpha - p \quad (\alpha = 1, 2) \quad \text{and} \quad p_3 = -p. \]
For convenience we also set
\[ d_3 = d_2 - d_1. \]

In what follows we denote by
\[ x^\ell = n^1 \ell d_1 + n^2 \ell d_2 + m \ell p, \quad (n^1, n^2, m) \in \mathbb{Z}^2 \times \{0, 1\} \]
the lattice points and label them by the triplets \((n^1, n^2, m)\): the points with \(m = 0\) belong to \(L_1(\ell)\), while those in \(L_2(\ell)\) correspond to \(m = 1\).

Graphene energetics depends on the description chosen to mimic atomic interactions. Our model stems on the 2nd-generation Brenner potential [5], which is one of the most used in molecular dynamics simulations of graphene. Accordingly, the binding energy \(V\) of an atomic aggregate is given as a sum over nearest neighbors:
\[ V = \sum_i \sum_{j < i} V_{ij}, \quad V_{ij} = V_R(l_{ij}) + b_{ij}(\vartheta_{hij}, \Theta_{hijk})V_A(l_{ij}), \]
where the individual effects of the repulsion and attraction functions \(V_R(l_{ij})\) and \(V_A(l_{ij})\), which model pair-wise interactions of atoms \(i\) and \(j\) depending on their distance \(l_{ij}\), are modulated by the bond-order function \(b_{ij}\): for a given bond chain of atoms \(h, i, j, k\) the function \(b_{ij}\) depends in a complex manner on the angle between the edges \(hi\) and \(ij\) and on the dihedral angle between the planes spanned by \((hi, ij)\) and \((ij, jk)\). This potential reveals that, in order to properly account for the mechanical behavior of graphene, it is necessary to consider three types of energetic contributions: binary interactions between next nearest atoms (edge bonds), three-bodies interactions between consecutive pairs of next nearest atoms (wedge bonds) and four-bodies interactions between three consecutive pairs of next nearest atoms (dihedral bonds). There are two types of relevant dihedral bonds: the \(Z\)-dihedra, in which the edges connecting the four atoms form a \(Z\)-shape, and the \(C\)-dihedra, in which the edges form a \(C\)-shape (see Fig. 2).

Following [9], we consider a harmonic approximation of the energy density. Moreover, it is possible to show [10] that the edge length at ease is \(\ell\), the dihedral angle at ease is null, while the angle at ease between consecutive edges is \(\frac{2}{3} \pi + \delta \vartheta_0\), where \(\delta \vartheta_0 \neq 0\). This means that the graphene sheet does not have a configuration at ease (\(i.e.\) stress-free).

With this in mind, we assume that the energy is given by the sum of the following terms:
\[ U^\ell = \frac{1}{2} \sum_k k^l (\delta l)^2, \]
\[ U^\vartheta = \tau_0 \sum_w \delta \vartheta + \frac{1}{2} \sum_w k^\vartheta (\delta \vartheta)^2, \]
\[ U^\Theta = \frac{1}{2} \sum_z k^z (\delta (z \Theta))^2 + \frac{1}{2} \sum_c k^c (\delta (c \Theta))^2. \]
(3)
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\[ l_{ij}, \vartheta_{hi}, (z)_{\Theta}, (c)_{\Theta} \]

Figure 2: Edge bond $l$, wedge bond $\vartheta$, Z-dihedron $\Theta$ and a C-dihedron $\Theta$.

$U^l_{\ell}, U^\vartheta_{\ell}$ and $U^\Theta_{\ell}$ are the energies of the edge bonds, the wedge bonds and the dihedral bonds, respectively; $\delta l$ denotes the change of distance between nearest neighbor atoms, $\delta \vartheta$ the change of angle between pairs of edges having a lattice point in common and $\delta (z)_{\Theta}$ and $\delta (c)_{\Theta}$ the Z- and C-dihedral change of angles between two consecutive wedges; finally,

$$\tau_0 := -k^\vartheta \delta \vartheta_0$$

is the wedge self-stress. The sums extend to all edges, $\mathcal{E}$, all wedges, $\mathcal{W}$, all Z-dihedra, $\mathcal{Z}$, and all C-dihedra $\mathcal{C}$. The bond constants $k^l, k^\vartheta, k^Z,$ and $k^C$ can be deduced by making use of the 2nd-generation Brenner potential. In (3) we approximate the strain measures to the lowest order that makes the energy quadratic in the displacement field.

In [9] we have shown that the change in length of edges and the first order variation of the change in angle of wedges depend on the in-plane components of the displacement. We have also shown that the energy splits into two contributions: one depends on the in-plane displacement and the other —the bending energy— is a function of the out-of-plane displacement $w : L_1(\ell) \cup L_2(\ell) \to \mathbb{R}$. The total bending energy associated to $w$ is given by

$$U_{\ell}(w) = U^Z_{\ell}(w) + U^C_{\ell}(w) + U^s_{\ell}(w),$$

where

$$U^Z_{\ell}(w) := \frac{1}{2} \sum_Z k^Z (\delta (z)_{\Theta})^2,$$

$$U^C_{\ell}(w) := \frac{1}{2} \sum_C k^C (\delta (c)_{\Theta})^2,$$

$$U^s_{\ell} := \tau_0 \sum_{\mathcal{W}} \delta \vartheta^{(2)}.$$

$U^Z_{\ell}$ and $U^C_{\ell}$ are the Z- and C-dihedral energy, while $U^s_{\ell}$ is the self-energy (corresponding to
the so-called cohesive energy in the literature); in (4), $\delta \vartheta^{(2)}$ is the second order variation of the wedge angle with respect to the reference angle $\frac{2}{3}\pi$.

Hereafter we write explicitly the dependence on $w$ of the strain measures. In particular, by $\Theta_{\ell,\ell+1}^{(z)}[w](x^\ell)$ we denote the Z-dihedral angle, associated to displacement $w$, that corresponds to the Z-dihedron with middle edge $\ell p_i$, starting from $x^\ell$ and the other two edges parallel to $p_{i+1}$. The C-dihedral angle $\Theta_{\ell,\ell+1}^{(c)}[w](x^\ell)$ is the angle corresponding to the C-dihedron with middle edge $\ell p_i$ and oriented as $p_i^\perp$, while $\Theta_{\ell,\ell+1}^{(c)}[w](x^\ell)$ is the angle corresponding to the C-dihedron oriented opposite to $p_i^\perp$ (see Fig. 3 for $i = 1$).

In [9] we have shown that the Z-dihedral energy has the following expression:

$$\mathcal{U}_Z^2(w) := \frac{1}{2} k Z \sum_{\ell \in L_2(\ell)} \sum_{i=1}^{3} \left( \Theta_{\ell,\ell+1}^{(z)}[w](x^\ell) \right)^2 + \left( \Theta_{\ell,\ell+2}^{(z)}[w](x^\ell) \right)^2, \quad (5)$$

where the change of Z-dihedral angles may be given in the following way:

$$\Theta_{\ell,\ell+1}^{(z)}[w](x^\ell) = \frac{2\sqrt{3}}{3\ell} [w(x^\ell + \ell p_i - \ell p_{i+1}) - w(x^\ell + \ell p_i) + w(x^\ell + \ell p_{i+1}) - w(x^\ell)], \quad (6)$$

$$\Theta_{\ell,\ell+2}^{(z)}[w](x^\ell) = \frac{2\sqrt{3}}{3\ell} [w(x^\ell + \ell p_i - \ell p_{i+2}) - w(x^\ell + \ell p_i) + w(x^\ell + \ell p_{i+2}) - w(x^\ell)].$$

Figure 3: Left: C-dihedral angles $\Theta_{p_i}^{(c)}$ (green) and Z-dihedral angle $\Theta_{p_i p_{i+1}}^{(z)}$ (blue). Right: C-dihedral angles $\Theta_{p_i}^{(c)}$ (green) and Z-dihedral angle $\Theta_{p_i p_{i+1}}^{(z)}$ (blue).
To make notation simpler, we have omitted the symbol $\delta$ to denote the variation; we will do the same throughout the paper without any further mention. Analogously, the C-dihedral energy can be written as:

$$U_C^\ell(w) := \frac{1}{2} k_C \sum_{x^\ell \in L_2(\ell)} \left( \Theta_{p_i}^+[w](x^\ell) \right)^2 + \left( \Theta_{p_i}^-[w](x^\ell) \right)^2,$$

with the change of C-dihedral angles given by:

$$\Theta_{p_i}^+[w](x^\ell) = +\sqrt{3} \sum_{i=1}^3 w(x^\ell - \ell p_i - \ell p_{i+2}) - w(x^\ell + \ell p_i),$$

$$\Theta_{p_i}^-[w](x^\ell) = -\sqrt{3} \sum_{i=1}^3 w(x^\ell + \ell p_i),$$

Concerning the self-energy, (4) becomes:

$$U_s^\ell(w) := -\frac{1}{2} \tau_0 \left[ \sum_{x^\ell \in L_1(\ell)} \left( \vartheta_1^+[w](x^\ell) \right)^2 + \sum_{x^\ell \in L_2(\ell)} \left( \vartheta_2^+[w](x^\ell) \right)^2 \right],$$

where:

$$\vartheta_1^+[w](x^\ell) = \sqrt{3} \sum_{i=1}^3 w(x^\ell - \ell p_i - \ell p_{i+2}) - w(x^\ell + \ell p_i),$$

$$\vartheta_2^+[w](x^\ell) = \sqrt{3} \sum_{i=1}^3 w(x^\ell + \ell p_i).$$

The reader is referred to [9] for detailed computations.

## 3 Main assumptions and results

The dual triangulation represented in Fig. 4 will play an important role in our analysis. This is composed by equilateral triangles of length side $\sqrt{3} \ell$ centered at the lattice points that tessellate $\mathbb{R}^2$. The triangle centered at point $x^\ell$ is denoted by $T^\ell(x^\ell)$.

In the place of displacements defined on the lattice points of $L_1(\ell) \cup L_2(\ell)$, as introduced in the previous section, we shall consider (equivalent) functions with domain $\mathbb{R}^2$ that are constant over each triangle of the dual triangulation. Thence, if $w$ is such a function the following representation holds:

$$w(x) = \sum_{x^\ell \in L_1(\ell) \cup L_2(\ell)} w(x^\ell) \chi_{T^\ell(x^\ell)}(x),$$
where $\chi_{T^\ell(x^\ell)}$ is the characteristic function of $T^\ell(x^\ell)$. The energies and the deformation measures defined in the previous section can be unambiguously evaluated on this kind of functions.

We consider a graphene sheet of finite extension corresponding to the nodes of lattice $L_1(\ell) \cup L_2(\ell)$ contained in some open and simply connected bounded set $\Omega$ of $\mathbb{R}^2$. The lattice size $\ell$ is assumed to be much smaller than the diameter of the largest ball contained in $\Omega$. For simplicity, we consider homogeneous Dirichlet boundary conditions, which we implement by considering out-of-plane displacements belonging to the set

$$A_\ell = \{ w \in L^2(\mathbb{R}^2) : w \text{ is constant over each } T^\ell(x^\ell) \text{ and } w = 0 \text{ over all } T^\ell(x^\ell) \notin \Omega \}.$$ 

Before stating our first result we make the following assumption:

$$k^Z > 0, \quad k^c \geq 0 \quad \text{and} \quad \tau_0 \leq 0$$

that will be maintained throughout the paper without any further mention.

The following compactness result holds.

**Theorem 1** Let $w_\ell \in A_\ell$ be a sequence that satisfy the energy bound:

$$\sup_{\ell} U_\ell(w_\ell) < +\infty.$$ (11)

Then, there exist $w \in H^2_0(\Omega)$ and a subsequence of $\{w_\ell\}$, not relabelled, such that

$$w_\ell \to w \quad \text{in } L^2(\Omega).$$ (12)
All the theorems stated in this section will be proved in the following sections. The next Theorem characterizes the bending behavior of graphene.

**Theorem 2** Assume that either \( k^C \neq 0 \) or \( \tau_0 \neq 0 \), and set

\[
U^e_\ell(w) := \begin{cases} U_\ell(w) & \text{if } w \in A_\ell, \\ +\infty & \text{if } w \in L^2(\Omega) \setminus A_\ell. \end{cases}
\] (13)

The functionals \( U^e_\ell \) \( \Gamma \)-converge with respect to the \( L^2(\Omega) \)-convergence to the functional

\[
U^e_0(w) := \begin{cases} U^{(b)}_0(w) & \text{if } w \in H^2_0(\Omega), \\ +\infty & \text{if } w \in L^2(\Omega) \setminus H^2_0(\Omega), \end{cases}
\]

where

\[
U^{(b)}_0(w) := \frac{1}{2} \int_\Omega \left( \frac{5\sqrt{3}}{3} k^Z + \frac{2\sqrt{3}}{3} k^C - \frac{\tau_0}{2} \right) (\Delta w)^2 \\
- \frac{8\sqrt{3}}{3} (k^Z + k^C) \det \nabla^2 w \, dx.
\] (14)

We close this section by looking at the case \( k^C = \tau_0 = 0 \). For \( w \in H^2_0(\Omega) \) we denote by

\[
(-\Delta)^{-1}(-\frac{2}{3}\partial_{p_1p_2p_3} w) \in H^1_0(\Omega)
\]

the solution of the following problem

\[
\begin{cases} \\
\gamma \in H^1_0(\Omega), \\
- \Delta \gamma = -\frac{2}{3}\partial_{p_1p_2p_3} w \ & \text{in } D'(\Omega). \\
\end{cases}
\]

The following theorem characterizes the \( \Gamma \)-limit when \( k^C = \tau_0 = 0 \), that is \( U_\ell(w) = U^Z_\ell(w) \).

We notice that in this case the \( \Gamma \)-limit is a non-local functional.

