DERIVATION OF A ROD THEORY FROM LATTICE SYSTEMS WITH INTERACTIONS BEYOND NEAREST NEIGHBOURS

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Abstract. We study continuum limits of discrete models for (possibly heterogeneous) nanowires. The lattice energy includes at least nearest and next-to-nearest neighbour interactions: the latter have the role of penalising changes of orientation. In the heterogeneous case, we obtain an estimate on the minimal energy spent to match different equilibria. This gives insight into the nucleation of dislocations in epitaxially grown heterostructured nanowires.

Introduction. In this paper we study an atomistic model for (possibly heterogeneous) nanowires. We consider a scaling of the energy that corresponds to a reduction of the system from N dimensions to one dimension and, in addition, accounts for transitions between different equilibria.

Specifically, in the homogeneous case, we study the asymptotic behaviour of the energy defined by

$$\mathcal{E}_\varepsilon(u) := \sum_{\substack{i,j\in\mathbb{Z}^N \\ |i-j|\leq R}} \left(\frac{|u(\varepsilon i) - u(\varepsilon j)|}{\varepsilon} - |i-j| \right)^p , \tag{0.1}$$

where $p > 1$ and u is a deformation of the portion of the lattice $\varepsilon\mathbb{Z}^N$ modelling the nanowire; the small parameter $\varepsilon > 0$ represents the atomic distance and $R > 0$ is sufficiently large to include a certain number of interactions beyond nearest neighbours. The above sum is taken over a "thin" domain, i.e., a domain consisting of a few lines of atoms (for the precise formula see (1.4)); as the lattice distance converges to zero, we perform a discrete to continuum limit and a dimension reduction simultaneously.

This model was first studied in [14, 15] under the assumption that the admissible deformations satisfy the non-interpenetration condition, namely, that the Jacobian determinant of a suitably defined piecewise affine interpolation of u is positive. Here we remove such assumption and we show that, by incorporating into the energy the effect of interactions in a certain finite range, one can recover the results of [14, 15] and get even further insight into the problem. More precisely, we obtain an effective energy that accounts for the effects of changes of orientation in the lattice. The latter are thus allowed, but energetically penalised. We remark that, in dimension two, our analysis corresponds to the first-order Γ-limit of a functional of the kind studied in [1, 18] without non-interpenetration assumptions. We also point out that the effects of long range interactions in non-convex lattice systems have already been analysed in [7, 5, 6] in the one-dimensional case.

For the scaling of (0.1), we obtain a complete description of the Γ-limit with respect to two different topologies (Theorems 5.1 and 5.4). It turns out that the Γ-limit with respect to the topology used in [14, 15] is trivial (see Remark 4), that is, one can exhibit recovery sequences for which the gradient always lies in the same energy well up to an asymptotically vanishing correction. In order to see the effects of changes of orientation in the nanowire, we introduce a stronger topology which is sensitive to them. In this case, for each change of orientation, the Γ-limit gives a finite positive contribution which is characterised by a discrete optimal transition problem. Moreover, one can prove that if we prescribe affine boundary conditions of the type $x \mapsto Bx$ with $\mathrm{dist}(B; SO(N))$ sufficiently small, then recovery sequences for minimisers will always preserve orientation (Remark 6). In this respect our model is consistent with the non-interpenetration condition. On the other hand, we also show that minimisers may violate such condition if we add to the functionals pathological loading terms which force the deformations to overcome the energetic barrier between equilibria with opposite orientation (see Section 6 and Remark 7).

The Γ-limit is nontrivial, also in the weaker topology, when one considers heterogeneous nanowires, which consist of components with different equilibria, arranged longitudinally; i.e., the interface between the components is a cross-section of the rod. In this case, we prove an estimate on the minimal energy spent to match the equilibria. Precisely, denoting by $k \in \mathbb{N}$ the number of atomic layers of the nanowire, we show that the minimal cost grows faster than k^{N-1}. The proof of such result (Theorem 2.2) follows as an application of [2, Theorem 3.1]. Such lower bound is to be compared with the estimate that one can prove in the case of a two- or three-dimensional model accounting for dislocations. This is discussed in Section

[7] where we compare the minimal energy of heterogeneous defect-free systems and the minimal energy of heterogeneous systems containing dislocations. It turns out that for sufficiently large values of k, the latter are energetically preferred since their energy may grow exactly like k^{N-1} (see Remark [8]). In this respect our result is consistent with the one proven in [14, 15] under the non-interpenetration assumption. We recall that the first variational justification of dislocation nucleation in nanowire heterostructures was obtained in [17] in the context of non-linear elasticity. This result was later generalised to a discrete to continuum setting in [14, 15] under the non-interpenetration condition, and is here validated without the latter assumption. More recently, variational models for misfit dislocations at semi-coherent interfaces and in elastic thin films have been proposed in [10] and [11] respectively.

The paper is organised as follows. In Section [1] we introduce the model. In Section [2] we introduce the minimal costs to bridge different equilibria and study their dependence on the thickness of the nanowire. In Sections [3]–[5], performing a discrete to continuum limit and a dimension reduction simultaneously, we characterise the Γ-limit of the energy functional for different choices of the topology (Theorems [5.1] and [5.4]). All the results are stated in the general case of heterogeneous nanowires. In Section [6] we discuss the effect of boundary conditions on the Γ-limit and briefly study a model including external forces (only in the homogeneous case, for simplicity). In the final part of the paper, Section [7], we compare the model for defect-free nanowires with models including dislocations at the interface, showing that the latter are energetically favoured.

Notation. We recall some basic notions of geometric measure theory for which we refer to [3]. Given a bounded open set $\Omega \subset \mathbb{R}^N$, $N \geq 2$, and $M \geq 1$, $BV(\Omega; \mathbb{R}^M)$ denotes the space of functions of bounded variation; i.e., of functions $u \in L^1(\Omega; \mathbb{R}^M)$ whose distributional gradient $\mathrm{D}u$ is a Radon measure on Ω with $|\mathrm{D}u|(\Omega) < +\infty$, where $|\mathrm{D}u|$ is the total variation of $\mathrm{D}u$. If $u \in BV(\Omega; \mathbb{R}^M)$, the symbol ∇u stands for the density of the absolutely continuous part of $\mathrm{D}u$ with respect to the N-dimensional Lebesgue measure $\mathcal{L}^N$. We denote by J_u the jump set of u, by u^+ and u^- the traces of u on J_u, and by $\nu_u(x)$ the measure theoretic inner normal to J_u at x, which is defined for $\mathcal{H}^{N-1}$-a.e. $x \in J_u$, where $\mathcal{H}^{N-1}$ is the $(N-1)$-dimensional Hausdorff measure. A function $u \in BV(\Omega; \mathbb{R}^M)$ is said to be a special function of bounded variation if $\mathrm{D}u - \nabla u\, \mathcal{L}^N$ is concentrated on J_u; in this case one writes $u \in SBV(\Omega; \mathbb{R}^M)$. Given a set $E \subset \Omega$, we denote by $P(E, \Omega)$ its relative perimeter in Ω and by $\partial^* E$ its reduced boundary. We recall that a partition $\{E_i\}_{i \in \mathbb{N}}$ of Ω is called a Caccioppoli partition if $\sum_{i \in \mathbb{N}} P(E_i, \Omega) < +\infty$. Given a rectifiable set $K \subset \Omega$, we say that a Caccioppoli partition $\{E_i\}_{i \in \mathbb{N}}$ of Ω is subordinated to K if for every $i \in \mathbb{N}$ the reduced boundary $\partial^* E_i$ of E_i is contained in K, up to a $\mathcal{H}^{N-1}$-negligible set.

For $N \geq 2$, $\mathbb{M}^{N \times N}$ is the set of real $N \times N$ matrices, $GL^+(N)$ is the set of matrices with positive determinant, $O(N)$ is the set of orthogonal matrices, and $SO(N)$ is the set of rotations. We denote by I the identity matrix and J the reflection matrix such that $Je_1 = -e_1$ and $Je_i = e_i$ for $i = 2, \ldots, N$, where $\{e_i : i = 2, \ldots, N\}$ is the canonical basis in $\mathbb{R}^N$. The symbol $\mathrm{co}(X)$ stands for the convex hull of a set X in $\mathbb{M}^{N \times N}$. Moreover, given $N+1$ points $x_0, x_1, \ldots, x_N \in \mathbb{R}^N$, we denote by $[x_0, x_1, \ldots, x_N]$ the simplex determined by all convex combinations of those points.

Finally, $\mathcal{U}$ is the class of subsets of $(-L, L)$ that are disjoint union of a finite number of open intervals.

In the paper, the same letter C denotes various positive constants whose precise value may change from place to place.

1. **Setting of the problem.** We study the dimension reduction of a discrete model for heterogeneous nanowires. Let $L > 0$, $k \in \mathbb{N}$, $\Omega_{k\varepsilon} := (-L, L) \times (-k\varepsilon, k\varepsilon)^{N-1}$. Up to an affine deformation $H \in GL^+(N)$, we can reduce to the case where the lattice is $\mathbb{Z}^N$. Thus we consider the discrete thin domain $\mathcal{L}_\varepsilon(k) \subset \mathbb{R}^N$ defined as

$$\mathcal{L}_\varepsilon(k) := \varepsilon \mathbb{Z}^N \cap \overline{\Omega}_{k\varepsilon}, \tag{1.1}$$

where $\overline{\Omega}_{k\varepsilon}$ is the union of all hypercubes with vertices in $\varepsilon\mathbb{Z}^N$ that have non-empty intersection with $\Omega_{k\varepsilon}$. In the physically relevant case of $N = 3$, the set $\mathcal{L}_\varepsilon(k)$ models the crystal structure of a nanowire of length $2L$ and thickness $2k\varepsilon$, where k is the number of parallel atomic planes. We will nonetheless state all the results for a general N, since their proof does not depend on the dimension. Notice that in definition (1.1) the dependence on k is explicit; this parameter will indeed play a major role in the subsequent analysis.