**Theorem 3** Let

\[
U^{Z\ell}_e(w) := \begin{cases} U^Z_\ell(w) & \text{if } w \in A_\ell, \\ +\infty & \text{if } w \in L^2(\Omega) \setminus A_\ell. \end{cases}
\]

The functionals \( U^{Z\ell}_e \) \( \Gamma \)-converge with respect to the \( L^2(\Omega) \)-convergence to the functional

\[
U^{Z_0}(w) := \begin{cases} U^{Z(b)}_0(w, (-\Delta)^{-1}(-\frac{2}{3}\partial_{p_1p_2p_3} w)) & \text{if } w \in H^2_0(\Omega), \\
+\infty & \text{if } w \in L^2(\Omega) \setminus H^2_0(\Omega), \end{cases}
\]

where

\[
U^{Z(b)}_0(w, \gamma) := \frac{5\sqrt{3}}{6} k^Z \int_\Omega (\Delta w)^2 - \frac{8}{5} \det \nabla^2 w \, dx \\
+ \sqrt{3} k^Z \int_\Omega (2\partial_{12} w e_1 + (\partial_{11} w - \partial_{22} w) e_2) \cdot \nabla \gamma \, dx \\
+ 3\sqrt{3} k^Z \int_\Omega |\nabla \gamma|^2 \, dx.
\] (15)
4 Interpolating functions and their limits

In this section we introduce three piecewise affine interpolants on strips of $\mathbb{R}^2$ that are naturally emerging in the study of the behavior of the $Z$-dihedral energy. These interpolants, besides shading light on the $Z$-dihedral energy, will play a crucial role also in the study of the other energies.

It is convenient to group the nodes of the 2–lattice as

\[
S^1_\ell(k) = \{ x^\ell \in \mathbb{R}^2 : x^\ell = (i d_1 + k d_2 + m p)\ell \text{ with } i \in \mathbb{Z}, \ m \in \{0,1\} \},
\]
\[
S^2_\ell(k) = \{ x^\ell \in \mathbb{R}^2 : x^\ell = (k d_1 + i d_2 + m p)\ell \text{ with } i \in \mathbb{Z}, \ m \in \{0,1\} \},
\]
\[
S^3_\ell(k) = \{ x^\ell \in \mathbb{R}^2 : x^\ell = ((k - i - m) d_1 + i d_2 + m p)\ell \text{ with } i \in \mathbb{Z}, \ m \in \{0,1\} \}.
\]

We denote by $cS^i_\ell(k)$ the convex hull of $S^i_\ell(k)$, see Fig. 5, and define

\[
S^i_\ell = \bigcup_{k \in \mathbb{Z}} S^i_\ell(k), \quad cS^i_\ell = \bigcup_{k \in \mathbb{Z}} cS^i_\ell(k), \quad \text{for } i = 1, 2, 3.
\]

![Figure 5: A representation of the strips $cS^i_\ell(k)$ and of the triangles $T^i(x^\ell)$.](image)

Each strip $cS^i_\ell(k)$ is naturally decomposed, by the lattice points, into isosceles triangles with base of the triangles parallel to the vector $d_i$, of length $\sqrt{3} \ell$, and the two equal sides of
length $\ell$. We denote by $T^{(i)}(x^\ell)$ the isosceles triangle belonging to $cS^{(i)}_\ell$ with vertex in $x^\ell$, see Fig. 5.

Thanks to these triangulations, we now define, over each strip $cS^{(i)}_\ell(k)$, a piecewise affine function $\hat{w}^{(i)}_\ell$ that interpolates the lattice values of a given function $w_\ell \in A_\ell$. The function $\hat{w}^{(i)}_\ell$ is set to be equal to zero in the complement of $cS^{(i)}_\ell$. We achieve this in two steps. For a given function $w_\ell \in A_\ell$ and for each $i = 1, 2, 3$, we first define the piecewise affine interpolant of $w_\ell$ over the strips composing $cS^{(i)}_\ell$. That is,

$$\hat{w}^{(i)}_\ell|_{cS^{(i)}_\ell} : cS^{(i)}_\ell \rightarrow \mathbb{R}$$

is a piecewise affine function with values

$$\hat{w}^{(i)}_\ell|_{cS^{(i)}_\ell}(x^\ell) = w_\ell(x^\ell)$$

for every $x^\ell \in L_1(\ell) \cup L_2(\ell)$. We also set $\hat{w}^{(i)}_\ell : \mathbb{R}^2 \rightarrow \mathbb{R}$ by

$$\hat{w}^{(i)}_\ell(x) = \begin{cases} 
\hat{w}^{(i)}_\ell|_{cS^{(i)}_\ell}(x) & x \in cS^{(i)}_\ell, \\
0 & \text{otherwise}
\end{cases}$$

(16)

Figure 6: The interpolating function $\hat{w}^{(i)}_\ell(x)$.

Hence, the point-wise gradient $\nabla \hat{w}^{(i)}_\ell$ is constant over each triangle $T^{(i)}(x^\ell)$; we denote this constant by $\nabla \hat{w}^{(i)}_\ell(x^\ell)$. Formally, we set

$$\nabla \hat{w}^{(i)}_\ell(x^\ell) := \nabla \hat{w}^{(i)}_\ell(x)$$
with \( \mathbf{x} \) any point in \( T^{(i)}(\mathbf{x}^\ell) \).

Among adjacent triangles we may compute the jump of the gradients. We denote by
\[
[\nabla \hat{w}^{(i)}_\ell]_{p_j}(\mathbf{x}^\ell)
\]
the jump of the gradient \( \nabla \hat{w}^{(i)}_\ell \) across triangles, in the union of strips \( cS^{(i)}_\ell \), that share a side passing by \( \mathbf{x}^\ell \) and parallel to \( p_j \). The sign of the jump is computed according to the orientation determined by \( \mathbf{d}_i \); that is, it is defined as the value of the gradient \( \nabla \hat{w}^{(i)}_\ell \) on the triangle on which \( \mathbf{d}_i \) is pointing to, minus the value of the gradient over the triangle opposite to the direction of \( \mathbf{d}_i \). To become accustomed with the notation introduced we compute (6) with \( \ell = 1 \) and \( \mathbf{x}^\ell \in L_2(\ell) \):
\[
\Theta^{(z)}_{p_1p_3}|w_\ell|^z(\mathbf{x}^\ell) = \frac{2\sqrt{3}}{3\ell} \left( \hat{w}^{(1)}_\ell(\mathbf{x}^\ell + \ell \mathbf{p}_1 - \ell \mathbf{p}_3) - \hat{w}^{(1)}_\ell(\mathbf{x}^\ell + \ell \mathbf{p}_1) \right)
= \frac{2\sqrt{3}}{3\ell} \left( \nabla \hat{w}^{(1)}_\ell(\mathbf{x}^\ell + \ell \mathbf{p}_1) \cdot (-\ell \mathbf{p}_3) + \nabla \hat{w}^{(1)}_\ell(\mathbf{x}^\ell) \cdot (\ell \mathbf{p}_3) \right)
= -\frac{2\sqrt{3}}{3} \left[ \nabla \hat{w}^{(1)}_\ell \right]_{p_3}(\mathbf{x}^\ell) \cdot p_3,
\]
where the first identity holds because \( \hat{w}^{(1)}_\ell \) is affine. Similarly, (6) with \( \ell = 3 \) and for \( \mathbf{x}^\ell \in L_2(\ell) \) rewrites as
\[
\Theta^{(z)}_{p_1p_3}|w_\ell|^z(\mathbf{x}^\ell) = \frac{2\sqrt{3}}{3\ell} \left( \nabla \hat{w}^{(1)}_\ell(\mathbf{x}^\ell + \ell \mathbf{p}_3) \cdot (-\ell \mathbf{p}_1) + \nabla \hat{w}^{(1)}_\ell(\mathbf{x}^\ell) \cdot (\ell \mathbf{p}_1) \right)
= +\frac{2\sqrt{3}}{3} \left[ \nabla \hat{w}^{(1)}_\ell \right]_{p_1}(\mathbf{x}^\ell) \cdot p_1.
\]

The \( Z \)-dihedral energy, (5), can be split into three parts as
\[
\frac{2U_\ell^Z(w_\ell)}{kZ} = \sum_{\mathbf{x}^\ell \in L_2(\ell)} \left( \Theta^{(z)}_{p_1p_3}|w_\ell|^z(\mathbf{x}^\ell) \right)^2 + \left( \Theta^{(z)}_{p_1p_3}|w_\ell|^z(\mathbf{x}^\ell) \right)^2 + \sum_{\mathbf{x}^\ell \in L_2(\ell)} \left( \Theta^{(z)}_{p_1p_3}|w_\ell|^z(\mathbf{x}^\ell) \right)^2 + \left( \Theta^{(z)}_{p_1p_3}|w_\ell|^z(\mathbf{x}^\ell) \right)^2 + \sum_{\mathbf{x}^\ell \in L_2(\ell)} \left( \Theta^{(z)}_{p_1p_3}|w_\ell|^z(\mathbf{x}^\ell) \right)^2 + \left( \Theta^{(z)}_{p_1p_3}|w_\ell|^z(\mathbf{x}^\ell) \right)^2,
\]
where only dihedral bonds contained in the strip \( cS^{(1)}_\ell \) are involved in the first line, as it appears also from (17) and (18), while the second and third lines could be written using \( \hat{w}^{(2)}_\ell \) and \( \hat{w}^{(3)}_\ell \), respectively. Thanks to this decomposition we are allowed to study the \( Z \)-dihedral energy only on \( cS^{(1)}_\ell \) and then extend the results “by rotation” to obtain the equivalent ones on the strips \( cS^{(2)}_\ell \) and \( cS^{(3)}_\ell \).

In the next Lemma we establish a bound on the \( L^2 \)-norm of the jumps of \( \nabla w^{(i)}_\ell \).
Lemma 4 Let \( w_\ell \in \mathcal{A}_\ell \) satisfy the energy bound (11) and let \( \hat{w}_\ell^{(i)} \) be the piecewise affine functions defined in (16). Then,

\[
\sup_\ell \sum_{i=1}^{3} \ell \int_{J(\nabla \hat{w}_\ell^{(i)}) \cap cS_\ell^{(i)}} \left| \frac{1}{\ell} [\nabla \hat{w}_\ell^{(i)}] \right|^2 ds < +\infty, \tag{20}
\]

where \( [\nabla \hat{w}_\ell^{(i)}] \) and \( J(\nabla \hat{w}_\ell^{(i)}) \) denote the jump and the jump set of \( \nabla \hat{w}_\ell^{(i)} \).

**Proof.** We prove the lemma for \( i = 1 \) only, since the other cases can be treated similarly. Recalling (17) and (18) we have that

\[
\sum_{x^i \in L_2(\ell)} \left( \Theta_{p_1, p_3}[w_\ell](x^i) \right)^2 + \left( \Theta_{p_3, p_1}[w_\ell](x^i) \right)^2
= \frac{4}{3} \sum_{x^i \in L_2(\ell)} \left( [\nabla \hat{w}_\ell^{(1)}]_{p_1}(x^i) \cdot p_3 \right)^2 + \left( [\nabla \hat{w}_\ell^{(1)}]_{p_3}(x^i) \cdot p_1 \right)^2. \tag{21}
\]

Thanks to the continuity of \( \hat{w}_\ell^{(1)} \) over the strip \( cS_\ell^{(1)} \), we find that

\[
[\nabla \hat{w}_\ell^{(1)}]_{p_1} = [\partial_{p_1} \hat{w}_\ell^{(1)}]_{p_1} + [\partial_{p_3} \hat{w}_\ell^{(1)}]_{p_3} = [\partial_{p_1} \hat{w}_\ell^{(1)}]_{p_1} \cdot p_3,
\]

and therefore

\[
([\nabla \hat{w}_\ell^{(1)}]_{p_1} \cdot p_3)^2 = \frac{3}{4} ([\partial_{p_1} \hat{w}_\ell^{(1)}]_{p_1})^2 = \frac{3}{4} [\nabla \hat{w}_\ell^{(1)}]_{p_1}^2,
\]

since \( |p_1^+ \cdot p_3| = \sqrt{3}/2 \). We may therefore rewrite (21) as

\[
\sum_{x^i \in L_2(\ell)} \left( \Theta_{p_1, p_3}[w_\ell](x^i) \right)^2 + \left( \Theta_{p_3, p_1}[w_\ell](x^i) \right)^2
= \sum_{x^i \in L_2(\ell)} \left| [\nabla \hat{w}_\ell^{(1)}]_{p_1}(x^i) \right|^2 + \left| [\nabla \hat{w}_\ell^{(1)}]_{p_3}(x^i) \right|^2
= \frac{1}{\ell} \int_{J(\nabla \hat{w}_\ell^{(1)}) \cap cS_\ell^{(1)}} \left| [\nabla \hat{w}_\ell^{(1)}] \right|^2 ds = \ell \int_{J(\nabla \hat{w}_\ell^{(1)}) \cap cS_\ell^{(1)}} \left| \frac{1}{\ell} [\nabla \hat{w}_\ell^{(1)}] \right|^2 ds.
\]

Since \( w_\ell \in \mathcal{A}_\ell \) satisfy the energy bound (11), we have that \( \sup_\ell \mathcal{U}_\ell^{(c)}(w_\ell) < +\infty \) and hence (20) follows by recalling (19).

We now prove that \( \hat{w}_\ell^{(i)} \) is \( H^1 \)-bounded over the region \( cS_\ell^{(i)} \).

Lemma 5 Let \( \hat{w}_\ell^{(i)} \) be as in Lemma 4. Then,

\[
\sup_\ell \| \hat{w}_\ell^{(i)} \|_{H^1(cS_\ell^{(i)})} < +\infty. \tag{22}
\]
Proof. Again we prove the lemma for $i = 1$. This proof is more transparent if we adopt a notation different from that used so far. For given $k$, we denote the triangles on the strip $cS^{(1)}_k(k)$ by $T_j$ (instead of $T^{(1)}(x')$), with $j \in \mathbb{Z}$ increasing in the direction $d_1$, and we write $\nabla \hat{w}^{(1)}_\ell(T_j)$ to indicate the constant value taken by $\nabla \hat{w}^{(1)}_\ell$ over the triangle $T_j$. Notice that the following identity
\[
\nabla \hat{w}^{(1)}_\ell(T_j) = \sum_{m=-\infty}^{j} \left( \nabla \hat{w}^{(1)}_\ell(T_m) - \nabla \hat{w}^{(1)}_\ell(T_{m-1}) \right)
\]
holds because on the right we have a telescoping sum and because $\hat{w}^{(1)}_\ell$ vanishes outside of $\Omega$. Hence,
\[
|\nabla \hat{w}^{(1)}_\ell(T_j)| \leq \sum_{m=-\infty}^{\infty} \left| \left( \nabla \hat{w}^{(1)}_\ell(T_m) - \nabla \hat{w}^{(1)}_\ell(T_{m-1}) \right) \right| = \int_{J(\nabla \hat{w}^{(1)}_\ell) \cap cS^{(1)}_k(k)} \frac{1}{\ell} \|[\nabla \hat{w}^{(1)}_\ell]|| ds,
\]
and by applying Jensen inequality we find
\[
|\nabla \hat{w}^{(1)}_\ell(T_j)|^2 \leq J(\nabla \hat{w}^{(1)}_\ell) \cap cS^{(1)}_k(k) \int_{J(\nabla \hat{w}^{(1)}_\ell) \cap cS^{(1)}_k(k)} \frac{1}{\ell} [\nabla \hat{w}^{(1)}_\ell]|^2 ds \leq C \int_{J(\nabla \hat{w}^{(1)}_\ell) \cap cS^{(1)}_k(k)} \frac{1}{\ell} [\nabla \hat{w}^{(1)}_\ell]|^2 ds.
\]
The last inequality follows because $|J(\nabla \hat{w}^{(1)}_\ell) \cap cS^{(1)}_k(k)| \leq c\ell (\text{diam}\Omega / \ell)$. Hence, multiplying by $|T_j|$ on both sides and summing over $j$ we get
\[
\|\nabla \hat{w}^{(1)}_\ell\|_{L^2(cS^{(1)}_k(k))} = \sum_{T_j \cap \Omega \neq \emptyset} |\nabla \hat{w}^{(1)}_\ell(T_j)|^2 |T_j| \leq c \sum_{T_j \cap \Omega \neq \emptyset} |T_j| \int_{J(\nabla \hat{w}^{(1)}_\ell) \cap cS^{(1)}_k(k)} \frac{1}{\ell} [\nabla \hat{w}^{(1)}_\ell]|^2 ds \leq c \text{diam} \Omega \ell \int_{J(\nabla \hat{w}^{(1)}_\ell) \cap cS^{(1)}_k(k)} \frac{1}{\ell} [\nabla \hat{w}^{(1)}_\ell]|^2 ds.
\]
Hence, summing over $k$ and taking Lemma 4 into account, we have
\[
\|\nabla \hat{w}^{(1)}_\ell\|_{L^2(cS^{(1)}_k(k))} < +\infty.
\]
With Poincaré inequality we deduce (22). □

We are now in a position to prove (12) of Theorem 1; the regularity of the limit function will be proved later.
Theorem 6 Let $w_\ell \in A_\ell$ satisfy the energy bound (11). Then, there exists $w \in L^2(\mathbb{R}^2)$ equal to zero almost everywhere outside of $\Omega$ such that, up to a subsequence,

\[ w_\ell \to w \text{ in } L^2(\mathbb{R}^2). \]

Proof. Note that $w_\ell$ is uniformly bounded in $L^2(\mathbb{R}^2)$. Indeed,

\[ w_\ell(x) = \sum_{x^\ell \in L_1(\ell) \cup L_2(\ell)} w_\ell(x^\ell) \chi_{T^\ell(x^\ell)}(x) = \sum_{x^\ell \in L_1(\ell) \cup L_2(\ell)} \hat{w}_\ell^{(1)}(x^\ell) \chi_{T^\ell(x^\ell)}(x), \]

hence

\[
\int_{\mathbb{R}^2} |w_\ell|^2 \, dx \leq \sum_{x^\ell \in L_1(\ell) \cup L_2(\ell)} |\hat{w}_\ell^{(1)}(x^\ell)|^2 |T^\ell(x^\ell)(x)| \\
\leq c \sum_{x^\ell \in L_1(\ell) \cup L_2(\ell)} \int_{T^\ell(x^\ell)} |\hat{w}_\ell^{(1)}(x)|^2 + |\nabla \hat{w}_\ell^{(1)}(x)|^2 \ell \, dx \\
\leq c \|\hat{w}_\ell^{(1)}\|_{H^1(cS^\ell_1)}^2 \leq C
\]

by Lemma 5. Then, there exists $w \in L^2(\mathbb{R}^2)$ equal to zero almost everywhere outside of $\Omega$ such that, up to a subsequence,

\[ w_\ell \to w \text{ in } L^2(\mathbb{R}^2). \]

We now prove that the convergence is in fact strong.

Let $h = h^1 d_1 + h^2 d_2 \in \mathbb{R}^2$ and write

\[
\int_{\mathbb{R}^2} |w_\ell(x + h) - w_\ell(x)|^2 \, dx \leq C \int_{\mathbb{R}^2} |w_\ell(x + h^1 d_1 + h^2 d_2) - w_\ell(x + h^1 d_1)|^2 \, dx \\
+ C \int_{\mathbb{R}^2} |w_\ell(x + h^1 d_1) - w_\ell(x)|^2 \, dx.
\]

Let us consider the second term on the right hand side (the first can be handled similarly). For each $x$ and each $h^1$ there exist two lattice points $y^\ell$ and $z^\ell$ such that

\[ x \in T^\ell(y^\ell), \quad \text{and} \quad x + h^1 d_1 \in T^\ell(z^\ell). \]

With the notation introduced in (2) we may also write

\[ y^\ell = n_y^\ell d_1 + k \ell d_2 + m_y^\ell p, \]
\[ z^\ell = n_z^\ell d_1 + k \ell d_2 + m_z^\ell p, \]

with $n_y, n_z, k \in \mathbb{Z}$ and $m_y, m_z \in \{0, 1\}$.

Without loss of generality we assume that $h^1 > 0$, which implies that $n_y \geq n_x$. 

We consider a “monotonic” path from $y^\ell$ to $z^\ell$ through the lattice points of the strip $S^{(1)}(k)$ and label these points by means of the index $j = 0, \ldots, j_f$, so that

$$x(0) = y^\ell \quad \text{and} \quad x(j_f) = z^\ell.$$ 

Then, the number of sides of the path are $2(n_z - n_y) + 1$ according to whether the initial and the final points belong to the same Bravais lattice, i.e., $m_z = m_y$.

With this notation we have:

$$|w_\ell(x + h_1 d_1) - w_\ell(x)|^2 = |w_\ell(y^\ell) - w_\ell(x^\ell)|^2 = |\tilde{w}_\ell^{(1)}(y^\ell) - \tilde{w}_\ell^{(1)}(x^\ell)|^2$$

$$= \left| \sum_{j=1}^{j_f} \tilde{w}_\ell^{(1)}(x(j)) - \tilde{w}_\ell^{(1)}(x(j-1)) \right|^2$$

$$\leq |2(n_z - n_y) + 1| \left| \sum_{j=1}^{j_f} \tilde{w}_\ell^{(1)}(x(j)) - \tilde{w}_\ell^{(1)}(x(j-1)) \right|^2$$

$$\leq |2(n_z - n_y) + 1| \left| \sum_{j \in \mathbb{Z}} \nabla \tilde{w}_\ell^{(1)}(x(j)) \right|^2 \ell^2$$

$$\leq c |2(n_z - n_y) + 1| \int_{cS^{(1)}(k)} |\nabla \tilde{w}_\ell^{(1)}|^2 d\mathbf{x}. \quad (26)$$

We now estimate $2(n_z - n_y) + 1$.

We first look at the case $h_1 > \ell$. From the obvious inequality

$$(2(n_z - n_y) - 1)\frac{\sqrt{3}}{2} \leq |(z^\ell - y^\ell) \cdot \frac{d_1}{|d_1|}| \leq |z^\ell - y^\ell|,$$

we find

$$2(n_z - n_y) + 1 \leq \frac{2\sqrt{3}}{3\ell} |z^\ell - y^\ell| + 2 \leq \frac{2\sqrt{3}}{3\ell} |z^\ell - y^\ell| + 2 \frac{h_1}{\ell},$$

and noting that $|z^\ell - y^\ell| \leq |h_1 d_1| + \ell = \sqrt{3} h_1 + \ell$, we deduce that

$$2(n_z - n_y) + 1 \leq \frac{2\sqrt{3}}{3\ell} (\sqrt{3} h_1 + \ell) + 2 \frac{h_1}{\ell} \leq c \frac{1}{\ell} |h|.$$ 

Then, by integrating (26) over the union of the triangles $T^{(1)}(x^\ell)$, with $x^\ell \in S^{(1)}(k) \cap \Omega$:

$$A(k) := \bigcup_{x^\ell \in S^{(1)}(k) \cap \Omega} T^{(1)}(x^\ell),$$

we get

$$\int_{A(k)} |w_\ell(x + h_1 d_1) - w_\ell(x)|^2 d\mathbf{x} \leq c \frac{|h|}{\ell} \text{diam}(\Omega) \frac{\ell}{2} \int_{cS^{(1)}(k)} |\nabla \tilde{w}_\ell^{(1)}|^2 d\mathbf{x}.$$
Hence, by summing over $k$ and applying Lemma 5, we have that

$$
\int_{\mathbb{R}^2} |w_\ell(x + h^1 d_1) - w_\ell(x)|^2 \, dx \leq C |h|.
$$

We now look at the case $h^1 < \ell$. We have

$$
\int_{\mathbb{R}^2} |w_\ell(x + h^1 d_1) - w_\ell(x)|^2 \, dx
= \sum_{x^\ell \in L_1(\ell) \cup L_2(\ell)} \int_{T^\ell(x^\ell)} |w_\ell(x + h^1 d_1) - w_\ell(x)|^2 \, dx
= \sum_{x^\ell \in L_1(\ell) \cup L_2(\ell)} \int_{T^\ell(x^\ell) \cap S^h(x^\ell)} |w_\ell(x + h^1 d_1) - w_\ell(x)|^2 \, dx,
$$

where $S^h(x^\ell)$ is a strip contained in $T^\ell(x^\ell)$ of width $|h^1 d_1|$, in the direction $d_1$, and sides parallel to $d_2$ or $d_3$, see Figure 7. The third equality follows since the difference $w_\ell(x + h^1 d_1) - w_\ell(x)$ vanishes for all $x \in T^\ell(x^\ell) \setminus S^h(x^\ell)$. In this case for every $x \in S^h(x^\ell)$ the

Figure 7: The strip $S^h(x^\ell)$

point $(x + h^1 d_1)$ has to belong to the next or after next neighbor triangle. With the notation above, one calculates that

$$
2(n_z - n_y) + 1 \leq 3,
$$
and from (26) and (28), we deduce

\[
\int_{\mathbb{R}^2} |w_\ell(x + h^1 d_1) - w_\ell(x)|^2 \, dx \\
\leq c \sum_{x^1 \in (L_1(\ell) \cup L_2(\ell)) \cap \Omega} \int_{\mathbb{T}^1} \left( \int_{cS_1^{(1)}(k) \cap cS_1^{(1)}(k)} |\nabla \hat{w}_\ell^{(1)}|^2 \, dx \right) \, dx \\
\leq c \sum_{x^1 \in (L_1(\ell) \cup L_2(\ell)) \cap \Omega} |h_\ell| \int_{cS_1^{(1)}(k)} |\nabla \hat{w}_\ell^{(1)}|^2 \, dx \\
= c \sum_{k \in \mathbb{Z}} \sum_{x^1 \in cS_1^{(1)}(k) \cap \Omega} |h_\ell| \int_{cS_1^{(1)}(k)} |\nabla \hat{w}_\ell^{(1)}|^2 \, dx \\
= c \sum_{k \in \mathbb{Z}} \text{diam}(\Omega) |h_\ell| \int_{cS_1^{(1)}(k)} |\nabla \hat{w}_\ell^{(1)}|^2 \, dx \\
\leq c |h_\ell| \int_{cS_1^{(1)}(k)} |\nabla \hat{w}_\ell^{(1)}|^2 \, dx \leq C|h_\ell|, \quad (29)
\]

where we have taken into account that the number of lattice points in \(S_1^{(1)}(k) \cap \Omega\) is of order \(\text{diam}(\Omega)/\ell\).

From (27) and (29) we get that

\[
\int_{\mathbb{R}^2} |w_\ell(x + h^1 d_1) - w_\ell(x)|^2 \, dx \leq C|h_\ell|
\]

uniformly in \(\ell\). Since the first term on the right hand side of (25) can be studied in exactly the same way, we have that for every \(h \in \mathbb{R}^2\)

\[
\int_{\mathbb{R}^2} |w_\ell(x + h) - w_\ell(x)|^2 \, dx \leq C|h|
\]

(30)

uniformly in \(\ell\). Then, by (30), (23), and Riesz-Kolmogorov’s theorem it follows that \(w_\ell\) has a strongly convergent subsequence. Thus the convergence stated in (24) is strong. \(\square\)

We end this section with two lemmas that address the convergence of \(\hat{w}_\ell^{(i)}\) and its derivatives.

**Lemma 7** Let \(\hat{w}_\ell^{(i)}\) be as in Lemma 4 and \(w\) be as in Theorem 6. Then, \(w \in H^1(\mathbb{R}^2)\) and there exists a subsequence, not relabeled, such that

\[
\hat{w}_\ell^{(i)} \to \frac{1}{3} w, \quad \partial_d \hat{w}_\ell^{(i)} \to \frac{1}{3} \partial_d w \quad \text{in } L^2(\mathbb{R}^2), \quad (31)
\]

for \(i = 1, 2, 3\).
PROOF. From the definition (16) of $\hat{w}^{(i)}$, we have that $\partial_d \hat{w}^{(i)} = 0$ in $\mathbb{R}^2 \setminus cS^{(i)}_\ell$. Hence, by Lemma 5 it follows that
\[ \| \hat{w}^{(i)}_\ell \|_{L^2(\mathbb{R}^2)} + \| \partial_d \hat{w}^{(i)}_\ell \|_{L^2(\mathbb{R}^2)} < +\infty. \]

Up to a subsequence, we have that
\[ \hat{w}^{(i)}_\ell \to \hat{w}^{(i)}, \quad \partial_d \hat{w}^{(i)}_\ell \to \partial_d \hat{w}^{(i)} \quad \text{in} \ L^2(\mathbb{R}^2), \]
for some $\hat{w}^{(i)} \in L^2(\mathbb{R}^2)$ with $\partial_d \hat{w}^{(i)} \in L^2(\mathbb{R}^2)$.