The bonds between the atoms are defined by means of the so-called Kuhn decomposition, which is relevant for modelling some specific Bravais lattices. (See [2, Remark 2.6] for details on the treatment of some lattices in dimension two and three, such as the hexagonal or equilateral triangular, the face-centred cubic, and the body-centred cubic.) First we define a partition $\mathcal{T}_0$ of the unit cube $(0, 1)^N$ into N-simplices: we say that $T \in \mathcal{T}_0$ if the $(N+1)$-tuple of its vertices belongs to the set

$$\left\{ \{0, e_{i_1}, e_{i_1} + e_{i_2}, \ldots, e_{i_1} + e_{i_2} + \cdots + e_{i_N}\} \colon \begin{pmatrix} 1 & 2 & \cdots & N \\ i_1 & i_2 & \cdots & i_N \end{pmatrix} \in S_N \right\},$$

where S_N is the set of permutations of N elements; see Figure 1. Next, we define $\mathcal{T}$ as the periodic extension of $\mathcal{T}_0$ to all of $\mathbb{R}^N$. We say that two nodes $x, y \in \mathbb{Z}^N$ are contiguous if there exists a simplex $T \in \mathcal{T}$ that has both x and y as its vertices. We set

$$B_1 := \{ \xi \in \mathbb{R}^N \colon x \text{ and } x + \xi \text{ are contiguous} \}. \tag{1.2}$$

If both simplices $[x_0, x_1, \ldots, x_N]$ and $[y_0, x_1, \ldots, x_N]$ belong to $\mathcal{T}$, then we say that $[x_0, x_1, \ldots, x_N]$ and $[y_0, x_1, \ldots, x_N]$ are neighbouring simplices (i.e., they share a
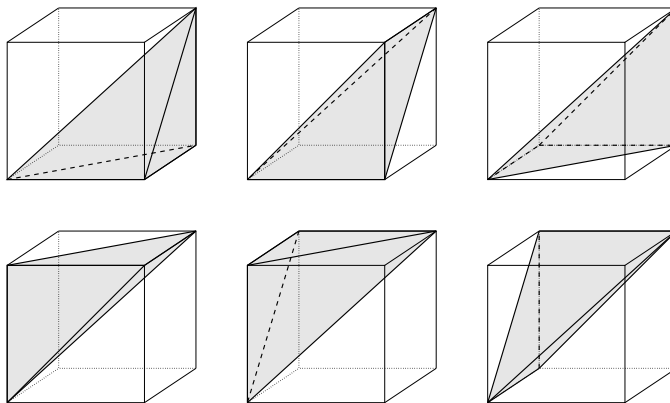

FIGURE 1. The six tetrahedra in the Kuhn decomposition of a three-dimensional cube.

facet) and x_0 and y_0 are opposite vertices. We set

$$B_2 := \{\xi \in \mathbb{R}^N : x \text{ and } x + \xi \text{ are opposite vertices}\}, \tag{1.3}$$

and remark that, by periodicity, B_1 and B_2 do not depend on x.

We assume that $\mathcal{L}_\varepsilon(k)$ is composed of two species of atoms, occupying the points contained in the subsets

$$\mathcal{L}_\varepsilon^-(k) := \{x \in \mathcal{L}_\varepsilon(k) : x_1 < 0\},$$
$$\mathcal{L}_\varepsilon^+(k) := \{x \in \mathcal{L}_\varepsilon(k) : x_1 \geq 0\},$$

respectively, where $x = (x_1, \ldots, x_N)$. The two species of atoms are characterised by equilibrium distances given by ε and $\lambda\varepsilon$, respectively, where $\lambda \in (0, 1]$ is fixed; the case $\lambda \in (0, 1)$ models a heterogeneous nanowire, while the case $\lambda = 1$ refers to a homogeneous nanowire. Specifically, the total interaction energy relative to a deformation $u \colon \mathcal{L}_\varepsilon(k) \to \mathbb{R}^N$ is defined as

$$\mathcal{E}_\varepsilon^{1,\lambda}(u, k) := \sum_{\substack{x \in \mathcal{L}_\varepsilon^-(k) \\ \xi \in B_1 \cup B_2 \\ x + \varepsilon\xi \in \mathcal{L}_\varepsilon(k)}} c(\xi) \left| \frac{|u(x + \varepsilon\xi) - u(x)|}{\varepsilon} - |H\xi| \right|^p$$
$$+ \sum_{\substack{x \in \mathcal{L}_\varepsilon^+(k) \\ \xi \in B_1 \cup B_2 \\ x + \varepsilon\xi \in \mathcal{L}_\varepsilon(k)}} c(\xi) \left| \frac{|u(x + \varepsilon\xi) - u(x)|}{\varepsilon} - \lambda|H\xi| \right|^p, \tag{1.4}$$

where $p > 1$, $H \in GL^+(N)$, and the coefficient $c(\xi)$ is equal to some $c_1 > 0$ for $\xi \in B_1$ and to $c_2 > 0$ for $\xi \in B_2$.

To simplify the presentation, we restrict our attention to the case of p-harmonic potentials, though our analysis applies, without any significant change, to more general potentials satisfying polynomial growth conditions. More precisely, we may replace $\mathcal{E}_\varepsilon^{1,\lambda}(u, k)$ with

$$\sum_{\substack{x \in \mathcal{L}_\varepsilon^-(k) \\ \xi \in B_1 \cup B_2 \\ x + \varepsilon\xi \in \mathcal{L}_\varepsilon(k)}} \phi^1\left(\xi, \frac{|u(x + \varepsilon\xi) - u(x)|}{\varepsilon} - |H\xi|\right) + \sum_{\substack{x \in \mathcal{L}_\varepsilon^+(k) \\ \xi \in B_1 \cup B_2 \\ x + \varepsilon\xi \in \mathcal{L}_\varepsilon(k)}} \phi^\lambda\left(\xi, \frac{|u(x + \varepsilon\xi) - u(x)|}{\varepsilon} - \lambda|H\xi|\right),$$

where $\phi \colon \mathbb{Z}^N \times \mathbb{R} \to [0, +\infty)$ is a positive potential such that

$$C_1|z|^p \leq \phi^\mu(\xi, z) \leq C_2|z|^p \quad \text{for } \mu = \lambda, 1,$$

for some positive constants C_1, C_2. One could consider the case of potentials depending also on x and satisfying suitable periodicity assumptions: this would require a more delicate analysis and would lead to a more complex formula for the Γ-limit.

In principle, all the results that we present in the sequel extend to the case when the two components of the nanowire have equilibria of the form H^- and H^+, where $H^-, H^+ \in GL^+(N)$. We have chosen to analyse the case when $H^+ = \lambda H^-$, since this is particularly meaningful in applications where one has misfit between two crystalline materials with the same lattice structure but different lattice distance at equilibrium (see e.g. [9, 13]).

We study the limit behaviour of $\mathcal{E}_\varepsilon^{1,\lambda}(\cdot, k)$ as $\varepsilon \to 0^+$, thus performing simultaneously a discrete to continuum limit and a dimension reduction to a one-dimensional system. The limit functional was derived in [14, 15] by means of Γ-convergence, under the assumption that the admissible deformations fulfil the non-interpenetration

condition, namely, that the Jacobian determinant of (the piecewise affine interpolation of) any deformation is strictly positive almost everywhere. The non-interpenetration assumption was used in several parts of the analysis; in particular, it was needed to prove that the limit functional (dependent on k) scales like k^N as $k \to \infty$.

The main novelty of the present paper is that we remove the non-interpenetration assumption made in [14, 15], allowing for changes of orientations. Furthermore, in the study of the Γ-limit we define a stronger topology that accounts for such changes. In the proof of the new results, only those parts that differ from [14, 15] will be shown in details.

In the sequel of the paper we will often consider the rescaled domain $\frac{1}{\varepsilon}\Omega_{k\varepsilon}$, which converges, as $\varepsilon \to 0^+$, to the unbounded strip

$$\Omega_{k,\infty} := \mathbb{R} \times (-k, k)^{N-1} \,.$$

We define the associated lattice and subsets

$$\mathcal{L}_\infty(k) := \mathbb{Z}^N \cap \overline{\Omega}_{k,\infty} \,,$$
$$\mathcal{L}_\infty^-(k) := \{x \in \mathcal{L}_\infty(k) : x_1 < 0\} \,,$$
$$\mathcal{L}_\infty^+(k) := \{x \in \mathcal{L}_\infty(k) : x_1 \geq 0\} \,,$$

where $\overline{\Omega}_{k,\infty}$ is the union of all hypercubes with vertices in $\mathbb{Z}^N$ that have non-empty intersection with $\Omega_{k,\infty}$. For $u : \mathcal{L}_\infty(k) \to \mathbb{R}^N$ we define

$$
\begin{aligned}
\mathcal{E}_\infty^{1,\lambda}(u, k) := &\sum_{\substack{x \in \mathcal{L}_\infty^-(k) \\ \xi \in B_1 \cup B_2 \\ x+\xi \in \mathcal{L}_\infty(k)}} c(\xi) \Big| |u(x+\xi) - u(x)| - |H\xi| \Big|^p \\
&+ \sum_{\substack{x \in \mathcal{L}_\infty^+(k) \\ \xi \in B_1 \cup B_2 \\ x+\xi \in \mathcal{L}_\infty(k)}} c(\xi) \Big| |u(x+\xi) - u(x)| - \lambda|H\xi| \Big|^p \,.
\end{aligned}
\tag{1.5}
$$

We identify every deformation u of the lattice $\mathcal{L}_\varepsilon(k)$ by its piecewise affine interpolation with respect to the triangulation $\varepsilon\mathcal{T}$. By a slight abuse of notation, such extension is still denoted by u. We can then define the domain of the functional (1.4) as

$$
\begin{aligned}
\mathcal{A}_\varepsilon(\Omega_{k\varepsilon}) := \big\{ u \in C^0(\overline{\Omega}_{k\varepsilon}; \mathbb{R}^N) : \ &u \text{ piecewise affine,} \\
&\nabla u \text{ constant on } \Omega_{k\varepsilon} \cap \varepsilon T \ \forall T \in \mathcal{T} \big\} \,.
\end{aligned}
$$

Similarly, for (1.5) we define

$$
\begin{aligned}
\mathcal{A}_\infty(\Omega_{k,\infty}) := \big\{ u \in C^0(\overline{\Omega}_{k,\infty}; \mathbb{R}^N) : \ &u \text{ piecewise affine,} \\
&\nabla u \text{ constant on } \Omega_{k,\infty} \cap T \ \forall T \in \mathcal{T} \big\} \,.
\end{aligned}
$$

As customary in dimension reduction problems, we rescale the domain $\Omega_{k\varepsilon}$ to a fixed domain Ω_k, independent of ε, by introducing the change of variables $z(x) := (x_1, \varepsilon x_2, \ldots, \varepsilon x_N)$. Accordingly, for each $u \in \mathcal{A}_\varepsilon(\Omega_{k\varepsilon})$ we define $\tilde{u}(x) := u(z(x))$. Moreover we set $\Omega_k := A_\varepsilon^{-1}(\Omega_{k\varepsilon}) = (-L, L) \times (-k, k)^{N-1}$, where $A_\varepsilon \in \mathbb{M}^{N \times N}$ is the diagonal matrix

$$A_\varepsilon := \mathrm{diag}(1, \varepsilon, \ldots, \varepsilon); \tag{1.6}$$

i.e., $z(x) = A_\varepsilon x$. In this way we can recast the functionals (1.4) defined over varying domains into functionals defined on deformations of the fixed domain Ω_k. Precisely we set

$$\mathcal{I}_\varepsilon^{1,\lambda}(\tilde{u}, k) := \mathcal{E}_\varepsilon^{1,\lambda}(u, k) \quad \text{for } \tilde{u} \in \widetilde{\mathcal{A}}_\varepsilon(\Omega_k), \tag{1.7}$$

with

$$\widetilde{\mathcal{A}}_\varepsilon(\Omega_k) := \left\{ \tilde{u} \in C^0(A_\varepsilon^{-1}(\overline{\Omega}_{k\varepsilon}); \mathbb{R}^N) \colon \tilde{u} \text{ piecewise affine,} \right.$$
$$\left. \nabla \tilde{u} \text{ constant on } \Omega_k \cap (A_\varepsilon^{-1}\varepsilon T) \ \forall\, T \in \mathcal{T} \right\}.$$

For later use it will be convenient to set the following notation:

$$\Omega_k^- := (-L, 0) \times (-k, k)^{N-1}, \quad \Omega_k^+ := (0, L) \times (-k, k)^{N-1}.$$

2. Definition and properties of minimal energies.

We recall that, throughout the paper, I is the identity matrix and J is the reflection matrix such that $Je_1 = -e_1$ and $Je_i = e_i$ for $i = 2, \ldots, N$.