Let $\psi \in C_0^\infty(\mathbb{R}^2)$. Then,
\[ \int_{\mathbb{R}^2} \hat{w}^{(i)}_\ell \psi \, dx = \int_{\mathbb{R}^2} \hat{w}^{(i)}_\ell \chi_{cS^{(i)}_\ell} \psi \, dx = \int_{\mathbb{R}^2} w_\ell \chi_{cS^{(i)}_\ell} \psi \, dx + \int_{cS^{(i)}_\ell} (\hat{w}^{(i)}_\ell - w_\ell) \psi \, dx. \quad (33) \]

The last integral on the right hand side tends to zero, since
\[
\left| \int_{cS^{(i)}_\ell} (\hat{w}^{(i)}_\ell - w_\ell) \psi \, dx \right| \leq \int_{cS^{(i)}_\ell} |\nabla \hat{w}^{(i)}_\ell| |\ell| \psi \, dx \leq \ell \| \nabla \hat{w}^{(i)}_\ell \|_{L^2(cS^{(i)}_\ell)} \| \psi \|_{L^2(\mathbb{R}^2)}.
\]

By Theorem 6 and taking into account that $\chi_{cS^{(i)}_\ell} \to 1/3$ in $L^\infty(\mathbb{R}^2)$, passing to the limit in (33) yields that
\[ \int_{\mathbb{R}^2} \hat{w}^{(i)} \psi \, dx = \int_{\mathbb{R}^2} \frac{1}{3} w \psi \, dx \]
from which we deduce that $\hat{w}^{(i)} = \frac{1}{3} w$, for $i = 1, 2, 3$. But, by (32), $\partial_d w \in L^2(\mathbb{R}^2)$ for $i = 1, 2, 3$ and, since $w \in L^2(\mathbb{R}^2)$, we have $w \in H^1(\mathbb{R}^2)$. \hfill \Box

In the previous lemma we have deduced the weak limit of $\partial_d \hat{w}^{(i)}_\ell$. We notice that, by the definition of $\hat{w}^{(i)}_\ell$, the pointwise derivative of $\hat{w}^{(i)}_\ell$ in the direction $d_i$ coincides with the distributional derivative in the same direction. This is not the case for other directional derivatives, because the distributional gradient of $\hat{w}^{(i)}_\ell$ is singular at $\partial cS^{(i)}_\ell$ due to the discontinuity of $\hat{w}^{(i)}_\ell$. Below we denote by $g^{(i)}_\ell$ the absolutely continuous part, with respect to the 2-dimensional Lebesgue measure, of the distributional gradient of $\hat{w}^{(i)}_\ell$ and give a characterization of its limit in the next theorem.

**Theorem 8** Let $\hat{w}^{(i)}_\ell$ be as in Lemma 4 and let
\[ g^{(i)}_\ell(x) = \begin{cases} \nabla \hat{w}^{(i)}_\ell(x) & x \in cS^{(i)}_\ell, \\ 0 & \text{otherwise.} \end{cases} \quad (34) \]

Then, up to subsequences,
\[ g^{(i)}_\ell \to g^{(i)} \quad \text{in} \ L^2(\mathbb{R}^2, \mathbb{R}^2), \]
where, with $w$ as in Lemma 7,
\[ g^{(1)} = \frac{1}{3} \nabla w + \gamma p_2, \quad g^{(2)} = \frac{1}{3} \nabla w + \gamma p_1, \quad g^{(3)} = \frac{1}{3} \nabla w + \gamma p_3, \quad (36) \]
with $\gamma \in L^2(\mathbb{R}^2)$ and equal to zero almost everywhere outside of $\Omega$. 
Proof. By Lemma 5, the weak convergence stated in (35) holds for $g^{(i)} \in L^2(\mathbb{R}^2; \mathbb{R}^2)$ and for a subsequence. By definition (34), the equalities

$$g^{(i)}_\ell \cdot \frac{d_i}{|d_i|} = \partial_{d_i} \hat{w}^{(i)}_\ell$$

hold true almost everywhere in $\mathbb{R}^2$ and not just in $cS^{(i)}_\ell$, because $\partial_{d_i} \hat{w}^{(i)}_\ell = 0$ in $\mathbb{R}^2 \setminus cS^{(i)}_\ell$. Then, from (31) and by passing to the limit we find that

$$g^{(i)}_\ell \cdot \frac{d_i}{|d_i|} = \frac{1}{3} \partial_{d_i} w$$

for $i = 1, 2, 3$.

Since $d_1 \cdot p_2 = d_2 \cdot p_1 = d_3 \cdot p_3 = 0$, we can write

$$g^{(1)} = \frac{1}{3} \nabla w + \gamma^{(1)} p_2, \quad g^{(2)} = \frac{1}{3} \nabla w + \gamma^{(2)} p_1, \quad g^{(3)} = \frac{1}{3} \nabla w + \gamma^{(3)} p_3$$

with $\gamma^{(i)} \in L^2(\mathbb{R}^2)$.

We now show that

$$g^{(1)} \cdot p_3 = g^{(2)} \cdot p_3, \quad g^{(1)} \cdot p_1 = g^{(3)} \cdot p_1, \quad g^{(3)} \cdot p_2 = g^{(2)} \cdot p_2,$$

hold almost everywhere in $\mathbb{R}^2$. We limit ourselves to the proof of $g^{(1)} \cdot p_1 = g^{(3)} \cdot p_1$, since the other equalities can be proved similarly.

Let $x^\ell \in L_2(\ell)$ and define

$$\mathcal{P}^{(1)}(x^\ell) := T^{(1)}(x^\ell) \cup T^{(1)}(x^\ell + \ell p_1),$$

$$\mathcal{P}^{(3)}(x^\ell) := T^{(3)}(x^\ell) \cup T^{(3)}(x^\ell + \ell p_1),$$

see Fig. 8.

Figure 8: The regions $\mathcal{P}^{(1)}(x^\ell)$ and $\mathcal{P}^{(3)}(x^\ell)$. 
Since the triangles $T^{(1)}(x^\ell)$ and $T^{(1)}(x^\ell + \ell p_1)$ have a common side parallel to $p_1$, it follows that $\partial_{p_1} w^{(1)}_\ell$ is constant on $\mathcal{P}^{(1)}(x^\ell)$. Similarly, $\partial_{p_1} w^{(3)}_\ell$ is constant on $\mathcal{P}^{(3)}(x^\ell)$. Furthermore, on the segment joining $x^\ell$ to $x^\ell + \ell p_1$ we have $\partial_{p_1} w^{(1)}_\ell = \partial_{p_1} w^{(3)}_\ell$. Hence, we have that

$$\int_{\mathcal{P}^{(1)}(x^\ell)} \partial_{p_1} w^{(1)}_\ell \, dx = \int_{\mathcal{P}^{(3)}(x^\ell)} \partial_{p_1} w^{(3)}_\ell \, dx$$

(39)

for all lattice point $x^\ell \in L_2(\ell)$. Let $B \subset \mathbb{R}^2$ be an open subset, and let $B_\ell := \{ x \in B : \text{dist}(x, \partial B) \geq \ell \}$. If the segment joining $x^\ell$ to $x^\ell + \ell p_1$ is contained in $B_\ell$ then $\mathcal{P}^{(1)}(x^\ell) \cup \mathcal{P}^{(3)}(x^\ell) \subset B$ and hence, by (39),

$$\int_{\mathcal{P}^{(1)}(x^\ell) \cap B} \partial_{p_1} w^{(1)}_\ell \, dx = \int_{\mathcal{P}^{(3)}(x^\ell) \cap B} \partial_{p_1} w^{(3)}_\ell \, dx.$$

Therefore,

$$\left| \int_B \partial_{p_1} w^{(1)}_\ell - \partial_{p_1} w^{(3)}_\ell \, dx \right| \leq \int_{B \setminus B_\ell} \left| \partial_{p_1} w^{(1)}_\ell - \partial_{p_1} w^{(3)}_\ell \right| \, dx \leq |B \setminus B_\ell| \frac{1}{2} \left\| \partial_{p_1} w^{(1)}_\ell - \partial_{p_1} w^{(3)}_\ell \right\|_{L^2(B)} \leq C\sqrt{\ell},$$

where to obtain the last bound we used (22). By the definition of $g^{(i)}_\ell$ it follows that

$$\left| \int_B g^{(1)}_\ell \cdot p_1 - g^{(3)}_\ell \cdot p_1 \, dx \right| \leq C\sqrt{\ell},$$

and by passing to the limit we find

$$\int_B g^{(1)} \cdot p_1 - g^{(3)} \cdot p_1 \, dx = 0.$$

Since this identity holds for every open set $B$ we deduce that $g^{(1)} \cdot p_1 = g^{(3)} \cdot p_1$ almost everywhere in $\mathbb{R}^2$. This proves (38).

From (37) and (38) we find that

$$g^{(1)} \cdot p_3 - g^{(2)} \cdot p_3 = \frac{1}{2} (\gamma^{(2)} - \gamma^{(1)}) = 0,$$

$$g^{(1)} \cdot p_1 - g^{(3)} \cdot p_1 = \frac{1}{2} (\gamma^{(3)} - \gamma^{(1)}) = 0,$$

and this implies that $\gamma^{(1)} = \gamma^{(2)} = \gamma^{(3)} = \gamma$. That $\gamma$ is equal to zero almost everywhere outside of $\Omega$ it follows since $\nabla \hat{w}^{(i)}_\ell$ is equal to zero in that region.

The results obtained so far hold for whatever $k^C$ and $\tau_0$. In the next theorem we show that we can further specify $g^{(i)}$ if either one of these two constants is different from zero.

**Theorem 9** Let $w_\ell \in \mathcal{A}_\ell$ and $\hat{w}^{(i)}_\ell$ be as in Lemma 4, and let $\gamma$ be as in Theorem 8. If either $k^C \neq 0$ or $\tau_0 \neq 0$, then $\gamma = 0$ almost everywhere in $\mathbb{R}^2$. 
Proof. Let us first consider the case $k^c \neq 0$. Then, by assumption $k^c > 0$, and since $w_\ell$ satisfies the energy bound (11) we find, among other things, that

$$\sum_{x^\ell \in L_2(\ell)} \left( \Theta_{p_2}^{(c)} [w_\ell](x^\ell) \right)^2 < +\infty.$$  \hfill (40)

Set

$$\ell_\ell(x) := \sum_{x^\ell \in L_2(\ell)} \Theta_{p_2}^{(c)} [w_\ell](x^\ell) \chi_{T^\ell(x^\ell)}(x).$$

Then, $\ell_\ell \to 0$ in $L^2(\mathbb{R}^2)$. Indeed, since the area of $T^\ell(x^\ell)$ is equal to $3\sqrt{3}\ell^2/4$, we have

$$\int_{\mathbb{R}^2} (\ell_\ell)^2 \, dx = \frac{3\sqrt{3}\ell^2}{4} \sum_{x^\ell \in L_2(\ell)} \left( \Theta_{p_2}^{(c)} [w_\ell](x^\ell) \right)^2,$$

which converges to zero, as $\ell$ goes to zero, by (40).

Let $B \subset \mathbb{R}^2$ be any bounded and open set. Then,

$$0 = \lim_{\ell \to 0} \int_B \ell_\ell \, dx = \lim_{\ell \to 0} \frac{3\sqrt{3}\ell^2}{4} \sum_{x^\ell \in L_2(\ell) \cap B} \Theta_{p_2}^{(c)} [w_\ell](x^\ell)$$

and since, by (8), we have that

$$\Theta_{p_2}^{(c)} [w_\ell](x^\ell) = \frac{2\sqrt{3}}{3\ell} (w_\ell(x^\ell + \ell p_2) - w_\ell(x^\ell + \ell p_1) - w_\ell(x^\ell + \ell p_3))$$

$$= \frac{2\sqrt{3}}{3} (-p_1 \cdot \nabla w_\ell^{(1)}(x^\ell + \ell p_2) - p_2 \cdot \nabla w_\ell^{(2)}(x^\ell) - p_3 \cdot \nabla w_\ell^{(1)}(x^\ell)), $$

we can write

$$0 = \lim_{\ell \to 0} \frac{3\ell^2}{2} \sum_{x^\ell \in L_2(\ell) \cap B} (-p_1 \cdot \nabla w_\ell^{(1)}(x^\ell + \ell p_2) - p_2 \cdot \nabla w_\ell^{(2)}(x^\ell))$$

$$- p_3 \cdot \nabla w_\ell^{(1)}(x^\ell))$$

$$= \lim_{\ell \to 0} \sqrt{3} \sum_{x^\ell \in L_2(\ell) \cap B} \left( - \int_{T^1(x^\ell + \ell p_2) \cup T^1(x^\ell + \ell p_2 - \ell p_1)} p_1 \cdot \nabla w_\ell^{(1)}(x) \, dx ight)$$

$$- \int_{T^2(x^\ell) \cup T^2(x^\ell + \ell p_2)} p_2 \cdot \nabla w_\ell^{(2)}(x) \, dx$$

$$- \int_{T^1(x^\ell + \ell p_2) \cup T^1(x^\ell + \ell p_3)} p_3 \cdot \nabla w_\ell^{(1)}(x) \, dx).$$
since, for instance, \( p_3 \cdot \nabla \hat{w}^{(1)}_\ell \) is constant on \( T^{(1)}(x^\ell) \cup T^{(1)}(x^\ell + \ell p_3) \). Recalling the definition of \( g^{(i)}_\ell \), we may rewrite the previous equality as

\[
0 = \lim_{\ell \to 0} \int_B p_1 \cdot g^{(1)}_\ell(x) + p_2 \cdot g^{(2)}_\ell(x) + p_3 \cdot g^{(1)}_\ell(x) \, dx,
\]

which, by (35), implies that

\[
\int_B p_1 \cdot g^{(1)}(x) + p_2 \cdot g^{(2)}(x) + p_3 \cdot g^{(1)}(x) \, dx = 0.
\]

From the arbitrariness of the set \( B \) we find that

\[
p_1 \cdot g^{(1)} + p_2 \cdot g^{(2)} + p_3 \cdot g^{(1)} = 0,
\]

almost everywhere in \( \mathbb{R}^2 \). This is equivalent, by (36), to

\[
\frac{1}{3} \nabla w \cdot (p_1 + p_2 + p_3) - \frac{3}{2} \gamma = 0,
\]

which implies that \( \gamma = 0 \), since \( p_1 + p_2 + p_3 = 0 \).