We will study the Γ-limit of the sequence $\mathcal{I}_\varepsilon^{1,\lambda}(\cdot, k)$ as $\varepsilon \to 0^+$ for every fixed k. For this purpose we introduce the quantity $\gamma(P_1, P_2; k)$ for $P_1, P_2 \in O(N) \cup \lambda O(N)$, which represents the minimum cost of a transition from a well to another. Specifically, for each $P_1 \in O(N)$ and $P_2 \in \lambda O(N)$ we define

$$\gamma(P_1, P_2; k) := \inf \left\{ \mathcal{E}_\infty^{1,\lambda}(v, k) \colon M > 0, \ v \in \mathcal{A}_\infty(\Omega_{k,\infty}), \right.$$
$$\nabla v = P_1 H \text{ for } x_1 \in (-\infty, -M), \tag{2.1a}$$
$$\left. \nabla v = P_2 H \text{ for } x_1 \in (M, +\infty) \right\};$$

for $P_1, P_2 \in O(N)$

$$\gamma(P_1, P_2; k) := \inf \left\{ \mathcal{E}_\infty^{1,1}(v, k) \colon M > 0, \ v \in \mathcal{A}_\infty(\Omega_{k,\infty}), \right.$$
$$\nabla v = P_1 H \text{ for } x_1 \in (-\infty, -M), \tag{2.1b}$$
$$\left. \nabla v = P_2 H \text{ for } x_1 \in (M, +\infty) \right\},$$

where

$$\mathcal{E}_\infty^{1,1}(v, k) := \sum_{\substack{x \in \mathcal{L}_\infty(k) \\ \xi \in B_1 \cup B_2 \\ x + \xi \in \mathcal{L}_\infty(k)}} c(\xi) \Big| |v(x + \xi) - v(x)| - |H\xi| \Big|^p;$$

for $P_1, P_2 \in \lambda O(N)$

$$\gamma(P_1, P_2; k) := \inf \left\{ \mathcal{E}_\infty^{\lambda,\lambda}(v, k) \colon M > 0, \ v \in \mathcal{A}_\infty(\Omega_{k,\infty}), \right.$$
$$\nabla v = P_1 H \text{ for } x_1 \in (-\infty, -M), \tag{2.1c}$$
$$\left. \nabla v = P_2 H \text{ for } x_1 \in (M, +\infty) \right\},$$

where

$$\mathcal{E}_\infty^{\lambda,\lambda}(v, k) := \sum_{\substack{x \in \mathcal{L}_\infty(k) \\ \xi \in B_1 \cup B_2 \\ x + \xi \in \mathcal{L}_\infty(k)}} c(\xi) \Big| |v(x + \xi) - v(x)| - \lambda|H\xi| \Big|^p.$$

The next proposition shows that the relevant quantities defined through (2.1) are in fact four: the minimal costs of the transition at the interface between the energy wells $O(N)$ and $\lambda O(N)$ are provided in (2.2b) and (2.2c); the minimal cost of the transition between $SO(N)$ and $O(N) \backslash SO(N)$ is provided in (2.2d); the one of the transition between $\lambda SO(N)$ and $\lambda O(N) \backslash SO(N)$ is given in (2.2e). Moreover, the constants in (2.2d) and in (2.2e) are related by the proportionality rule (2.3).

Proposition 1. *For each $k \in \mathbb{N}$, the function γ satisfies for every $R, R' \in SO(N)$ and $Q, Q' \in O(N) \backslash SO(N)$*

$$\gamma(R, R'; k) = \gamma(Q, Q'; k) \quad = \gamma(\lambda R, \lambda R'; k) = \gamma(\lambda Q, \lambda Q'; k) = 0, \qquad (2.2a)$$

$$\gamma(R, \lambda R'; k) = \gamma(Q, \lambda Q'; k) \quad = \gamma(I, \lambda I; k), \qquad (2.2b)$$

$$\gamma(R, \lambda Q; k) = \gamma(Q, \lambda R; k) \quad = \gamma(I, \lambda J; k), \qquad (2.2c)$$

$$\gamma(R, Q; k) = \gamma(Q, R; k) \quad = \gamma(I, J; k), \quad and \qquad (2.2d)$$

$$\gamma(\lambda R, \lambda Q; k) = \gamma(\lambda Q, \lambda R; k) = \gamma(\lambda I, \lambda J; k). \qquad (2.2e)$$

Moreover,

$$\gamma(\lambda P_1, \lambda P_2; k) = \lambda^p \gamma(P_1, P_2; k) \quad for\ every\ P_1, P_2 \in O(N). \qquad (2.3)$$

Proof. First one notices that $\gamma(P_1, P_2; k) = \gamma(J P_1, J P_2; k)$. Hence, the proof of (2.2) relies on the construction of low energy transitions between two given rotations or two given rotoreflections, see [14, Proposition 2.4]. Finally, standard comparison arguments yield (2.3). □

We now prove estimates on the asymptotic behaviour of $\gamma(I, \lambda I)$ and $\gamma(I, \lambda J)$ as $k \to \infty$, which have interesting consequences towards the comparison of this model with those accounting for dislocations in nanowires, see Section 7 below. Indeed, in Theorem 2.2 below we show that for $\lambda \neq 1$ (heterogeneous nanowire) these constants grow faster than k^{N-1}, while it is known that the corresponding minimum cost for nanowires with dislocations scales like k^{N-1} (see discussion at the end of Section 7). In contrast, we remark that for $\lambda = 1$ one has $\gamma(I, I) = 0$ and $\gamma(I, J) \simeq C k^{N-1}$. An essential tool in the proof of Theorem 2.2 is the following result.

Theorem 2.1. [2, Theorem 3.1] *Let $u_\varepsilon \in \mathcal{A}_\varepsilon((0,1)^N)$ be a sequence such that*

$$\varepsilon^{N-1} \sum_{\xi \in B_1 \cup B_2} \sum_{\substack{x, x+\varepsilon\xi \in \\ \varepsilon\mathbb{Z}^N \cap (0,1)^N}} \left| \frac{|u_\varepsilon(x+\varepsilon\xi) - u_\varepsilon(x)|}{\varepsilon} - |H\xi| \right|^p < C. \qquad (2.4)$$

Then there are a subsequence (not relabelled) and a function $u \in W^{1,\infty}((0,1)^N; \mathbb{R}^N)$ such that $\nabla u_\varepsilon \to \nabla u$ in $L^p((0,1)^N; \mathbb{M}^{N \times N})$ and

$$\nabla u \in SBV((0,1)^N; O(N)H). \qquad (2.5)$$

Specifically, u is a collection of an at most countable family of rigid deformations, i.e., there exists a Caccioppoli partition $\{E_i\}_{i \in \mathbb{N}}$ subordinated to the reduced boundary $\partial^*\{\nabla u \in SO(N)H\}$, such that

$$u(x) = \sum_{i \in \mathbb{N}} (R_i H x + b_i) \chi_{E_i}(x), \qquad (2.6)$$

where $R_i \in O(N)$ and $b_i \in \mathbb{R}^N$. Moreover, if $\partial^* E_i \cap \partial^* E_j \neq \emptyset$, then $\det R_i \det R_j = -1$ and $\partial^* E_i \cap \partial^* E_j$ is flat, i.e., the measure theoretic normal vector to $\partial^* E_i \cap \partial^* E_j$ is constant (up to the sign).

We now prove the main result of this section.

Theorem 2.2. *Let $\lambda \in (0,1)$ and $(P_1, P_2) \in \{(I, \lambda I), (I, \lambda J)\}$. There exists $C > 0$ such that*

$$\gamma(P_1, P_2; k) \leq C k^N. \qquad (2.7)$$

Moreover,

$$\lim_{k \to \infty} \frac{\gamma(P_1, P_2; k)}{k^{N-1}} = +\infty. \qquad (2.8)$$

Proof. The upper bound (2.7) is proven by comparing test functions for $\gamma(P_1, P_2; k)$ with those for $\gamma(P_1, P_2; 1)$. Namely, let $v \in A_\infty(\Omega_{1,\infty})$ be such that $v(x) = P_1 H x$ for every $x \in \mathcal{L}_\infty^-(k)$ and $v(x) = P_2 H x$ for every $x \in \mathcal{L}_\infty^+(k)$; in particular, $\nabla v = P_1 H$ for $x_1 \in (-\infty, -1)$ and $\nabla v = P_2 H$ for $x_1 \in (0, +\infty)$. Then one defines $u \in \mathcal{A}_\infty(\Omega_{k,\infty})$ by $u(x) := k v(x/k)$, which yields $\gamma(P_1, P_2; k) \leq \mathcal{E}_\infty^{1,\lambda}(u, k) \leq C \mathcal{E}_\infty^{1,\lambda}(v, 1) k^N$, and thus $\gamma(P_1, P_2; k) \leq C \gamma(P_1, P_2; 1) k^N$. Note that in the previous inequalities one uses the fact that $\nabla v \in L^\infty$ and that the energy of the interactions in B_2 can be bounded, using the Mean Value Theorem, by the energy of the interactions in B_1.

For the proof of the lower bound (2.8) we will use Theorem 2.1 in each of the subsets $(-1, 0) \times (-1, 1)^{N-1}$ and $(0, 1) \times (-1, 1)^{N-1}$. By contradiction, suppose that there exist a sequence $k_j \nearrow \infty$ and a sequence $\{u_j\} \subset \mathcal{A}_\infty(\Omega_{k_j, \infty})$ such that

$$\frac{1}{k_j^{N-1}} \mathcal{E}_\infty^{1,\lambda}(u_j, k_j) < C, \tag{2.9}$$

for some positive C. Define $v_j \colon \Omega_{1,\infty} \to \mathbb{R}^N$ as $v_j(x) := \frac{1}{k_j} u_j(k_j x)$. Accordingly, we consider the rescaled lattices

$$\mathcal{L}_j := \frac{1}{k_j} \mathbb{Z}^N \cap \overline{\Omega}_{1,\infty}, \quad \mathcal{L}_j^+ := \mathcal{L}_j \cap \{x_1 > 0\}, \quad \mathcal{L}_j^- := \mathcal{L}_j \cap \{x_1 < 0\}.$$

Expressing $\mathcal{E}_\infty^{1,\lambda}(u_j, k_j)$ in terms of v_j, one finds

$$\begin{aligned}
\mathcal{E}_\infty^{1,\lambda}(u_j, k) = &\sum_{\substack{x \in \mathcal{L}_j^- \\ \xi/k_j \in B_1 \cup B_2 \\ x + \xi/k_j \in \mathcal{L}_j}} c(\xi) \left| \frac{|v_j(x + \frac{\xi}{k_j}) - v_j(x)|}{\frac{1}{k_j}} - |H\xi| \right|^p \\
&+ \sum_{\substack{x \in \mathcal{L}_j^+ \\ \xi/k_j \in B_1 \cup B_2 \\ x + \xi/k_j \in \mathcal{L}_j}} c(\xi) \left| \frac{|v_j(x + \frac{\xi}{k_j}) - v_j(x)|}{\frac{1}{k_j}} - \lambda |H\xi| \right|^p .
\end{aligned} \tag{2.10}$$