The proof for the case \( \tau_0 \neq 0 \) is similar; hereafter we only sketch it. For

\[
\sum_{x^\ell \in L_2(\ell)} \sum_{x^\ell \in L_2(\ell)} \hat{q}_\ell(x) := \sum_{x^\ell \in L_2(\ell)} \hat{q}_\ell(\{w_\ell\}(x^\ell)) \chi_{T^\ell(x^\ell)}(x),
\]

we have that

\[
\lim_{\ell \to 0} \int_B \hat{q}_\ell \, dx = 0
\]

for any bounded open set \( B \) of \( \mathbb{R}^2 \). Hence, thanks to (10), we may write

\[
\hat{q}_\ell(\{w_\ell\}(x^\ell)) = \frac{\sqrt{3} \sqrt{3}}{3} (p_1 \cdot \nabla \hat{w}_\ell^{(1)}(x^\ell) + p_2 \cdot \nabla \hat{w}_\ell^{(2)}(x^\ell) - p_3 \cdot \nabla \hat{w}_\ell^{(1)}(x^\ell)),
\]

which let us arrive at

\[
\lim_{\ell \to 0} \int_B p_1 \cdot g^{(1)}_\ell(x) + p_2 \cdot g^{(2)}_\ell(x) + p_3 \cdot g^{(1)}_\ell(x) \, dx = 0.
\]

This identity implies, as shown above, that \( \gamma = 0 \) almost everywhere in \( \mathbb{R}^2 \).

\[\square\]

5 Lower bounds and proof of Theorem 1

We start by studying the behavior of the \( Z \)-dihedral energy. From (17) we see that the dihedral angle \( \hat{\Theta}_{p_1, p_3}[w_\ell](x^\ell) \) is proportional to \( [\nabla \hat{w}_\ell^{(1)}]^Z_{p_1}(x^\ell) \cdot p_3 \). Hence, to understand the
limit behavior of the dihedral angles we may study the behavior of particular jumps. With this in mind, we set

\[ J^{(1)}_{3\ell}(x) := \sum_{x^f \in L_2} \frac{[\nabla \hat{w}^{(1)}_{x^f}](x^f) \cdot p_3}{\sqrt{3}\ell} \chi_{P_{3\ell}^{(1)}(x^f)}(x), \]  

(41)

with \( P_{3\ell}^{(1)}(x^f) \) the parallelograms of height \( \frac{3}{2}\ell \) and base \( \sqrt{3}\ell \), with sides parallel to \( d_1 \) and \( p_1 \) passing through the nodes \( x^f + \ell p_1 \) and \( x^f + \ell p_3 \), cf. Fig. 9.

Figure 9: The regions \( P_{3\ell}^{(1)}(x^f) \) and \( P_{1\ell}^{(1)}(x^f) \).

Note that \( \cup_{x^f \in L_2(\ell)} P_{3\ell}^{(1)}(x^f) \) is equal to \( \mathbb{R}^2 \), up to a set of measure zero. By (17) we may also write

\[ J^{(1)}_{3\ell}(x) = -\sum_{x^f \in L_2} \frac{1}{2\ell} \Theta_{p_1 p_3}[w_{x^f}](x^f) \chi_{P_{3\ell}^{(1)}(x^f)}(x). \]  

(42)

Similarly, we set

\[ J^{(1)}_{1\ell}(x) := \sum_{x^f \in L_2} \frac{[\nabla \hat{w}^{(1)}_{x^f}](x^f) \cdot p_1}{\sqrt{3}\ell} \chi_{P_{1\ell}^{(1)}(x^f)}(x), \]  

(43)

with \( P_{1\ell}^{(1)}(x^f) \) the parallelograms with sides parallel to \( d_1 \) and \( p_3 \) passing through the nodes \( x^f + \ell p_1 \) and \( x^f + \ell p_3 \).

**Lemma 10** Let \( \hat{w}^{(1)}_{x^f} \) be as in Lemma 4, \( g^{(1)} \) be as in Theorem 8, \( J^{(1)}_{3\ell} \) and \( J^{(1)}_{1\ell} \) be the functions defined in (41) and (43), respectively. Then, there exists a subsequence, not relabeled, such that

\[ J^{(1)}_{3\ell} \rightharpoonup 3 \partial_{d_1} g^{(1)} \cdot p_3, \quad \text{and} \quad J^{(1)}_{1\ell} \rightharpoonup 3 \partial_{d_1} g^{(1)} \cdot p_1 \quad \text{in} \quad L^2(\mathbb{R}^2). \]  

(44)

**Proof.** By integrating (42) we find that

\[ \int_{\mathbb{R}^2} (J^{(1)}_{3\ell})^2 \, dx = \sum_{x^f \in L_2} \frac{1}{4\ell^2} \Theta_{p_1 p_3}[w_{x^f}](x^f)^2 \frac{3\sqrt{3}}{2} \ell^2 \leq C, \]
where the last inequality follows since, by assumption, $w_\ell$ satisfies the energy bound (11). Hence, there exists a subsequence of $J_{3\ell}^{(1)}$ weakly convergent in $L^2(\mathbb{R}^2)$. We now characterize its limit.

By writing explicitly the jump in (41) we find

$$J_{3\ell}^{(1)}(x) = \sum_{x^\ell \in L_2} p_3 \cdot \nabla \hat{w}_{\ell}^{(1)}(x^\ell + \ell p_1) - \nabla \hat{w}_{\ell}^{(1)}(x^\ell) \sqrt{\frac{3\ell}{3}} \chi_{P_{3\ell}^{(1)}(x^\ell)}(x),$$

which we may rewrite more compactly as

$$J_{3\ell}^{(1)}(x) = \sum_{x^\ell \in L_2} \frac{\partial_{p_3} \hat{w}_{\ell}^{(1)}(x^\ell + \ell p_1) - \partial_{p_3} \hat{w}_{\ell}^{(1)}(x^\ell)}{\sqrt{3\ell}} \chi_{P_{3\ell}^{(1)}(x^\ell)}(x).$$

Let $\varphi \in C_0^\infty(\mathbb{R}^2)$. Since

$$P_{3\ell}^{(1)}(x^\ell) := P_{3\ell}^{(1)}(x^\ell) \cap cS_\ell^{(1)},$$

the pointwise derivative $\partial_{p_3} \hat{w}_{\ell}^{(1)}$ is constant, and since for every $x \in \bar{P}_{3\ell}^{(1)}(x^\ell)$ we have that $x + \ell d_1 \in \bar{P}_{3\ell}^{(1)}(x^\ell + \ell d_1)$, the identity

$$\partial_{p_3} \hat{w}_{\ell}^{(1)}(x^\ell + \ell p_1) - \partial_{p_3} \hat{w}_{\ell}^{(1)}(x^\ell) = \partial_{p_3} \hat{w}_{\ell}^{(1)}(x + \ell d_1) - \partial_{p_3} \hat{w}_{\ell}^{(1)}(x)$$

holds for every $x \in \bar{P}_{3\ell}^{(1)}(x^\ell)$. Then,

$$\int_{\mathbb{R}^2} J_{3\ell}^{(1)} \varphi \, dx = \sum_{x^\ell \in L_2} \int_{P_{3\ell}^{(1)}(x^\ell)} \frac{\partial_{p_3} \hat{w}_{\ell}^{(1)}(x^\ell + \ell p_1) - \partial_{p_3} \hat{w}_{\ell}^{(1)}(x^\ell)}{\sqrt{3\ell}} \varphi(x) \, dx$$

$$= \sum_{x^\ell \in L_2} \int_{\bar{P}_{3\ell}^{(1)}(x^\ell)} \frac{\partial_{p_3} \hat{w}_{\ell}^{(1)}(x + \ell d_1) - \partial_{p_3} \hat{w}_{\ell}^{(1)}(x)}{\sqrt{3\ell}} \varphi(x) \, dx$$

$$+ \sum_{x^\ell \in L_2} \int_{P_{3\ell}^{(1)}(x^\ell)} \frac{\partial_{p_3} \hat{w}_{\ell}^{(1)}(x + \ell d_1) - \partial_{p_3} \hat{w}_{\ell}^{(1)}(x)}{\sqrt{3\ell}} \varphi(x + \ell/2 p_1) \, dx$$

$$+ \sum_{x^\ell \in L_2} \int_{P_{3\ell}^{(1)}(x^\ell)} \frac{\partial_{p_3} \hat{w}_{\ell}^{(1)}(x + \ell d_1) - \partial_{p_3} \hat{w}_{\ell}^{(1)}(x)}{\sqrt{3\ell}} \varphi(x - \ell/2 p_1) \, dx.$$

Hence, by a change of variables and a rearrangement of the sums we deduce

$$\int_{\mathbb{R}^2} J_{3\ell}^{(1)} \varphi \, dx = \sum_{x^\ell \in L_2} \int_{\bar{P}_{3\ell}^{(1)}(x^\ell)} \frac{\varphi(x - \ell d_1) - \varphi(x)}{\sqrt{3\ell}} \partial_{p_3} \hat{w}_{\ell}^{(1)}(x) \, dx$$

$$+ \sum_{x^\ell \in L_2} \int_{P_{3\ell}^{(1)}(x^\ell)} \frac{\varphi(x - \ell d_1 + \ell/2 p_1) - \varphi(x + \ell/2 p_1)}{\sqrt{3\ell}} \partial_{p_3} \hat{w}_{\ell}^{(1)}(x) \, dx$$

$$+ \sum_{x^\ell \in L_2} \int_{P_{3\ell}^{(1)}(x^\ell)} \frac{\varphi(x - \ell d_1 - \ell/2 p_1) - \varphi(x - \ell/2 p_1)}{\sqrt{3\ell}} \partial_{p_3} \hat{w}_{\ell}^{(1)}(x) \, dx.$$
After observing that $\partial_p \hat{w}^{(1)}_\ell(x) = g^{(1)}_\ell(x) \cdot p_3$ for every $x \in cS^{(1)}_\ell$ and recalling (35), we pass to the limit to obtain
\[
\lim_{\ell \to 0} \int_{\mathbb{R}^2} J^{(1)}_{3\ell} \varphi \, dx = 3 \int_{\mathbb{R}^2} -\partial_1 \varphi \, g^{(1)}_\ell \cdot p_3 \, dx, \quad \forall \varphi \in C^\infty_0(\mathbb{R}^2),
\]
that is,
\[
J^{(1)}_{3\ell} \rightharpoonup 3 \partial_1 \varphi g^{(1)}_\ell \cdot p_3 \text{ in } L^2(\mathbb{R}^2).
\]
The statement about $J^{(1)}_{1\ell}$ is proved similarly.

**Remark 1** To contain the notation, in Lemma 10 we stated the result just for the jumps of $\hat{w}^{(1)}_\ell$. But similarly, we may define the functions $J^{(2)}_{3\ell}$ and $J^{(2)}_{2\ell}$ for the piecewise affine interpolant $\hat{w}^{(2)}_\ell$ along the nodes of $cS^{(2)}_\ell$, and the functions $J^{(3)}_{3\ell}$ and $J^{(3)}_{2\ell}$ for the interpolant $\hat{w}^{(3)}_\ell$ along $cS^{(3)}_\ell$, and find
\[
J^{(2)}_{3\ell} \rightharpoonup 3 \partial_1 \varphi g^{(2)}_\ell \cdot p_3 \quad \text{and} \quad J^{(2)}_{2\ell} \rightharpoonup 3 \partial_1 \varphi g^{(2)}_\ell \cdot p_2,
\]
\[
J^{(3)}_{1\ell} \rightharpoonup 3 \partial_1 \varphi g^{(3)}_\ell \cdot p_1 \quad \text{and} \quad J^{(3)}_{2\ell} \rightharpoonup 3 \partial_1 \varphi g^{(2)}_\ell \cdot p_2,
\]
in $L^2(\mathbb{R}^2)$.

The next lemma deals with the regularity of $w$ and $\gamma$.

**Lemma 11** Let $w$ be as in Theorem 6 and $\gamma$ as in Theorem 8. Then $w \in H^2(\mathbb{R}^2)$, $\gamma \in H^1(\mathbb{R}^2)$, and both functions are equal to zero almost everywhere outside of $\Omega$.

**Proof.** We already know that $w \in H^1(\mathbb{R}^2)$, $\gamma \in L^2(\mathbb{R}^2)$, and that both functions are equal to zero almost everywhere outside of $\Omega$, cf. Theorem 6, Lemma 7, and Theorem 8. By Lemma 10,
\[
\partial_1 g^{(1)}_\ell \cdot p_3 \in L^2(\mathbb{R}^2), \quad \text{and} \quad \partial_1 g^{(1)}_\ell \cdot p_1 \in L^2(\mathbb{R}^2),
\]
and hence $\partial_1 g^{(1)}_\ell \in L^2(\mathbb{R}^2; \mathbb{R}^2)$. Similarly by Remark 1, we deduce that
\[
\partial_1 g^{(i)}_\ell \in L^2(\mathbb{R}^2; \mathbb{R}^2), \quad i = 1, 2, 3.
\]
By scalar multiplication by $d_i$ and $d_i^\perp$, this and (36) imply that
\[
\partial_1 d_i w \in L^2(\mathbb{R}^2), \quad \partial_1 d_i \gamma \in L^2(\mathbb{R}^2)
\]
for $i = 1, 2, 3$. This implies $w \in H^2(\mathbb{R}^2)$ and $\gamma \in H^1(\mathbb{R}^2)$.