The above term controls the (piecewise constant) gradient of v_j. From (2.9), (2.10), and Theorem 2.1 we deduce that, up to subsequences, $\nabla v_j \to \nabla v$ in $L^p((-1, 1)^N; \mathbb{M}^{N \times N})$, for some $v \in W^{1,\infty}((-1, 1)^N; \mathbb{R}^N)$, where $\nabla v \in O(N)H$ for a.e. $x \in (-1, 0) \times (-1, 1)^{N-1}$ and $\nabla v \in \lambda O(N)H$ for a.e. $x \in (0, 1) \times (-1, 1)^{N-1}$. Precisely,

$$v(x) = \sum_{i \in \mathbb{N}} (R_i H x + a_i) \chi_{E_i^-}(x) + \sum_{j \in \mathbb{N}} (\lambda Q_j H x + b_j) \chi_{E_j^+}(x),$$

where $R_i, Q_j \in O(N)$, $a_i, b_j \in \mathbb{R}^N$, and $\{E_i^-\}$ (respectively $\{E_j^+\}$) is a Caccioppoli partition of $(-1, 0) \times (-1, 1)^{N-1}$ (respectively of $(0, 1) \times (-1, 1)^{N-1}$). Then, since $\{E_i^-\} \cup \{E_j^+\}$ is a Caccioppoli partition of $(-1, 1)^N$, by the local structure of Caccioppoli partitions (see e.g. [3, Theorem 4.17]), we find that, for $\mathcal{H}^{N-1}$-a.e. $x \in \{0\} \times (-k, k)^{N-1}$, $x \in \partial^* E_i^- \cap \partial^* E_j^+$ for some i, j (where $\partial^* E$ denotes the reduced boundary of E). Therefore, using a blow-up argument and the fact that $v \in W^{1,\infty}((-1, 1)^N; \mathbb{R}^N)$, we deduce that there exist rank-1 connections between $O(N)H$ and $\lambda O(N)H$; see [2, Lemma 3.2]. This implies in particular that $\lambda = 1$, which is a contradiction to $\lambda \in (0, 1)$. Hence (2.8) follows. $\qquad\square$

Remark 1. An estimate similar to (2.8) was proven in [14, 15] (for a hexagonal lattice in dimension two and a class of three-dimensional lattices) via a different argument, based on the non-interpenetration condition. In fact, in [14, 15] a stronger result is proven, namely, that $\gamma(I, \lambda I; k)$ scales like k^N.

The non-interpenetration assumption turns out to be necessary if the energy involves only nearest neighbour interactions; indeed, in such a case, one can exhibit deformations that violate the non-interpenetration condition and for which (2.8) does not hold, see [14, Section 4.2]. Such deformations, which consist of suitable foldings of the lattice, would be energetically expensive (and, in particular, would not provide a counterexample to (2.8)) in the present setting, exactly because of the effect of the interactions across neighbouring cells. It is the latter ones that prevent folding phenomena and allow one to prove (2.8), via Theorem 2.1.

3. **Compactness and lower bound.** Before characterising the Γ-convergence for the rescaled functionals (1.7), we show a compactness theorem for sequences with equibounded energy, as well as bounds from above and from below on those functionals in terms of the changes of orientation in the wire. Such bounds will be used in the proof of the Γ-convergence results, Theorems 5.1 and 5.4.

Essential tools for the compactness and the lower bound are provided by the following rigidity estimates.

Theorem 3.1. [12, Theorem 3.1] *Let $N \geq 2$, and let $1 < p < \infty$. Suppose that $U \subset \mathbb{R}^N$ is a bounded Lipschitz domain. Then there exists a constant $C = C(U)$ such that for each $u \in W^{1,p}(U; \mathbb{R}^N)$ there exists a constant matrix $R \in SO(N)$ such that*

$$\|\nabla u - R\|_{L^p(U; \mathbb{M}^{N \times N})} \leq C(U)\|\mathrm{dist}(\nabla u, SO(N))\|_{L^p(U)}. \qquad (3.1)$$

The constant $C(U)$ is invariant under dilation and translation of the domain.

It is convenient to define the energy of a single simplex T with vertices $x_0, \ldots, x_N$,

$$E_{\mathrm{cell}}(u_F; T) := \sum_{i \leq j = 0}^{N} \left| |F(x_i - x_j)| - |H(x_i - x_j)| \right|^p \quad \text{for every } F \in \mathbb{M}^{N \times N},$$

where u_F is the affine map $u_F(x) := Fx$. The following lemma provides a lower bound on $E_{\mathrm{cell}}(u_F; T)$ in terms of the distance of F from $O(N)$. It will be instrumental in using Theorem 3.1.

Lemma 3.2. [2, Lemma 2.2] *There exists a constant $C > 0$ such that*

$$\mathrm{dist}^p(F, SO(N)H) \leq C\, E_{\mathrm{cell}}(u_F; T) \quad \forall F \in \mathbb{M}^{N \times N}: \det F \geq 0, \quad (3.2\mathrm{a})$$

$$\mathrm{dist}^p(F, (O(N)\backslash SO(N))H) \leq C\, E_{\mathrm{cell}}(u_F; T) \quad \forall F \in \mathbb{M}^{N \times N}: \det F \leq 0. \quad (3.2\mathrm{b})$$

The next lemma asserts that if in two neighbouring simplices the sign of $\det \nabla u$ has different sign, then the energy of those two simplices is larger than a positive constant. It will be convenient to define the energetic contribution of the interactions within two neighbouring simplices $T = [x_0, x_1, \ldots, x_N]$, $S = [y_0, x_1, \ldots, x_N]$ as

$$E_{\mathrm{cell}}(u; S \cup T) := \sum_{i \leq j = 0}^{N} \left| |u(x_i) - u(x_j)| - |H(x_i - x_j)| \right|^p$$

$$+ \sum_{j=1}^{N} \left| |u(y_0) - u(x_j)| - |H(y_0 - x_j)| \right|^p$$

$$+ \left| |u(y_0) - u(x_0)| - |H(y_0 - x_0)| \right|^p.$$

Lemma 3.3. [2, Lemma 2.3] *There exists a positive constant C_0 (depending on H) with the following property: if two neighbouring N-simplices S, T have different orientations in the deformed configuration, i.e.,*

$$\det \left(\nabla u|_S \right) \det \left(\nabla u|_T \right) \leq 0,$$

then $E_{\mathrm{cell}}(u; S \cup T) \geq C_0$.

Lemma 3.2 will allow us to apply Theorem 3.1. More precisely, in the part of the wire with $x_1 \in (-L, 0)$ we use (3.1) or its "symmetric" version for $O(N) \backslash SO(N)$ in subdomains that scale in such a way that the constant of the rigidity estimate does not change; for $x_1 \in (0, L)$ we use corresponding estimates for $\lambda SO(N)$ or $\lambda(O(N) \backslash SO(N))$. Thus we approximate the deformation gradient with piecewise constant matrices in $O(N)$, respectively $\lambda O(N)$.

Due to the fact that a minimum energy has to be paid for each change of orientation, see Lemma 3.3, the parts with positive determinant do not mix with those with negative determinant. Hence, passing to the weak* limit we obtain functions taking values in $\mathrm{co}(SO(N)) \cup \mathrm{co}(O(N) \backslash SO(N))$, respectively $\lambda \mathrm{co}(SO(N)) \cup \lambda \mathrm{co}(O(N) \backslash SO(N))$. Here, $\mathrm{co}(X)$ denotes the convex hull of a set X in $\mathbb{M}^{N \times N}$.

Remark 2. It is well known that $\mathrm{co}(SO(N)) \cap \mathrm{co}(O(N) \backslash SO(N)) \neq \emptyset$: indeed, the intersection always contains the zero matrix, here denoted by 0. In dimension $N = 2$, one can see that

$$\mathrm{co}(SO(2)) = \left\{ \begin{pmatrix} \alpha & -\beta \\ \beta & \alpha \end{pmatrix} : \alpha^2 + \beta^2 \leq 1 \right\},$$

$$\mathrm{co}(O(2) \backslash SO(2)) = \left\{ \begin{pmatrix} \alpha & \beta \\ \beta & -\alpha \end{pmatrix} : \alpha^2 + \beta^2 \leq 1 \right\}.$$

In particular, $\mathrm{co}(SO(2)) \cap \mathrm{co}(O(2) \backslash SO(2)) = \{0\}$. For $N > 2$, the intersection is nontrivial. For example, $\mathrm{co}(SO(3)) \cap \mathrm{co}(O(3) \backslash SO(3))$ contains the matrix $-\frac{1}{3} I$. Moreover, one can see that

$$\mathrm{co}(SO(N)) \cup \mathrm{co}(O(N) \backslash SO(N)) \subsetneq \mathrm{co}(O(N))$$

for $N \geq 2$.

Henceforth, the symbol $\mathcal{U}$ stands for the class of subsets of $(-L, L)$ that are disjoint union of a finite number of open intervals.

Proposition 2. *Let $\tilde{u}_\varepsilon \in \widetilde{\mathcal{A}}_\varepsilon(\Omega_k)$ be a sequence such that*

$$\limsup_{\varepsilon \to 0^+} \mathcal{I}_\varepsilon^{1,\lambda}(\tilde{u}_\varepsilon, k) \leq C. \tag{3.3}$$

Then there exist functions $\tilde{u} \in W^{1,\infty}(\Omega_k; \mathbb{R}^N)$, $d_1, \ldots, d_N \in L^\infty(\Omega_k; \mathbb{R}^N)$, and a subsequence (not relabelled) such that

$$\tilde{u}_\varepsilon - \fint_{\Omega_k} \tilde{u}_\varepsilon \, \mathrm{d}x \overset{*}{\rightharpoonup} \tilde{u} \qquad \qquad weakly* \text{ in } W^{1,\infty}(\Omega_k; \mathbb{R}^N),$$

$$\nabla \tilde{u}_\varepsilon A_\varepsilon^{-1} = (\nabla u_\varepsilon) \circ A_\varepsilon \overset{*}{\rightharpoonup} (\partial_1 \tilde{u} \,|\, d_2 \,|\, \cdots \,|\, d_N) \quad weakly* \text{ in } L^\infty(\Omega_k; \mathbb{M}^{N \times N}), \tag{3.4}$$

and $\tilde{u}$, $d_1, \ldots, d_N$, are independent of $x_2, \ldots, x_N$, i.e., $\partial_j \tilde{u} = \partial_j d_i = 0$, for each $i = 2, \ldots, N$ and $j = 2, \ldots, N$. Moreover, there exists $U \in \mathcal{U}$ such that

$$(\partial_1 \tilde{u} \,|\, d_2 \,|\, \cdots \,|\, d_N) \in \begin{cases} \mathrm{co}(SO(N))H & \text{a.e. in } (-L, 0) \cap U \,, \\ \mathrm{co}(O(N) \backslash SO(N))H & \text{a.e. in } (-L, 0) \setminus U \,, \\ \lambda \, \mathrm{co}(SO(N))H & \text{a.e. in } (0, L) \cap U \,, \\ \lambda \, \mathrm{co}(O(N) \backslash SO(N))H & \text{a.e. in } (0, L) \setminus U \,, \end{cases} \tag{3.5}$$

and

$$\liminf_{\varepsilon \to 0^+} \mathcal{I}_\varepsilon^{1,\lambda}(\tilde{u}_\varepsilon, k) \geq \gamma(I, J; k)\, \mathcal{H}^0(\partial U \cap (-L, 0)) + \gamma(\lambda I, \lambda J; k)\, \mathcal{H}^0(\partial U \cap (0, L))$$

$$+ \gamma(I, \lambda I; k)\,[1 - \chi_{\partial U}(0)] + \gamma(I, \lambda J; k)\, \chi_{\partial U}(0) \,. \tag{3.6}$$

Remark 3. The right-hand side of (3.6) contains different contributions. The first term corresponds to the minimal energy needed to bridge a rotation with a rotoreflection, or viceversa, in the left part of the nanowire; the energy spent depends on the number of changes of orientation, i.e., on the cardinality of ∂U. The second term plays an analogous role for the right part of the nanowire. The remaining terms describe the interfacial energy spent to bridge the two energy wells $O(N)H$ and $\lambda O(N)H$: that contribution also depends on whether or not the orientation is preserved across the interface, i.e., on whether 0 is an inner or external, or boundary point for U.