**Proof of Theorem 1.** The proof follows by putting together Theorem 6 and Lemma 11.

We now prove a lower bound for the lim inf of the $Z$- dihedral energy.
Lemma 12 Let $w_\ell \in \mathcal{A}_\ell$ satisfy the energy bound (11), let $w \in H^2(\mathbb{R}^2)$ and $\gamma \in H^1(\mathbb{R}^2)$ be as in Theorem 11. Then,
\[
\liminf_{\ell \to 0} U_\ell^Z(w_\ell) \geq U_0^Z(w, \gamma),
\]
where
\[
U_0^Z(w, \gamma) := \frac{4\sqrt{3}}{9} k^Z \int_{\mathbb{R}^2} \left( (\partial_{d_1} p_3 w - \frac{3}{2} \partial_{d_1} \gamma)^2 + (\partial_{d_2} p_3 w - \frac{3}{2} \partial_{d_2} \gamma)^2 + (\partial_{d_3} p_1 w - \frac{3}{2} \partial_{d_3} \gamma)^2 + (\partial_{d_3} p_2 w - \frac{3}{2} \partial_{d_3} \gamma)^2 \right) d\mathbf{x}.
\]

Proof. Consider the first term of (19) and use (42) to find that
\[
\sum_{x^\ell \in L_2(\ell)} \left( \Theta^{(z)} p_{1,3} [w_\ell](x^\ell) \right)^2 = \frac{8\sqrt{3}}{9} \int_{\mathbb{R}^2} (J_{3\ell}^{(1)})^2 d\mathbf{x}.
\]
Hence, by (44),
\[
\liminf_{\ell \to 0} \frac{1}{2} k^Z \sum_{x^\ell \in L_2(\ell)} \left( \Theta^{(z)} p_{1,3} [w_\ell](x^\ell) \right)^2 \geq \frac{4\sqrt{3}}{9} k^Z \int_{\mathbb{R}^2} (\partial_{d_1} g^{(1)} \cdot p_3)^2 d\mathbf{x}.
\]
Since all the other terms of (19) can be treated similarly, we find that
\[
\liminf_{\ell \to 0} U_\ell^Z(w_\ell) \geq 4\sqrt{3} k^Z \int_{\mathbb{R}^2} (\partial_{d_1} g^{(1)} \cdot p_3)^2 + (\partial_{d_2} g^{(2)} \cdot p_1)^2 + (\partial_{d_3} g^{(2)} \cdot p_3)^2 + (\partial_{d_3} g^{(3)} \cdot p_2)^2 d\mathbf{x}.
\]
Thanks to (36), the integral on the right hand side is equal to $U_0^Z(w, \gamma)$. \qed

Remark 2 We notice that, by expressing the derivatives that appear in (45) in terms of partial derivatives with respect to Cartesian coordinates, it is possible to show that $U_0^Z(w, \gamma)$ coincides with the functional $U_0^{Z(b)}(w, \gamma)$ introduced in (15), see [9] for the details.

We now prove a lower bound for the lim inf of the $C$–dihedral energy.

Lemma 13 Let $w_\ell \in \mathcal{A}_\ell$ satisfy the energy bound (11), let $w \in H^2(\mathbb{R}^2)$ be as in Theorem 11. Then,
\[
\liminf_{\ell \to 0} U_\ell^C(w_\ell) \geq U_0^C(w),
\]
where
\[
U_0^C(w) := \frac{8\sqrt{3}}{9} k^C \int_{\mathbb{R}^2} \sum_{i=1}^3 (\partial_{p_i} w)^2 d\mathbf{x}.
\]
Proof. For $k^C = 0$ the statement of the lemma trivially holds. Hence, we suppose $k^C > 0$.

For $x^\ell \in L_2(\ell)$, denote by $T_{2\ell}^+(x^\ell)$ the trapezoid with one base the bond edge starting at $x^\ell$ and ending at $x^\ell + \ell p_2$ and the other base the segment joining the points $x^\ell + \ell p_2$ and $x^\ell + \ell p_2 - \ell p_1$. Let $T_{2\ell}^-(x^\ell)$ be the trapezoid obtained by reflecting $T_{2\ell}^+(x^\ell)$ with respect to the bond edge starting at $x^\ell$ and parallel to $p_2$, see Fig. 10.

![Diagram with trapezoids and points labeled](image)

Figure 10: The trapezoids $T_{2\ell}^+(x^\ell)$ and $T_{2\ell}^-(x^\ell)$.

Denote by $A_\ell := \frac{3\sqrt{3}}{4} \ell^2$ the area of the trapezoids, and let

$$p_{2\ell}(x) := \sum_{x^\ell \in L_2} \frac{1}{\sqrt{A_\ell}} \left( \Theta_{p_2}^{(c)} [w_\ell](x^\ell) \chi_{T_{2\ell}^+(x^\ell)}(x) - \Theta_{p_2}^{(c)} [w_\ell](x^\ell) \chi_{T_{2\ell}^-(x^\ell)}(x) \right).$$  \hspace{1cm} (47)

It follows that

$$\int_{\mathbb{R}^2} |p_{2\ell}|^2 \, dx = \sum_{x^\ell \in L_2(\ell)} \left( \Theta_{p_2}^{(c)} [w_\ell](x^\ell) \right)^2 + \left( \Theta_{p_2}^{(c)} [w_\ell](x^\ell) \right)^2 \leq C,$$  \hspace{1cm} (48)

where the last inequality follows since $w_\ell$ satisfies the energy bound (11) and because $k^C > 0$, see (7). Then, up to a subsequence, $p_{2\ell}$ weakly converges to some $\tilde{p}_2 \in L^2(\mathbb{R}^2)$. 
Since a REBO-potential-based model for graphene bending by \( \Gamma \)-convergence

Then, with (47), (49), and (50), we may compute

\[
\Theta_{p_2}[w_2](x^e) = \frac{2\sqrt{3}}{3\ell} \left[ w_\ell(x^e) - w_\ell(x^e + \ell p_3) - w_\ell(x^e + \ell p_2) \right.
\]

\[
- \left( w_\ell(x^e + \ell p_2) - w_\ell(x^e + \ell p_2 - \ell p_1) - w_\ell(x^e) \right),
\]

\[
= \frac{2\sqrt{3}}{3\ell} \left[ \tilde{w}_\ell^{(2)}(x^e) - \tilde{w}_\ell^{(2)}(x^e + \ell p_3) - \tilde{w}_\ell^{(2)}(x^e + \ell p_2) \right.
\]

\[
- \left( \tilde{w}_\ell^{(3)}(x^e + \ell p_2) - \tilde{w}_\ell^{(3)}(x^e + \ell p_2 - \ell p_1) - \tilde{w}_\ell^{(3)}(x^e) \right),
\]

\[
= \left( \nabla \tilde{w}_\ell^{(3)}(x^e + \ell p_2) - \nabla \tilde{w}_\ell^{(3)}(x^e) \right) \cdot (p_2^\perp), \quad (49)
\]

where the last identity follows by an easy calculation. Similarly, one finds

\[
\Theta_{p_2}[w_2](x^e) = \left( \nabla \tilde{w}_\ell^{(2)}(x^e + \ell p_2) - \nabla \tilde{w}_\ell^{(3)}(x^e) \right) \cdot (-p_2^\perp). \quad (50)
\]

Let

\[
A_{2\ell}(x^e) := \mathcal{T}^{+}_{2\ell}(x^e) \cup \mathcal{T}^{-}_{2\ell}(x^e).
\]

Then, with (47), (49), and (50), we may compute

\[
\int_{A_{2\ell}(x^e)} \hat{p}_{2\ell} \, d\mathbf{x} = \sqrt{A_{\ell}} \left( \Theta_{p_1}^{(c)}[w_\ell](x^e) - \Theta_{p_2}^{(c)}[w_\ell](x^e) \right)
\]

\[
= \sqrt{A_{\ell}} \left( \nabla \tilde{w}_\ell^{(3)}(x^e + \ell p_2) - \nabla \tilde{w}_\ell^{(2)}(x^e) \right)
\]

\[
+ \left( \nabla \tilde{w}_\ell^{(3)}(x^e + \ell p_2) - \nabla \tilde{w}_\ell^{(3)}(x^e) \right) \cdot p_2^\perp
\]

\[
= \sqrt{A_{\ell}} \left( \left[ \nabla \tilde{w}_\ell^{(3)}(x^e) \right]_{p_2}(x^e) \right) \cdot p_2^\perp.
\]

Since

\[
p_2^\perp = \frac{\sqrt{3}}{3} p_2 + \frac{2\sqrt{3}}{3} p_3 = -\frac{\sqrt{3}}{3} p_2 - \frac{2\sqrt{3}}{3} p_1,
\]

and since, by continuity, \( \left[ \nabla \tilde{w}_\ell^{(3)}(x^e) \right]_{p_2}(x^e) = \left[ \nabla \tilde{w}_\ell^{(2)}(x^e) \right]_{p_2}(x^e) \cdot p_2 = 0 \), we have that

\[
\int_{A_{2\ell}(x^e)} \hat{p}_{2\ell} \, d\mathbf{x} = -\frac{2\sqrt{3}}{3} \sqrt{A_{\ell}} \left( \left[ \nabla \tilde{w}_\ell^{(3)}(x^e) \right]_{p_2}(x^e) \cdot p_1 - \left[ \nabla \tilde{w}_\ell^{(2)}(x^e) \right]_{p_2}(x^e) \cdot p_3 \right).
\]

Let \( P_{1\ell}^{(3)}(x^e) \) and \( P_{3\ell}^{(2)}(x^e) \) be the rhomboidal regions used in the definition of the functions \( J_{1\ell}^{(3)} \) and \( J_{3\ell}^{(2)} \), respectively. Since the area of these regions are equal to \( 3\sqrt{3}\ell^2 / 2 \) we may write

\[
\int_{A_{2\ell}(x^e)} \hat{p}_{2\ell} \, d\mathbf{x} = -\frac{2\sqrt{3}}{3} \sqrt{A_{\ell}} \left[ \int_{P_{1\ell}^{(3)}(x^e)} \left[ \nabla \tilde{w}_\ell^{(3)}(x^e) \right]_{p_2}(x^e) \cdot p_1 \, d\mathbf{x}
\]

\[
- \int_{P_{3\ell}^{(2)}(x^e)} \left[ \nabla \tilde{w}_\ell^{(2)}(x^e) \right]_{p_2}(x^e) \cdot p_3 \, d\mathbf{x} \right]
\]

\[
= -\frac{2\sqrt{3}}{3} \sqrt{A_{\ell}} \left( \int_{P_{1\ell}^{(3)}(x^e)} J_{1\ell}^{(3)} \, d\mathbf{x} - \int_{P_{3\ell}^{(2)}(x^e)} J_{3\ell}^{(2)} \, d\mathbf{x} \right).
\]

(51)
Let $B \subset \mathbb{R}^2$ be an open set, and let
\begin{align*}
B_{\ell} &:= \{ \cup_{x^\ell \in L_2(\ell)} A_{2\ell}(x^\ell) : A_{2\ell}(x^\ell) \subset B \}, \\
B_{\ell}^{(2)} &:= \{ \cup_{x^\ell \in L_2(\ell)} P_{3\ell}^{(2)}(x^\ell) : A_{2\ell}(x^\ell) \subset B \}, \\
B_{\ell}^{(3)} &:= \{ \cup_{x^\ell \in L_2(\ell)} P_{1\ell}^{(3)}(x^\ell) : A_{2\ell}(x^\ell) \subset B \}.
\end{align*}

Then, by (51) we have
\begin{align*}
\int_{B} \frac{c}{\varepsilon} \, dx &= \lim_{\ell \to 0} \int_{B_{\ell}} \frac{c}{\varepsilon} \, dx \\
&= -\frac{2}{\sqrt{3 \sqrt{3}}} \lim_{\ell \to 0} \left( \int_{B_{\ell}^{(3)}} J_{1\ell}^{(3)} \, dx - \int_{B_{\ell}^{(2)}} J_{3\ell}^{(2)} \, dx \right) \\
&= -\frac{2}{\sqrt{3 \sqrt{3}}} \int_{B} 3 \, \partial_{d_2} g^{(3)} \cdot p_3 - 3 \, \partial_{d_3} g^{(2)} \cdot p_1 \, dx. \tag{52}
\end{align*}

By taking the characterization of the $g^{(i)}$ into account, see (36), it follows that
\begin{align*}
3(\partial_{d_2} g^{(2)} \cdot p_3 - \partial_{d_3} g^{(3)} \cdot p_1) &= (\partial_{d_2} p_3 w - \partial_{d_3} p_1 w - \frac{3}{2}(\partial_{d_2} \gamma - \partial_{d_3} \gamma)).
\end{align*}

But $\gamma = 0$ by Theorem 9. Furthermore, as it is easily seen, the following relations hold:
\begin{align*}
\partial_{d_2} p_3 w - \partial_{d_3} p_1 w &= 2 \partial_{p_2 p_2} w.
\end{align*}

Thus, (52) rewrites as
\begin{align*}
\int_{B} \frac{c}{\varepsilon} \, dx &= \frac{4}{\sqrt{3 \sqrt{3}}} \int_{B} \partial_{p_2 p_2} \, w \, dx,
\end{align*}
and since this identity holds for every open set $B$, we deduce that
\begin{align*}
\frac{c}{\varepsilon} &= \frac{4}{\sqrt{3 \sqrt{3}}} \partial_{p_2 p_2} w.
\end{align*}

Finally, from (48)
\begin{align*}
\liminf_{\ell \to 0} \sum_{x^\ell \in L_2(\ell)} \left( \Theta_{p_2}^{(c)} [w] (x^\ell) \right)^2 + \left( \Theta_{p_2}^{(c)} [w] (x^\ell) \right)^2 &= \liminf_{\ell \to 0} \int_{\mathbb{R}^2} |\frac{c}{\varepsilon}|^2 \, dx \\
&\geq \int_{\mathbb{R}^2} |\frac{c}{\varepsilon}|^2 \, dx = \frac{16 \sqrt{3}}{9} \int_{\mathbb{R}^2} (\partial_{p_2 p_2} w)^2 \, dx.
\end{align*}

Similar inequalities can be proved also for $p_1$ and $p_3$; hence, from (7) we deduce the statement of the Lemma. \qed

Next, we consider the self-energy.
Lemma 14 \ Let \( w_\ell \in \mathcal{A}_\ell \) satisfy the energy bound (11), let \( w \in H^2(\mathbb{R}^2) \) be as in Theorem 11. Then,

\[
\liminf_{\ell \to 0} U_\ell^s(w_\ell) \geq U_0^s(w),
\]

where

\[
U_0^s(w) := -\frac{\tau_0}{18} \int_{\mathbb{R}^2} \left( \sum_{i=1}^3 \partial_{p_i} p_i w \right)^2 \, dx.
\] (53)

Proof. Since the inequality trivially holds for \( \tau_0 = 0 \), we may assume \( \tau_0 < 0 \). Set

\[
\hat{s}_\ell(x) := \frac{2}{\sqrt{3} \sqrt{3} \ell} \left( \sum_{x' \in L_1(\ell)}^{(s)} \vartheta_1[w_\ell](x') \chi_{T^\ell(x')}(x) + \sum_{x' \in L_2(\ell)}^{(s)} \vartheta_2[w_\ell](x') \chi_{T^\ell(x')}(x) \right).
\]

Then, since the area of \( T^\ell(x) \) is equal to \( 3\sqrt{3}\ell^2/4 \), with (9),

\[
\int_{\mathbb{R}^2} |\hat{s}_\ell|^2 \, dx = \sum_{x' \in L_1(\ell)}^{(s)} \left( \vartheta_1[w_\ell](x') \right)^2 + \sum_{x' \in L_2(\ell)}^{(s)} \left( \vartheta_2[w_\ell](x') \right)^2 \leq C,
\] (54)

where the inequality follows because \( w_\ell \) satisfies the energy bound (11). Hence, up to a subsequence,

\[
\hat{s}_\ell \rightharpoonup \hat{p} \quad \text{in} \quad L^2(\mathbb{R}^2),
\]

for some \( \hat{p} \in L^2(\mathbb{R}^2) \).

From (10) we compute the strain measures

\[
\vartheta_1[w_\ell](x') = \frac{\sqrt{3\sqrt{3}}}{3\ell} \left( \hat{w}_\ell^{(3)}(x' - \ell p_1) - \hat{w}_\ell^{(3)}(x') \right)
\]

\[
+ \hat{w}_\ell^{(2)}(x' - \ell p_2) - \hat{w}_\ell^{(2)}(x')
\]

\[
+ \hat{w}_\ell^{(1)}(x' - \ell p_3) - \hat{w}_\ell^{(1)}(x'),
\]

\[
= -\frac{\sqrt{3\sqrt{3}}}{3} \left( \partial_{p_1} \hat{w}_\ell^{(3)}(x') + \partial_{p_2} \hat{w}_\ell^{(2)}(x') + \partial_{p_3} \hat{w}_\ell^{(1)}(x') \right).
\]

and

\[
\vartheta_2[w_\ell](x') = \frac{\sqrt{3\sqrt{3}}}{3} \left( \partial_{p_1} \hat{w}_\ell^{(3)}(x') + \partial_{p_2} \hat{w}_\ell^{(2)}(x') + \partial_{p_3} \hat{w}_\ell^{(1)}(x') \right).
\]
Therefore the function \( \hat{p}_l \) takes the form

\[
\hat{p}_l(x) = \frac{2}{3\ell} \left( \sum_{x^i \in L_2(\ell)} \left( \partial_{p_1} \hat{w}_l^{(3)}(x^i) + \partial_{p_2} \hat{w}_l^{(2)}(x^i) + \partial_{p_3} \hat{w}_l^{(1)}(x^i) \right) \chi_{T^l(x^i)}(x) \right)
- \sum_{x^i \in L_1(\ell)} \left( \partial_{p_1} \hat{w}_l^{(3)}(x^i) + \partial_{p_2} \hat{w}_l^{(2)}(x^i) + \partial_{p_3} \hat{w}_l^{(1)}(x^i) \right) \chi_{T^l(x^i)}(x) \right)

= \frac{2}{3}(\hat{p}_{1l}(x) + \hat{p}_{2l}(x) + \hat{p}_{3l}(x)),
\]

where we have set

\[
\hat{p}_{1l}(x) := \frac{1}{\ell} \left( \sum_{x^i \in L_2(\ell)} \partial_{p_1} \hat{w}_l^{(3)}(x^i) \chi_{T^l(x^i)}(x) - \sum_{x^i \in L_1(\ell)} \partial_{p_1} \hat{w}_l^{(3)}(x^i) \chi_{T^l(x^i)}(x) \right),
\]

\[
\hat{p}_{2l}(x) := \frac{1}{\ell} \left( \sum_{x^i \in L_2(\ell)} \partial_{p_2} \hat{w}_l^{(2)}(x^i) \chi_{T^l(x^i)}(x) - \sum_{x^i \in L_1(\ell)} \partial_{p_2} \hat{w}_l^{(2)}(x^i) \chi_{T^l(x^i)}(x) \right),
\]

\[
\hat{p}_{3l}(x) := \frac{1}{\ell} \left( \sum_{x^i \in L_2(\ell)} \partial_{p_3} \hat{w}_l^{(1)}(x^i) \chi_{T^l(x^i)}(x) - \sum_{x^i \in L_1(\ell)} \partial_{p_3} \hat{w}_l^{(1)}(x^i) \chi_{T^l(x^i)}(x) \right).
\]

Let \( \varphi \in C_0^\infty(\mathbb{R}^2) \). Then

\[
\int_{\mathbb{R}^2} \hat{p}_l \varphi \, dx = \frac{2}{3} \sum_{i=1}^3 \int_{\mathbb{R}^2} \hat{p}_{il} \varphi \, dx. \tag{55}
\]

We focus on the case \( i = 3 \), the other cases are treated similarly. We have

\[
\int_{\mathbb{R}^2} \hat{p}_{3l} \varphi \, dx = \frac{1}{\ell} \left( \sum_{x^i \in L_2(\ell)} \partial_{p_3} \hat{w}_l^{(1)}(x^i) \int_{T^l(x^i)} \varphi \, dx \right)
- \sum_{x^i \in L_1(\ell)} \partial_{p_3} \hat{w}_l^{(1)}(x^i) \int_{T^l(x^i)} \varphi \, dx

= \frac{1}{\ell} \left( \sum_{x^i \in L_2(\ell)} \partial_{p_3} \hat{w}_l^{(1)}(x^i) \int_{T^l(x^i)} \varphi \, dx \right)
- \partial_{p_3} \hat{w}_l^{(1)}(x^i + \ell p_3) \int_{T(x^i + \ell p_3)} \varphi \, dx

= \frac{1}{\ell} \sum_{x^i \in L_2(\ell)} \partial_{p_3} \hat{w}_l^{(1)}(x^i) \left( \int_{T^l(x^i)} \varphi \, dx - \int_{T(x^i + \ell p_3)} \varphi \, dx \right),
\]

where we have used that \( \partial_{p_3} \hat{w}_l^{(1)}(x^i) = \partial_{p_3} \hat{w}_l^{(1)}(x^i + \ell p_3) \).

By using Taylor’s expansion theorem we get

\[
\varphi(x) = \varphi(x^i) + \nabla \varphi(x^i) \cdot (x - x^i) + O(|x - x^i|^2),
\]
Similarly, and from (55), it follows that
\[
\frac{1}{\ell} \left( \int_{T^t(x^{\ell})} \varphi \, dx - \int_{T(x^t+\ell p_3)} \varphi \, dx \right) = \frac{3\sqrt{3} \ell^2}{4} \left( - \nabla \varphi(x^{\ell}) \cdot p_3 + O(\ell^3) \right)
\]
\[
= \frac{3}{2} \int_{T^{(1)}(x^{\ell}) \cup T^{(1)}(x^{\ell}+\ell p_3)} \partial_{p_3} \varphi(x^{\ell}) \, dx + O(\ell^3)
\]
\[
= -\frac{3}{2} \int_{T^{(1)}(x^{\ell}) \cup T^{(1)}(x^{\ell}+\ell p_3)} \partial_{p_3} \varphi(x) \, dx + O(\ell^3).
\]

Taking into account that \( \partial_{p_3} \hat{w}_i^{(1)}(x^{\ell}) \) is constant on \( T^{(1)}(x^{\ell}) \cup T^{(1)}(x^{\ell}+\ell p_3) \), we have
\[
\int_{\mathbb{R}^2} \hat{p}_3 \varphi \, dx = -\frac{3}{2} \sum_{x^{\ell} \in L_2(\ell)} \int_{T^{(1)}(x^{\ell}) \cup T^{(1)}(x^{\ell}+\ell p_3)} \partial_{p_3} \hat{w}_i^{(1)}(x) \partial_{p_3} \varphi(x) \, dx + O(\ell)
\]
\[
= -\frac{3}{2} \int_{S_3^{(1)}} \partial_{p_3} \hat{w}_i^{(1)}(x) \partial_{p_3} \varphi(x) \, dx + O(\ell)
\]
\[
= -\frac{3}{2} \int_{\mathbb{R}^2} p_3 \cdot g_i^{(1)}(x) \partial_{p_3} \varphi(x) \, dx + O(\ell),
\]
that leads to
\[
\lim_{\ell \to 0} \int_{\mathbb{R}^2} \hat{p}_3 \varphi \, dx = -\frac{3}{2} \int_{\mathbb{R}^2} p_3 \cdot g^{(1)} \partial_{p_3} \varphi \, dx = \frac{3}{2} \int_{\mathbb{R}^2} p_3 \cdot \partial_{p_3} g^{(1)} \varphi \, dx.
\]

Similarly,
\[
\lim_{\ell \to 0} \int_{\mathbb{R}^2} \hat{p}_1 \varphi \, dx = \frac{3}{2} \int_{\mathbb{R}^2} p_1 \cdot \partial_{p_1} g^{(3)} \varphi \, dx,
\]
\[
\lim_{\ell \to 0} \int_{\mathbb{R}^2} \hat{p}_2 \varphi \, dx = \frac{3}{2} \int_{\mathbb{R}^2} p_2 \cdot \partial_{p_2} g^{(2)} \varphi \, dx,
\]
and, from (55), it follows that
\[
\hat{p} = p_1 \cdot \partial_{p_1} g^{(3)} + p_2 \cdot \partial_{p_2} g^{(2)} + p_1 \cdot \partial_{p_1} g^{(3)}
\]
\[
= \frac{3}{3} \sum_{i=1} \partial_{p_i} w_i - \frac{1}{2} \partial_{p_i} \gamma = \frac{1}{3} \sum_{i=1} \partial_{p_i} w_i
\]
where we used (36) and the fact that \( \gamma = 0 \) since we have assumed \( \tau_0 < 0 \), cf. Theorem 9.

Finally, from (54) we find
\[
\liminf_{\ell \to 0} U^s_\ell(w_\ell) = \liminf_{\ell \to 0} \frac{-\tau_0}{2} \int_{\mathbb{R}^2} \hat{p}_\ell^2 \, dx
\]
\[
\geq \frac{-\tau_0}{2} \int_{\mathbb{R}^2} \hat{p}^2 \, dx = \frac{-\tau_0}{18} \int_{\mathbb{R}^2} \left( \sum_{i=1} \partial_{p_i} w_i \right)^2 \, dx.
\]
\[\square\]
6 Proofs of Theorems 2 and 3

In this final section we prove that the lower bounds obtained in Section 5 provide in fact the $\Gamma$-limit of the energy functional in the two cases envisaged in Theorems 2 and 3. To accomplish the task we need to show that the lower bounds can be achieved; in the case of smooth target functions, this is done in the next Lemma.

Lemma 15 Let $w \in C^\infty(\mathbb{R}^2)$ and $\gamma \in C^\infty(\mathbb{R}^2)$ be two functions with support in $\Omega$. Then,

1. if $k^c = \tau_0 = 0$, there exists a $w_\ell \in \mathcal{A}_\ell$ such that $w_\ell \to w$ in $L^2(\mathbb{R}^2)$, and
   \[
   \lim_{\ell \to 0} U_\ell(w_\ell) = U^Z_0(w, \gamma),
   \]
   with $U^Z_0(w, \gamma)$ defined in (45);

2. if either $k^c \neq 0$ or $\tau_0 \neq 0$, there exists a $w_\ell \in \mathcal{A}_\ell$ such that $w_\ell \to w$ in $L^2(\mathbb{R}^2)$, and
   \[
   \lim_{\ell \to 0} U_\ell(w_\ell) = U_0(w),
   \]
   with
   \[
   U_0(w) := U^Z_0(w, 0) + U^C_0(w) + U^s_0(w),
   \]
   cf. (45), (46), and (53).