Proof. (*Compactness*) The assumption (3.3) implies that $\{\nabla u_\varepsilon\}$, resp. $\{\nabla \tilde{u}_\varepsilon A_\varepsilon^{-1}\}$, is uniformly bounded in $L^\infty(\Omega_{k\varepsilon}; \mathbb{M}^{N \times N})$, respectively $L^\infty(\Omega_k; \mathbb{M}^{N \times N})$. (Recall that $u_\varepsilon(x) = \tilde{u}_\varepsilon(A_\varepsilon^{-1} x)$.) Therefore there exist a subsequence of $\{\tilde{u}_\varepsilon\}$ (not relabelled) and functions $\tilde{u} \in W^{1,\infty}(\Omega_k; \mathbb{R}^N)$ and $d_i \in L^\infty(\Omega_k; \mathbb{R}^N)$ for $i = 2, \ldots, N$, such that $\partial_1 \tilde{u}_\varepsilon \overset{*}{\rightharpoonup} \partial_1 \tilde{u}$ weakly* in $L^\infty(\Omega_k; \mathbb{M}^{N \times N})$, where $\tilde{u}$ is independent of x_i for all $i = 2, \ldots, N$, and $\frac{1}{\varepsilon} \partial_i \tilde{u}_\varepsilon \overset{*}{\rightharpoonup} d_i$ for each $i = 2, \ldots, N$.

In order to show $\partial_j d_i = 0$ and (3.5), we apply the rigidity estimate (3.1) to the sequence u_ε. To this aim, we divide the domain $\overline{\Omega}_{k\varepsilon}$ into subdomains that are the Cartesian product of intervals $(a_i, a_i + \varepsilon)$, $a_i \in \varepsilon \mathbb{Z}$, and the cross-section $(-k\varepsilon, k\varepsilon)^{N-1}$. We first observe that, by Lemma 3.3 and assumption (3.3), the number of changes of orientation of u_ε is uniformly bounded in ε. More precisely, we can find a uniformly bounded number of subdomains $(a_i, a_i + \varepsilon) \times (-k\varepsilon, k\varepsilon)^{N-1}$, $i \in I_\varepsilon$, $\#I_\varepsilon \leq C$, such that if $i \notin I_\varepsilon$ then $\det \nabla u_\varepsilon$ has constant sign in $(a_i, a_i + \varepsilon) \times (-k\varepsilon, k\varepsilon)^{N-1}$. In each of these subdomains, we use (3.2) to apply the rigidity estimate (3.1), or its "symmetric" version for $O(N) \backslash SO(N)$.

Specifically, for each a_i with $a_i < 0$ and $i \notin I_\varepsilon$, there exists $P_\varepsilon(a_i) \in O(N)H$ such that

$$\int_{(a_i, a_i + \varepsilon) \times (-k\varepsilon, k\varepsilon)^{N-1}} |\nabla u_\varepsilon - P_\varepsilon(a_i)|^p \, \mathrm{d}x \leq C \int_{(a_i, a_i + \varepsilon) \times (-k\varepsilon, k\varepsilon)^{N-1}} \mathrm{dist}^p(\nabla u_\varepsilon, O(N)H) \, \mathrm{d}x \,,$$

and for every $a_i > 0$ with $i \notin I_\varepsilon$ there exists $P_\varepsilon(a_i) \in \lambda O(N)H$ such that

$$\int_{(a_i, a_i + \varepsilon) \times (-k\varepsilon, k\varepsilon)^{N-1}} |\nabla u_\varepsilon - P_\varepsilon(a_i)|^p \, \mathrm{d}x \leq C \int_{(a_i, a_i + \varepsilon) \times (-k\varepsilon, k\varepsilon)^{N-1}} \mathrm{dist}^p(\nabla u_\varepsilon, \lambda O(N)H) \, \mathrm{d}x \,.$$

Moreover for $i \in I_\varepsilon$ we set $P_\varepsilon(a_i) = I$ if $a_i < 0$ and $P_\varepsilon(a_i) = \lambda I$ if $a_i \geq 0$. By interpolation one defines a piecewise constant matrix field $P_\varepsilon : (-L, L) \rightarrow$

$O(N)H \cup \lambda O(N)H$ such that $P_\varepsilon(x_1) = P_\varepsilon(a_i)$ if $x_1 \in (a_i, a_i + \varepsilon)$. Summing up over i and rescaling the variables, one gets

$$\int_{\Omega_k^-} |\nabla \tilde{u}_\varepsilon A_\varepsilon^{-1} - P_\varepsilon(x_1)|^p \, dx \leq C \int_{A_\varepsilon^{-1}(\overline{\Omega}_{k\varepsilon}) \cap \{x_1 < 0\}} \text{dist}^p(\nabla \tilde{u}_\varepsilon A_\varepsilon^{-1}, O(N)H) \, dx \leq C\varepsilon, \quad (3.7a)$$

$$\int_{\Omega_k^+} |\nabla \tilde{u}_\varepsilon A_\varepsilon^{-1} - P_\varepsilon(x_1)|^p \, dx \leq C \int_{A_\varepsilon^{-1}(\overline{\Omega}_{k\varepsilon}) \cap \{x_1 > 0\}} \text{dist}^p(\nabla \tilde{u}_\varepsilon A_\varepsilon^{-1}, \lambda O(N)H) \, dx \leq C\varepsilon, (3.7b)$$

where the last inequality of each line follows by applying Lemma 3.2 to each subdomain with $i \notin I_\varepsilon$ and by recalling that each subdomain has volume proportional to ε after rescaling.

We now define the sets

$$K_\varepsilon := \{a_i^\varepsilon \in (-L, L) : P_\varepsilon(x_1) \in SO(N)H \cup \lambda SO(N)H \text{ for } x_1 \in [a_i^\varepsilon, a_i^\varepsilon + \varepsilon)\},$$

$$U_\varepsilon := \bigcup_{a_i^\varepsilon \in K_\varepsilon} [a_i^\varepsilon, a_i^\varepsilon + \varepsilon),$$

and remark that Lemma 3.2, Lemma 3.3, and assumption (3.3) imply that the cardinality of ∂U_ε is uniformly bounded. Therefore the sequence $\{\chi_{U_\varepsilon}\}$ converges, up to subsequences, to χ_U strongly in $L^1(-L, L)$, where

$$U = \bigcup_{i=1}^{n} (\alpha_i, \beta_i), \quad -L \leq \alpha_1 < \beta_1 < \alpha_2 < \beta_2 < \cdots < \alpha_n < \beta_n \leq L. \quad (3.8)$$

Since we can write

$$P_\varepsilon(x_1) = R_\varepsilon(x_1)\left(\chi_{U_\varepsilon \cap (-L,0)} H + \chi_{U_\varepsilon \cap (0,L)} \lambda H\right)$$
$$+ J R_\varepsilon(x_1)\left((1 - \chi_{U_\varepsilon \cap (-L,0)}) H + (1 - \chi_{U_\varepsilon \cap (0,L)}) \lambda H\right),$$

where $R_\varepsilon : (-L, L) \to SO(N)$ is piecewise constant, we deduce that P_ε converges, up to subsequences, to some $P \in L^\infty((-L, L); \mathbb{M}^{N \times N})$ in the weak* topology of $L^\infty((-L, L); \mathbb{M}^{N \times N})$. From (3.7) it follows that the weak* limit of $\nabla \tilde{u}_\varepsilon A_\varepsilon^{-1}$ coincides with P and therefore does not depend on x_j for each $j = 2, \ldots, N$. Moreover, inclusion (3.5) follows from the fact that $\chi_{U_\varepsilon} P_\varepsilon$ converges weakly* to $\chi_U P$.

(*Lower bound*) Inequality (3.6) is proven by a standard argument which can be found, for example, in [14, 16, 17]. We will briefly sketch the main ideas and refer the reader to [14, 16, 17] for full details. First recall that ∂U consists of a finite number of points, cf. (3.8). Since $\chi_{U_\varepsilon} \to \chi_U$ and since the number of points of ∂U_ε is uniformly bounded, one can find $\sigma > 0$, $\alpha_i^\varepsilon \to \alpha_i$, $\beta_i^\varepsilon \to \beta_i$ such that

$$(\alpha_i^\varepsilon - 2\sigma, \alpha_i^\varepsilon - \sigma) \subset (-L, L) \setminus U_\varepsilon, \quad (\alpha_i^\varepsilon + \sigma, \alpha_i^\varepsilon + 2\sigma) \subset U_\varepsilon, \quad (3.9a)$$
$$(\beta_i^\varepsilon - 2\sigma, \beta_i^\varepsilon - \sigma) \subset U_\varepsilon, \quad (\beta_i^\varepsilon + \sigma, \beta_i^\varepsilon + 2\sigma) \subset (-L, L) \setminus U_\varepsilon. \quad (3.9b)$$

Moreover, if σ is sufficiently small, all the intervals $(\alpha_i^\varepsilon - 2\sigma, \alpha_i^\varepsilon + 2\sigma)$ and $(\beta_i^\varepsilon - 2\sigma, \beta_i^\varepsilon + 2\sigma)$ are mutually disjoint and therefore it suffices to prove the lower bound for one of such intervals. Suppose that $\alpha_i^\varepsilon \in (0, L)$ and define

$$v_\varepsilon(x_1, x_2, \ldots, x_N) := \tfrac{1}{\varepsilon} \tilde{u}_\varepsilon(\varepsilon x_1 + \alpha_i^\varepsilon, x_2, \ldots, x_N) = \tfrac{1}{\varepsilon} u_\varepsilon(\varepsilon x_1 + \alpha_i^\varepsilon, \varepsilon x_2, \ldots, \varepsilon x_N).$$

Then, $\nabla v_\varepsilon(x) = \nabla \tilde{u}_\varepsilon(\varepsilon x_1 + \alpha_i^\varepsilon, x_2, \ldots, x_N) A_\varepsilon^{-1} = \nabla u_\varepsilon(\varepsilon x_1 + \alpha_i^\varepsilon, \varepsilon x_2, \ldots, \varepsilon x_N)$, and, by (3.7), we have

$$\int_{(-\frac{2\sigma}{\varepsilon}, -\frac{\sigma}{\varepsilon}) \times (-k,k)^{N-1}} \mathrm{dist}^p(\nabla v_\varepsilon, \lambda(O(N)\backslash SO(N))H) \, \mathrm{d}x$$
$$+ \int_{(\frac{\sigma}{\varepsilon}, \frac{2\sigma}{\varepsilon}) \times (-k,k)^{N-1}} \mathrm{dist}^p((\nabla v_\varepsilon, \lambda\, SO(N)H) \, \mathrm{d}x \le C \,. \tag{3.10}$$

From (3.10), Theorem 3.1 and the Poincaré inequality, we deduce that there exists a unit interval contained in $(-\frac{2\sigma}{\varepsilon}, -\frac{\sigma}{\varepsilon})$ such that in the Cartesian product of such interval with the cross-section $(-k,k)^{N-1}$, the $W^{1,p}$-norm of the difference between v_ε and an affine map of the form $\lambda QHx + a$, with $Q \in O(N)\backslash SO(N)$ and $a \in \mathbb{R}^N$, is bounded by $C\varepsilon/\sigma$. By the same argument one can find a unit interval contained in $(\frac{\sigma}{\varepsilon}, \frac{2\sigma}{\varepsilon})$ such that in the Cartesian product of such interval with the cross-section $(-k,k)^{N-1}$, the $W^{1,p}$-norm of the difference between v_ε and an affine map of the form $\lambda RHx + b$, with $R \in SO(N)$ and $b \in \mathbb{R}^N$, is bounded by $C\varepsilon/\sigma$. By gluing the function v_ε with these maps on such intervals, one can define a function $\hat{v}_\varepsilon \in \mathcal{A}_\infty(\Omega_{k,\infty})$ that is a competitor for $\gamma(\lambda J, \lambda I; k)$ and such that (cf. (2.2))

$$\mathcal{I}_\varepsilon^{1,\lambda}(\tilde{u}_\varepsilon, k)|_{(\alpha_i^\varepsilon - 2\sigma, \alpha_i^\varepsilon + 2\sigma) \times (-k,k)^{N-1}} \ge \mathcal{E}_\infty^{\lambda,\lambda}(\hat{v}_\varepsilon, k) - C\frac{\varepsilon}{\sigma} \,,$$

where $\mathcal{I}_\varepsilon^{1,\lambda}(\tilde{u}_\varepsilon, k)|_{(\alpha_i^\varepsilon - 2\sigma, \alpha_i^\varepsilon + 2\sigma) \times (-k,k)^{N-1}}$ only takes into account the interactions between atoms lying in the subset $(\alpha_i^\varepsilon - 2\sigma, \alpha_i^\varepsilon + 2\sigma) \times (-k,k)^{N-1}$. Arguing in a similar way for the other intervals in (3.9) yields (3.6). □

4. **Upper bound.** We prove that the bound (3.6) is in fact optimal.

Proposition 3. *Let $F \in L^\infty((-L,L); \mathbb{M}^{N \times N})$ and $U \in \mathcal{U}$ satisfy*

$$F \in \begin{cases} \mathrm{co}(SO(N))H & \text{a.e. in } (-L,0) \cap U \,, \\ \mathrm{co}(O(N)\backslash SO(N))H & \text{a.e. in } (-L,0) \setminus U \,, \\ \lambda\, \mathrm{co}(SO(N))H & \text{a.e. in } (0,L) \cap U \,, \\ \lambda\, \mathrm{co}(O(N)\backslash SO(N))H & \text{a.e. in } (0,L) \setminus U \,. \end{cases} \tag{4.1}$$

Then there exists a sequence $\{\tilde{u}_\varepsilon\} \subset \widetilde{\mathcal{A}}_\varepsilon(\Omega_k)$ such that

$$\nabla \tilde{u}_\varepsilon A_\varepsilon^{-1} \overset{*}{\rightharpoonup} F \quad \text{weakly* in } L^\infty(\Omega_k; \mathbb{M}^{N \times N}) \,, \tag{4.2}$$

and

$$\limsup_{\varepsilon \to 0^+} \mathcal{I}_\varepsilon^{1,\lambda}(\tilde{u}_\varepsilon, k) \le \gamma(I, J; k)\, \mathcal{H}^0(\partial U \cap (-L,0)) + \gamma(\lambda I, \lambda J; k)\, \mathcal{H}^0(\partial U \cap (0,L))$$
$$+ \gamma(I, \lambda I; k)\, [1 - \chi_{\partial U}(0)] + \gamma(I, \lambda J; k)\, \chi_{\partial U}(0) \,. \tag{4.3}$$

Proof. Using a standard approximation argument we may assume that $x_1 \mapsto F(x_1)$ is piecewise constant, with values in $O(N)H$ for a.e. $x_1 \in (-L,0)$ and values in $\lambda O(N)H$ for a.e. $x_1 \in (0,L)$. We may also assume that this approximation process does not modify the set U of (4.1). More precisely, there exist $m, n \in \mathbb{Z}$, $m < 0$, $n \ge 0$, $-L = a_m < a_{m+1} < \cdots < a_{-1} < a_0 = 0 < a_1 < \cdots < a_n < a_{n+1} = L$, and $R_i \in O(N)$ for $i = m, \ldots, -1, 0, \ldots, n$ such that

$$F = \sum_{i=m}^{-1} \chi_{(a_i, a_{i+1})} R_i H + \sum_{i=0}^{n} \chi_{(a_i, a_{i+1})} \lambda R_i H$$

and

$$U = \mathrm{int} \bigcup \left\{ [a_i, a_{i+1}] \colon R_i \in SO(N) \, , \ m \leq i \leq n - 1 \right\} .$$

The following construction is similar to that in [14, Proposition 3.2], so we will show the details only for what concerns the changes of orientation. We introduce a mesoscale $\{\sigma_\varepsilon\}$ such that $\varepsilon \ll \sigma_\varepsilon \ll 1$ as $\varepsilon \to 0^+$. Next we define $\tilde{u}_\varepsilon$ in the sets of the type $(a_i + \sigma_\varepsilon, a_{i+1} - \sigma_\varepsilon) \times (-k, k)^{N-1}$ in such a way that its gradient equals $R_i H A_\varepsilon$ if $a_{i+1} \leq 0$ and equals $\lambda R_i H A_\varepsilon$ if $a_i \geq 0$. This determines $\tilde{u}_\varepsilon$ in those regions, up to some additive constants that will have to be fixed at the end of the construction in order to make $\tilde{u}_\varepsilon$ continuous.

We now complete the definition of $\tilde{u}_\varepsilon$ in the sets of the type $(a_i - \sigma_\varepsilon, a_i + \sigma_\varepsilon) \times (-k, k)^{N-1}$. Let us first assume $i < 0$, i.e., $a_i < 0$. Since R_{i-1} and R_i may be in $SO(N)$ or in $O(N) \backslash SO(N)$, one can have four cases. If both R_{i-1} and R_i are in $SO(N)$, it is possible to define $\tilde{u}_\varepsilon$ by interpolating R_{i-1} and R_i so that the cost of the transition has order $O(\varepsilon / \sigma_\varepsilon)$, so it gives no contribution to (4.3); we refer to [14] for details. The case $R_{i-1}, R_i \in O(N) \backslash SO(N)$ is completely analogous.

If $R_{i-1} \in SO(N)$ and $R_i \in O(N) \backslash SO(N)$ or viceversa, we define $\tilde{u}_\varepsilon$ in the set $(a_i - \sigma_\varepsilon, a_i + \sigma_\varepsilon) \times (-k, k)^{N-1}$ as a rescaling of a quasiminimiser of (2.1b). More precisely, we fix $\eta > 0$ and apply the definition of $\gamma(R_{i-1}, R_i; k)$, thus finding $M > 0$ and $v \in \mathcal{A}_\infty(\Omega_{k,\infty})$ such that

$$\nabla v = R_{i-1} H \ \text{for} \ x_1 \in (-\infty, -M) \, , \quad \nabla v = R_i H \ \text{for} \ x_1 \in (M, +\infty)$$

and

$$\mathcal{E}_\infty^{1,1}(v, k) \leq \gamma(I, J; k) + \eta \, ,$$

where we used also Proposition 1. With this at hand, we define $\tilde{u}_\varepsilon$ in the set $(a_i - \sigma_\varepsilon, a_i + \sigma_\varepsilon) \times (-k, k)^{N-1}$ as

$$\tilde{u}_\varepsilon(x) := \varepsilon v(\tfrac{1}{\varepsilon} A_\varepsilon x) + b \, .$$

The constant vector b in the last equation is chosen in such a way that $\tilde{u}_\varepsilon$ is continuous. Since each point of ∂U gives the same contribution $\gamma(I, J; k)$ to the upper bound, we obtain the first term of (4.3).

The case $i > 0$, i.e., $a_i > 0$, is treated similarly to $i < 0$ and gives rise to the second term of (4.3). Finally, for $i = 0$, i.e., $a_i = a_0 = 0$, we argue as above and define $\tilde{u}_\varepsilon$ by using a rescaling of a quasiminimiser of (2.1a) and applying the definition of $\gamma(R_{-1}, \lambda R_0; k)$. We then get an interfacial contribution in (4.3) that differs in the two cases $0 \in \partial U$ and $0 \notin \partial U$. $\qquad \square$

5. **Limit functionals with respect to different topologies.** In the next theorem we characterise the Γ-limit of the sequence $\{\mathcal{I}_\varepsilon^{1,\lambda}(\cdot, k)\}$ with respect to the weak* convergence in $W^{1,\infty}(\Omega_k; \mathbb{R}^N)$; see [4, 8] for an introduction to Γ-convergence. As it can be inferred from the compactness result in Proposition 2, the domain of the Γ-limit turns out to be

$$\mathcal{A}^{1,\lambda}(k) := \big\{ u \in W^{1,\infty}(\Omega_k; \mathbb{R}^N) \colon \partial_2 u = \cdots = \partial_N u = 0 \ \text{a.e. in} \ \Omega_k \, ,$$
$$|\partial_1 u| \leq 1 \ \text{a.e. in} \ \Omega_k^- \, , \ |\partial_1 u| \leq \lambda \ \text{a.e. in} \ \Omega_k^+ \big\} . \tag{5.1}$$

We show that on such domain the Γ-limit is constant. Hence, the macroscopic description of the model is similar to that of [14, 15]; in particular, it does not have memory of the changes of orientation in minimising sequences. In order to keep

track of the orientation changes, we need to introduce a stronger topology for the Γ-convergence, as we see in Theorem 5.4.