Proof. We start by proving 1. Let

\[
\Theta_{p, p+1}[w_\ell](x) = \frac{2\sqrt{3}}{3\ell} \left[ w(x^\ell + \ell p_i - \ell p_{i+1}) + \frac{3}{2} \ell \gamma(x^\ell + \ell p_i - \ell p_{i+1}) - w(x^\ell + \ell p_i) + w(x^\ell + \ell p_{i+1}) - w(x^\ell) - \frac{3}{2} \ell \gamma(x^\ell) \right],
\]

and by Taylor expanding $w$ up to second order and $\gamma$ up to first order, we find:

\[
\Theta_{p, p+1}[w_\ell](x^\ell) = \frac{2\sqrt{3}}{3} \left( \nabla^2 w(x^\ell)p_{i+1} \cdot (p_{i+1} - p_i) + \frac{3}{2} \nabla \gamma(x^\ell) \cdot (p_i - p_{i+1}) + o(1) \right),
\]

\[
= 2\ell \left( \nabla^2 w(x^\ell)p_{i+1} - \frac{3}{2} \nabla \gamma(x^\ell) \right) \cdot \frac{p_{i+1} - p_i}{|p_{i+1} - p_i|} + o(\ell).
\]
Similarly, we find:

\[ (z) \Theta_{\vec{p}_i,\vec{p}_{i+2}}[w_\ell](x^\ell) = \frac{2\sqrt{3}\ell}{3} \left( \nabla^2 w(x^\ell) \vec{p}_{i+2} - \frac{3}{2} \nabla \gamma(x^\ell) \right) \cdot \frac{\vec{p}_{i+2} - \vec{p}_i}{|\vec{p}_{i+2} - \vec{p}_i|} + o(\ell). \]

The \( Z \)-dihedral energy (5) takes the form

\[
U^Z_\ell(w_\ell) = 2\ell^2 k^Z \sum_{x^\ell \in L_2(\ell)} \sum_{i=1}^{3} \left\{ \left( \nabla^2 w(x^\ell) \vec{p}_{i+1} - \frac{3}{2} \nabla \gamma(x^\ell) \right) \cdot \frac{\vec{p}_{i+1} - \vec{p}_i}{|\vec{p}_{i+1} - \vec{p}_i|} \right\}^2 + \left( \nabla^2 w(x^\ell) \vec{p}_{i+2} - \frac{3}{2} \nabla \gamma(x^\ell) \right) \cdot \frac{\vec{p}_{i+2} - \vec{p}_i}{|\vec{p}_{i+2} - \vec{p}_i|} \right\}^2 \right\} + o(1). \tag{57}
\]

Let \( E^\ell(x^\ell) \) be the hexagon of side length \( \ell \) centered at \( x^\ell \) and with two sides parallel to \( \vec{p}_1 \), see Fig. 11, and observe that the area of the hexagon \( E^\ell(x^\ell) \) is \( 3\sqrt{3}\ell^2/2 \). Thence, (57) can be written as

\[
U^Z_\ell(w_\ell) = \frac{4\sqrt{3}}{9} k^Z \int_{\mathbb{R}^2} W^Z_\ell(x) d\vec{x} + o(1),
\]

with \( W^Z_\ell \) defined by

\[
W^Z_\ell(x) := \sum_{x^\ell \in L_2(\ell)} \sum_{i=1}^{3} \left\{ \left( \nabla^2 w(x^\ell) \vec{p}_{i+1} - \frac{3}{2} \nabla \gamma(x^\ell) \right) \cdot \frac{\vec{p}_{i+1} - \vec{p}_i}{|\vec{p}_{i+1} - \vec{p}_i|} \right\}^2 + \left( \nabla^2 w(x^\ell) \vec{p}_{i+2} - \frac{3}{2} \nabla \gamma(x^\ell) \right) \cdot \frac{\vec{p}_{i+2} - \vec{p}_i}{|\vec{p}_{i+2} - \vec{p}_i|} \right\} \chi_{E^\ell(x^\ell)}(x).
\]

Figure 11: The hexagon \( E^\ell(x^\ell) \).
Hence, by passing to the limit we find
\[
\lim_{\ell \to 0} \mathcal{U}_\ell(w_\ell) = \lim_{\ell \to 0} \mathcal{U}^Z_\ell(w_\ell) = \frac{4\sqrt{3}}{9} k^z \int_{\mathbb{R}^2} W^Z_0(x) \, dx,
\]
where
\[
W^Z_0(x) := \sum_{i=1}^3 \left\{ \left( (\nabla^2 w(x)p_{i+1} - \frac{3}{2} \nabla \gamma(x)) \cdot \frac{p_{i+1} - p_i}{|p_{i+1} - p_i|} \right)^2 
+ \left( (\nabla^2 w(x)p_{i+2} - \frac{3}{2} \nabla \gamma(x)) \cdot \frac{p_{i+2} - p_i}{|p_{i+2} - p_i|} \right)^2 \right\}.
\]

From the definitions of \(p_i\) and \(d_i\) it is
\[
p_2 - p_1 = d_3, \quad p_3 - p_2 = d_2, \quad \text{and} \quad p_1 - p_3 = d_1.
\]

Then, we easily check that the limit energy coincides with \(\mathcal{U}^Z_0(w, \gamma)\).

We now prove 2. Let
\[
w_\ell(x) := \sum_{x^\ell \in L_1(\ell) \cup L_2(\ell)} w(x^\ell) \chi_{T^\ell(x^\ell)}(x).
\]
Then, \(w_\ell \to w\) in \(L^2(\mathbb{R}^2)\) and for \(\ell\) small enough \(w_\ell \in A_\ell\). Setting \(\gamma = 0\) in the proof of 1., we find
\[
\lim_{\ell \to 0} \mathcal{U}^Z_\ell(w_\ell) = \mathcal{U}^Z_0(w, 0).
\]

Let us consider the \(C\)-dihedral energy. By Taylor expanding \(w\) around \(x^\ell\) up to second order, from (8) we find that
\[
\Theta^{(c)}_{p_i^1}[w_\ell](x^\ell) = 2\ell \nabla^2 w(x^\ell) p_i^1 \cdot p_i^1 + o(\ell),
\]
\[
\Theta^{(c)}_{p_i^-}[w_\ell](x^\ell) = 2\ell \nabla^2 w(x^\ell) p_i^- \cdot p_i^- + o(\ell),
\]
see Appendix A.3 of [9] if further details are needed. Then, (7) writes as
\[
\mathcal{U}_\ell^C(w_\ell) = 4k^c \sum_{x^\ell \in L_2(\ell)} \sum_{i=1}^3 \left( 2\ell \nabla^2 w(x^\ell) p_i \cdot p_i^1 + o(\ell) \right)^2
= \frac{8\sqrt{3}}{9} k^c \int_{\mathbb{R}^2} \sum_{x^\ell \in L_2(\ell)} \sum_{i=1}^3 \left( \nabla^2 w(x^\ell) p_i \cdot p_i^1 \right)^2 \chi_{E^\ell(x^\ell)}(x) \, dx + o(1),
\]
where \(E^\ell(x^\ell)\) is the hexagon defined above of area \(3\sqrt{3} \ell^2/2\). From this identity we immediately deduce that
\[
\lim_{\ell \to 0} \mathcal{U}_\ell^C(w_\ell) = \mathcal{U}^C_0(w).
\]
Similarly, from (10) we find
\[
\vartheta_1^{(s)}[w_{\ell}](x^L) = \frac{\sqrt{3\sqrt{3}}}{6} \nabla^2 w(x^L)p_i \cdot p_i + o(\ell),
\]
and hence the self-stress energy (9) writes as
\[
U_{ss}^{(s)}(w_{\ell}) = -\frac{\sqrt{3}}{24} \tau_0 \sum_{x^L \in L_1(\ell) \cup L_2(\ell)} \left( \ell \nabla^2 w(x^L)p_i \cdot p_i + o(\ell) \right)^2
\]
\[
= -\frac{1}{18} \tau_0 \int_{\mathbb{R}^2} \sum_{x^L \in L_1(\ell) \cup L_2(\ell)} \left( \nabla^2 w(x^L)p_i \cdot p_i \right)^2 \chi_{T^L(x^L)}(x) \, dx + o(1),
\]
since the area of $T^L(x^L)$ is $3\sqrt{3} \ell^2/4$. It follows that
\[
\lim_{\ell \to 0} U_{ss}^{(s)}(w_{\ell}) = U_0^{(s)}(w). \tag{60}
\]
From (58), (59), and (60), and recalling the definition (56) of $U_0$ we conclude the proof. \qed

**Proof of Theorem 2.** We first note that $U_0$, as defined in (56), coincides with $U_0^{(b)}$ as given in (14). Indeed, it suffices to rewrite the derivatives appearing in $U_0$ with respect to the coordinates $x_1$ and $x_2$ of a Cartesian orthogonal system, see [9] for further details. We need to prove that:

1. **(LIMINF Inequality)** for every $w \in L^2(\Omega)$ and for every sequence $w_{\ell}$ converging to $w$ in $L^2(\Omega)$
   \[
   \liminf_{\ell \to 0} U_{ss}^{(s)}(w_{\ell}) \geq U_0^{(s)}(w);
   \]
2. **(Recovery Sequence)** for every $w \in L^2(\Omega)$ there exists a sequence $w_{\ell}$ converging to $w$ in $L^2(\Omega)$ such that
   \[
   \limsup_{\ell \to 0} U_{ss}^{(s)}(w_{\ell}) \leq U_0^{(s)}(w).
   \]

We start by proving 1. Let $w, w_{\ell} \in L^2(\Omega)$ such that $w_{\ell} \to w$ in $L^2(\Omega)$ and, without loss of generality, $\liminf_{\ell \to 0} U_{ss}^{(s)}(w_{\ell}) < +\infty$. Then, up to a subsequence (not relabeled), by (13) we have that
\[
U_{ss}^{(s)}(w_{\ell}) = U_0(w_{\ell}), \quad \sup_\ell U_{ss}(w_{\ell}) < +\infty, \quad w_{\ell} \in A_{\ell}.
\]
By Lemma 11, $w \in H^3_0(\Omega)$, and by Theorem 9 we find $\gamma = 0$. By combining Lemmas 12, 13, and 14, we deduce that
\[
\liminf_{\ell \to 0} U_{ss}(w_{\ell}) \geq U_0(w).
\]
We now prove 2. Let \( w \in L^2(\Omega) \) be such that, without loss of generality, \( \mathcal{U}_0^e(w) < +\infty \). Then, from the definition of \( \mathcal{U}_0^e \) we infer that \( w \in H_0^2(\Omega) \). Let \( w^k \in C_0^\infty(\Omega) \) be a sequence such that \( w^k \to w \) in \( H^2(\Omega) \) as \( k \) tends to \( +\infty \), so that
\[
\lim_{k \to +\infty} \mathcal{U}_0^e(w^k) = \mathcal{U}_0^e(w).
\]

By Lemma 15, for every \( k \) there exists a sequence \( w^k_\ell \) such that \( w^k_\ell \to w^k \) in \( L^2(\Omega) \), as \( \ell \to 0 \), and
\[
\limsup_{\ell \to 0} \mathcal{U}_\ell(w^k_\ell) \leq \mathcal{U}_0^e(w^k).
\]

Combining the two limits we find
\[
\lim_{k \to +\infty} \limsup_{\ell \to 0} \mathcal{U}_\ell(w^k_\ell) \leq \lim_{k \to +\infty} \mathcal{U}_0^e(w^k) = \mathcal{U}_0^e(w).
\]

By a diagonal argument there exists an increasing mapping \( \ell \mapsto k(\ell) \) such that \( w^{k(\ell)}_\ell \to w \) in \( L^2(\Omega) \) and
\[
\limsup_{\ell \to 0} \mathcal{U}_\ell(w^{k(\ell)}_\ell) \leq \mathcal{U}_0^e(w).
\]

Hence, part 2. is proven. \( \square \)

**Proof of Theorem 3.** We recall that \( \mathcal{U}_0^Z \) defined in (15) takes also the form given in (45).

We start by proving the liminf inequality. Let \( w, w_\ell \in L^2(\Omega) \) such that \( w_\ell \to w \) in \( L^2(\Omega) \). Arguing as in the proof of Theorem 2, from the assumption that \( \sup_\ell \mathcal{U}_\ell^Z < \infty \) we deduce that \( \mathcal{U}_\ell^Z(w_\ell) = \mathcal{U}_\ell^Z(w) \), that \( w_\ell \in \mathcal{A}_\ell \) and that \( w \in H_0^2(\Omega) \). By Lemma 12, it follows that
\[
\liminf_{\ell \to 0} \mathcal{U}_\ell^Z(w_\ell) \geq \mathcal{U}_0^Z(w, \gamma) \geq \inf_{\gamma \in H_0^1(\Omega)} \mathcal{U}_0^Z(w, \gamma)
\]
\[
= \mathcal{U}_0^Z(w, (-\Delta)^{-1}(-2/3 \partial_{p_1p_2p_3} w)),
\]

where the last identity can be found by writing the Euler-Lagrange equation that the minimizer \( \gamma \) satisfies.

We now prove the recovery sequence condition. Without loss of generality, let \( w \in L^2(\Omega) \) be such that \( \mathcal{U}_0^Z(w) < +\infty \). Then, from the definition of \( \mathcal{U}_0^Z \) we infer that \( w \in H_0^2(\Omega) \). Set \( \gamma := (-\Delta)^{-1}(-2/3 \partial_{p_1p_2p_3} w) \in H_0^1(\Omega) \).

Let \( w^k, \gamma^k \in C_0^\infty(\Omega) \) be two sequences such that \( w^k \to w \) in \( H^2(\Omega) \) and \( \gamma^k \to \gamma \) in \( H^1(\Omega) \), as \( k \) tends to \( +\infty \). Then,
\[
\lim_{k \to +\infty} \mathcal{U}_0^Z(w^k, \gamma^k) = \mathcal{U}_0^Z(w, \gamma).
\]

By Lemma 15, for every \( k \) there exists a sequence \( w^k_\ell \) such that \( w^k_\ell \to w^k \) in \( L^2(\Omega) \), as \( \ell \to 0 \), and
\[
\limsup_{\ell \to 0} \mathcal{U}_\ell^Z(w^k_\ell) \leq \mathcal{U}_0^Z(w^k, \gamma^k).
\]
So, passing to the limit on the two sides of (61) yields that
\[
\lim_{k \to +\infty} \limsup_{\ell \to 0} \mathcal{U}_\ell^Z(w_k^\ell) \leq \lim_{k \to +\infty} \mathcal{U}_0^Z(w_k, \gamma_k) = \mathcal{U}_0^Z(w, \gamma).
\]
Again, by a diagonal argument there exist \(w_k^{k(\ell)}\) such that \(w_k^{k(\ell)} \to w\) in \(L^2(\Omega)\) and
\[
\limsup_{\ell \to 0} \mathcal{U}_\ell(w_k^{k(\ell)}) \leq \mathcal{U}_0^Z(w, (-\Delta)^{-1}(-\frac{2}{3}\partial_{p_1p_2p_3}w)),
\]
which completes the proof. \(\Box\)

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