Theorem 5.1. *The sequence of functionals $\{\mathcal{I}_\varepsilon^{1,\lambda}(\cdot, k)\}$ Γ-converges, as $\varepsilon \to 0^+$, to the functional*

$$\mathcal{I}^{1,\lambda}(u, k) = \begin{cases} \gamma(k) & \text{if } u \in \mathcal{A}^{1,\lambda}(k), \\ +\infty & \text{otherwise,} \end{cases} \tag{5.2}$$

with respect to the weak* convergence in $W^{1,\infty}(\Omega_k; \mathbb{R}^N)$, where

$$\gamma(k) := \min\left\{\gamma(I, \lambda I; k), \gamma(I, \lambda J; k)\right\}. \tag{5.3}$$

Proof. (*Liminf inequality*) Let $\tilde{u}_\varepsilon \in \widetilde{\mathcal{A}}_\varepsilon(\Omega_k)$ be a sequence of functions converging to a function u weakly* in $W^{1,\infty}(\Omega_k; \mathbb{R}^N)$. We have to show that

$$\mathcal{I}^{1,\lambda}(u, k) \leq \liminf_{\varepsilon \to 0^+} \mathcal{I}_\varepsilon^{1,\lambda}(\tilde{u}_\varepsilon, k).$$

We assume that $\liminf_{\varepsilon \to 0^+} \mathcal{I}_\varepsilon^{1,\lambda}(\tilde{u}_\varepsilon, k) \leq C$, the other case being trivial. By applying Proposition 2 we find a set $U \in \mathcal{U}$ and functions $\tilde{u} \in W^{1,\infty}(\Omega_k; \mathbb{R}^N)$, $d_2, \ldots, d_N \in L^\infty(\Omega_k; \mathbb{R}^N)$ independent of $x_2, \ldots, x_N$, such that (3.4), (3.5), and (3.6) hold. This implies that $\partial_1 u = \partial_1 \tilde{u}$ a.e., the function u is independent of $x_2, \ldots, x_N$, and $u \in \mathcal{A}^{1,\lambda}(k)$. Notice that the right-hand side of (3.6) is greater than or equal to $\gamma(k)$, since $\gamma(\cdot, \cdot; k)$ is positive.

(*Limsup inequality*) Given a function $u \in W^{1,\infty}(\Omega_k; \mathbb{R}^N)$ we have to find a sequence $\{\tilde{u}_\varepsilon\} \subset \widetilde{\mathcal{A}}_\varepsilon(\Omega_k)$ such that $\tilde{u}_\varepsilon \overset{*}{\rightharpoonup} u$ weakly* in $W^{1,\infty}(\Omega_k; \mathbb{R}^N)$ and

$$\limsup_{\varepsilon \to 0^+} \mathcal{I}_\varepsilon^{1,\lambda}(\tilde{u}_\varepsilon, k) \leq \mathcal{I}^{1,\lambda}(u, k). \tag{5.4}$$

We assume that $u \in \mathcal{A}^{1,\lambda}(k)$, the other case being trivial.

The construction of the recovery sequence depends on the precise value of the minimum in (5.3). Since we do not know such value, we explain how to proceed in the case when $\gamma(k)$ is any of the two quantities therein.

- If $\gamma(k) = \gamma(I, \lambda I; k)$, we set $U := (-L, L)$ and, following e.g. [16, Theorem 4.1], we construct measurable functions $d_2, \ldots, d_N \in L^\infty(\Omega_k; \mathbb{R}^N)$, independent of $x_2, \ldots, x_N$, such that

$$(\partial_1 u \,|\, d_2 \,|\, \cdots \,|\, d_N) \in \begin{cases} \text{co}(SO(N))H & \text{a.e. in } \Omega_k^-, \\ \lambda \,\text{co}(SO(N))H & \text{a.e. in } \Omega_k^+. \end{cases}$$

- If $\gamma(k) = \gamma(I, \lambda J; k)$ we set $U := (-L, 0)$ and construct $d_2, \ldots, d_N$ in such a way that

$$(\partial_1 u \,|\, d_2 \,|\, \cdots \,|\, d_N) \in \begin{cases} \text{co}(SO(N))H & \text{a.e. in } \Omega_k^-, \\ \lambda \,\text{co}(O(N)\backslash SO(N))H & \text{a.e. in } \Omega_k^+. \end{cases}$$

Proposition 3 can be now applied to $F := (\partial_1 u \,|\, d_2 \,|\, \cdots \,|\, d_N)$, hence providing us with a sequence $\{\tilde{u}_\varepsilon\} \subset \widetilde{\mathcal{A}}_\varepsilon(\Omega_k)$ satisfying (4.2)–(4.3). In particular we have $\nabla \tilde{u}_\varepsilon \overset{*}{\rightharpoonup} \nabla u$ weakly* in $L^\infty(\Omega_k; \mathbb{M}^{N \times N})$ and (5.4) holds because of the choice of U and the definition of $\gamma(k)$. $\square$
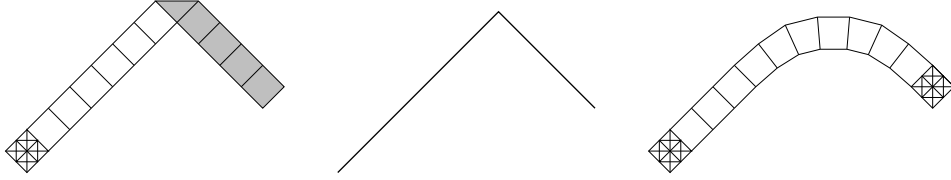
FIGURE 2. Two possible recovery sequences for the profile at the centre of the figure. Here we picture only a part of the wire containing just one species of atoms, therefore the transition at the interface is not represented. A kink in the profile may be reconstructed by folding the strip, i.e., mixing rotations and rotoreflections (left); or by a gradual transition involving only rotations or only rotoreflections (right). In the limit, the former recovery sequence gives a positive cost, while the latter gives no contribution. If the stronger topology is chosen, the appropriate recovery sequence will depend on the value of the internal variable, which defines the orientation of the wire.

Remark 4. As long as the Γ-convergence is taken with respect to the weak* topology of $W^{1,\infty}(\Omega_k; \mathbb{R}^N)$, (5.2) only accounts for the cost of transitions at the interface between the two species of atoms. Indeed, away from the interface it is always possible to construct recovery sequences without mixing rotations and rotoreflections, as done in the proof of the limsup inequality; such transitions have low interaction energy, since $\gamma(I, I) = \gamma(J, J) = 0$, see also Proposition 1. In particular, for $\lambda = 1$ the limit functional is trivial, since $\mathcal{I}^{1,1}(u, k) = 0$ if $u \in \mathcal{A}^{1,1}(k)$.

Below we show that, if a stronger topology is chosen, the value of the Γ-limit changes. The resulting limit functional depends on an internal variable, D in (5.7), that keeps track of the changes of orientation throughout the thin wire. In fact, different transitions between the energy wells must now be employed according to the value of D; two examples are provided in Figure 2.

We introduce the sequence of functionals defined for $u \in W^{1,\infty}(\Omega_k; \mathbb{R}^N)$ and $D \in L^\infty(\Omega_k; \mathbb{M}^{N \times N})$ by

$$\hat{\mathcal{I}}^{1,\lambda}_\varepsilon(\tilde{u}, D, k) := \begin{cases} \mathcal{I}^{1,\lambda}_\varepsilon(\tilde{u}, k) & \text{if } \tilde{u} \in \widetilde{\mathcal{A}}_\varepsilon(\Omega_k) \text{ and } D = (\partial_1 \tilde{u} \,|\, \varepsilon^{-1}\partial_2 \tilde{u} \,|\, \cdots \,|\, \varepsilon^{-1}\partial_N \tilde{u}), \\ +\infty & \text{otherwise.} \end{cases}$$

In the next theorem we study the Γ-limit of the sequence $\{\hat{\mathcal{I}}^{1,\lambda}_\varepsilon(\cdot, \cdot, k)\}$ as $\varepsilon \to 0^+$ with respect to the weak* convergence in $W^{1,\infty}(\Omega_k; \mathbb{R}^N) \times L^\infty(\Omega_k; \mathbb{M}^{N \times N})$. As a consequence of Proposition 2, the domain of the Γ-limit turns out to be

$$\begin{aligned} \hat{\mathcal{A}}^{1,\lambda}(k) := \big\{ (u, D) \colon\, & u \in \mathcal{A}^{1,\lambda}(k), \; D \in L^\infty(\Omega_k; \mathbb{M}^{N \times N}), \\ & De_1 = \partial_1 u, \; \partial_2 D = \cdots = \partial_N D = 0 \text{ a.e. in } \Omega_k, \\ & D \in \mathrm{co}(SO(N))H \cup \mathrm{co}(O(N)\backslash SO(N))H \text{ a.e. in } \Omega_k^-, \\ & D \in \lambda \, \mathrm{co}(SO(N))H \cup \lambda \, \mathrm{co}(O(N)\backslash SO(N))H \text{ a.e. in } \Omega_k^+ \big\}, \end{aligned}$$

where $\mathcal{A}^{1,\lambda}(k)$ is defined by (5.1). It is convenient to introduce the following definition, where the functional $\mathcal{J}$ coincides with the right-hand sides of (3.6) and (4.3).

Definition 5.2. Given $(u, D) \in \hat{\mathcal{A}}^{1,\lambda}(k)$, let $\mathcal{U}(u, D)$ be the collection of all subsets $U \in \mathcal{U}$ such that

$$D \in \begin{cases} \operatorname{co}(SO(N))H & \text{for a.e. } x_1 \in (-L, 0) \cap U, \\ \operatorname{co}(O(N) \backslash SO(N))H & \text{for a.e. } x_1 \in (-L, 0) \setminus U, \\ \lambda \operatorname{co}(SO(N))H & \text{for a.e. } x_1 \in (0, L) \cap U, \\ \lambda \operatorname{co}(O(N) \backslash SO(N))H & \text{for a.e. } x_1 \in (0, L) \setminus U. \end{cases} \tag{5.5}$$

For $U \in \mathcal{U}(u, D)$ we set

$$\mathcal{J}(U) := \gamma(I, J; k) \, \mathcal{H}^0(\partial U \cap (-L, 0)) + \gamma(\lambda I, \lambda J; k) \, \mathcal{H}^0(\partial U \cap (0, L))$$
$$+ \gamma(I, \lambda I; k) \, [1 - \chi_{\partial U}(0)] + \gamma(I, \lambda J; k) \, \chi_{\partial U}(0)$$

and

$$\mathcal{J}_{\min}(u, D) := \min_{U \in \mathcal{U}(u, D)} \mathcal{J}(U). \tag{5.6}$$

The last definition will be used to apply Propositions 2 and 3 towards the characterisation of the Γ-limit with respect to the stronger topology. To this end, each pair $(u, D) \in \hat{\mathcal{A}}^{1,\lambda}(k)$ is associated with a set U realising (5.5). Such U is in general not unique, since $\operatorname{co}(SO(N)) \cap \operatorname{co}(O(N) \backslash SO(N)) \neq \emptyset$. Therefore, we choose it to be "optimal", i.e., minimising (5.6). Notice that the minimum in (5.6) is attained since

$$\{ \mathcal{J}(U) : U \in \mathcal{U}(u, D) \}$$
$$\subset \{ m_1 \gamma(I, J; k) + m_2 \gamma(I, \lambda I; k) + m_3 \gamma(I, \lambda J; k) + m_4 \gamma(\lambda I, \lambda J; k) : m_i \in \mathbb{N} \}.$$

A minimiser needs not be unique as shown in the following example.

Example 5.3. Fix $a_1 < a_2 < 0$ and assume that $D(x_1) \in (O(N) \backslash SO(N))H$ for $x_1 < a_1$, $D(x_1) = 0$ for $a_1 < x_1 < a_2$, $D(x_1) \in SO(N)H$ for $a_2 < x_1 < 0$, and $D(x_1) \in \lambda SO(N)H$ for $x_1 > 0$. Then any interval of the type $U = (a, +\infty)$, with $a_1 \le a \le a_2$, is a minimiser of (5.6).

Theorem 5.4. *The sequence of functionals $\{\hat{\mathcal{I}}_\varepsilon^{1,\lambda}(\cdot, \cdot, k)\}$ Γ-converges, as $\varepsilon \to 0^+$, to the functional*

$$\hat{\mathcal{I}}^{1,\lambda}(u, D, k) := \begin{cases} \mathcal{J}_{\min}(u, D) & \text{if } (u, D) \in \hat{\mathcal{A}}^{1,\lambda}(k), \\ +\infty & \text{otherwise,} \end{cases} \tag{5.7}$$

with respect to the weak* convergence in $W^{1,\infty}(\Omega_k; \mathbb{R}^N) \times L^\infty(\Omega_k; \mathbb{M}^{N \times N})$, where $\mathcal{J}_{\min}(u, D)$ is defined by (5.6).

Proof. The liminf inequality is obtained by applying Proposition 2 and arguing as in Theorem 5.1. Also the derivation of the limsup inequality is similar to the one performed in Theorem 5.1; let us simply point out that, while in the proof of Theorem 5.1 the matrix field F needed to be reconstructed, here we set $F := D$ and choose U as a minimiser of (5.6). The conclusion follows by applying Proposition 3. $\qquad \square$

Remark 5. We underline that Theorem 5.4 provides a nontrivial Γ-limit also in the case when $\lambda = 1$. Indeed, one has $\hat{\mathcal{I}}^{1,1}(u, D, k) = \gamma(I, J; k) \, \mathcal{H}^0(\partial U \cap (-L, L))$ if $(u, D) \in \hat{\mathcal{A}}^{1,1}(k)$ and U miminises (5.6), where $\gamma(I, J; k) > 0$.

6. **Boundary conditions and external forces.** In the present section we discuss how the previous results extend to the case when the functional (1.4) is complemented by boundary conditions or external forces. Although our considerations apply to the case of general $H \in GL^+(N)$ and $\lambda \in (0,1]$, for simplicity we will focus on the case $H = I$ and $\lambda = 1$. We will also test the consistency of the present model with the non-interpenetration condition by looking at minimisers of the Γ-limit when boundary conditions or forces are prescribed. We will see that the continuum limit that keeps track of such constraints is the one provided by the stronger topology (5.7).

Boundary conditions. Let $B^-, B^+ \in GL^+(N)$ and suppose that the functional (1.4) is now defined on deformations $u \in \mathcal{A}_\varepsilon(\Omega_{k\varepsilon})$ that satisfy

$$\begin{cases} \nabla u(x) = B^- x & \text{if } -L < x_1 < -L + \varepsilon\,, \\ \nabla u(x) = B^+ x & \text{if } L - \varepsilon < x_1 < L\,. \end{cases} \tag{6.1}$$

It is easy to see that while the compactness result of Proposition 2 remains valid, the Γ-limit (5.2) will now contain additional terms corresponding to the minimal energy spent to fix the atoms in the vicinity of the lateral boundaries. However, such extra terms do not depend on the limiting deformations, therefore they do not encode any information about the behaviour of minimising sequences. As far as the stronger topology is concerned, one can see that the limit functional (5.7) will contain the additional quantities $\gamma(B^-, P; k)$ and $\gamma(P, B^+; k)$ defined, for $P \in \{I, J\}$, by

$$\begin{aligned} \gamma(B^-, P; k) := \inf \big\{ \mathcal{E}_M^{1,1}(v, k) \colon \ & M > 0\,, \ v \in \mathcal{A}_\infty(\Omega_{k,\infty})\,, \\ & \nabla v = B^- \text{ for } x_1 \in (-\infty, -M)\,, \\ & \nabla v = P \text{ for } x_1 \in (M, +\infty) \big\}\,, \end{aligned} \tag{6.2}$$

$$\begin{aligned} \gamma(P, B^+; k) := \inf \big\{ \mathcal{E}_M^{1,1}(v, k) \colon \ & M > 0\,, \ v \in \mathcal{A}_\infty(\Omega_{k,\infty})\,, \\ & \nabla v = P \text{ for } x_1 \in (-\infty, -M)\,, \\ & \nabla v = B^+ \text{ for } x_1 \in (M, +\infty) \big\}\,, \end{aligned} \tag{6.3}$$

where $\mathcal{E}_M^{1,1}$ is as in (2.1b), except that the sum is taken over all atoms contained in the bounded strip $(-M, M) \times (-k, k)^{N-1}$. The choice of $P = I$ or $P = J$ depends on whether or not $\pm L \in \partial \bar{U}$, where $\bar{U}$ is a minimiser of (5.6). Precisely, if $-L \in \partial \bar{U}$ (resp. $L \in \partial \bar{U}$), then in (6.2) (resp. (6.3)) we take $P = I$, otherwise we take $P = J$.

Remark 6. By Proposition 2 and the properties of Γ-convergence, minimisers of (1.4) subjected to (6.1) converge, up to subsequences, to minimisers of (5.7) complemented with the above extra terms. Moreover, if $\text{dist}(B^\pm; SO(N))$ is sufficiently small, then such minimisers will not have transitions between $\text{co}\big(SO(N)\big)$ and $\text{co}\big(O(N) \backslash SO(N)\big)$. This follows from the fact that

$$\gamma(I, B^\pm; k) \to 0 \quad \text{as} \quad \text{dist}(B^\pm; SO(N)) \to 0$$

and therefore, as long as $\gamma(I, B^+; k) + \gamma(B^-, I; k) < \gamma(I, J; k)$, the optimal transitions will fulfil the non-interpenetration condition. In this respect the quantity $\gamma(I, J; k)$ can be regarded as an energetic barrier that must be overcome in order to have folding effects.

External forces. We study a class of tangential/radial forces acting along the rod. Let $F_1 \in \mathbb{R}^N$, $F_2, \ldots, F_N \in C^0(\mathbb{R}^N; \mathbb{R}^N)$ be a collection of vector fields such that $F_i = F_i(x_1)$ for every $2 = 1, \ldots, N$. We denote by F the matrix field whose columns are $F_1, \ldots, F_N$. For each $u \colon \mathcal{L}_\varepsilon(k) \to \mathbb{R}^N$, consider the functional

$$\mathcal{F}_\varepsilon(u, k) :=$$
$$\sum_{(\pm L_\varepsilon, x_2, \ldots, x_N) \in \mathcal{L}_\varepsilon(k)} F_1 \cdot \big(u(L_\varepsilon, x_2, \ldots, x_N) - u(-L_\varepsilon, x_2, \ldots, x_N)\big)$$
$$+ \sum_{(x_1, \pm \varepsilon k, \ldots, x_N) \in \mathcal{L}_\varepsilon(k)} F_2(x_1) \cdot \big(u(x_1, \varepsilon k, x_3, \ldots, x_N) - u(x_1, -\varepsilon k, x_3, \ldots, x_N)\big) + \cdots$$
$$\cdots + \sum_{(x_1, \ldots, x_{N-1}, \pm \varepsilon k) \in \mathcal{L}_\varepsilon(k)} F_N(x_1) \cdot \big(u(x_1, \ldots, x_{N-1}, \varepsilon k) - u(x_1, \ldots, x_{N-1}, -\varepsilon k)\big),$$

$$(6.4)$$

where $L_\varepsilon := L$ if L is an integer multiple of ε, and $L_\varepsilon := ([L/\varepsilon] + 1)\varepsilon$ otherwise. The functional $\mathcal{F}_\varepsilon$ consists of several terms: the first sum represents a tangential force, while the other terms define a radial force acting on the external atoms of the lattice and enforcing the average displacements along the coordinate directions $e_2, \ldots, e_N$ to be aligned with the given vector fields $F_2, \ldots, F_N$. Note that $\mathcal{F}_\varepsilon(u, k)$ can be written as

$$\mathcal{F}_\varepsilon(u, k) =$$
$$\sum_{x_1 = -L_\varepsilon}^{L_\varepsilon - \varepsilon} \sum_{(x_1, \ldots, x_N) \in \mathcal{L}_\varepsilon(k)} F_1 \cdot \big(u(x_1 + \varepsilon, \ldots, x_N) - u(x_1, \ldots, x_N)\big)$$
$$+ \sum_{x_2 = -\varepsilon k}^{\varepsilon(k-1)} \sum_{(x_1, \ldots, x_N) \in \mathcal{L}_\varepsilon(k)} F_2(x_1) \cdot \big(u(x_1, x_2 + \varepsilon, \ldots, x_N) - u(x_1, x_2, \ldots, x_N)\big) + \cdots$$
$$\cdots + \sum_{x_N = -\varepsilon k}^{\varepsilon(k-1)} \sum_{(x_1, \ldots, x_N) \in \mathcal{L}_\varepsilon(k)} F_N(x_1) \cdot \big(u(x_1, \ldots, x_N + \varepsilon) - u(x_1, \ldots, x_N)\big),$$

hence we have that $\mathcal{F}_\varepsilon(u, k) \simeq \frac{1}{\varepsilon^{N-1}} \int_{\Omega_{k\varepsilon}} F : \nabla u \, dx$.

Introducing the new variables $z(x) := A_\varepsilon x$ defined by (1.6), and adopting the notation used in Section 1, (6.4) can be equivalently expressed in terms of $\tilde{u}(x) := u(z(x))$, namely

$$\widetilde{\mathcal{F}}_\varepsilon(\tilde{u}, k) :=$$
$$\sum_{(\pm L_\varepsilon, x_2, \ldots, x_N) \in A_\varepsilon^{-1} \mathcal{L}_\varepsilon(k)} F_1 \cdot \big(\tilde{u}(L_\varepsilon, x_2, \ldots, x_N) - \tilde{u}(-L_\varepsilon, x_2, \ldots, x_N)\big)$$
$$+ \sum_{(x_1, \pm k, \ldots, x_N) \in A_\varepsilon^{-1} \mathcal{L}_\varepsilon(k)} F_2(x_1) \cdot \big(\tilde{u}(x_1, k, x_3, \ldots, x_N) - \tilde{u}(x_1, -k, x_3, \ldots, x_N)\big) + \ldots$$
$$\cdots + \sum_{(x_1, \ldots, x_{N-1}, \pm k) \in A_\varepsilon^{-1} \mathcal{L}_\varepsilon(k)} F_N(x_1) \cdot \big(\tilde{u}(x_1, \ldots, x_{N-1}, k) - \tilde{u}(x_1, \ldots, x_{N-1}, -k)\big)$$
$$= \mathcal{F}_\varepsilon(u, k),$$

so that $\widetilde{\mathcal{F}}_\varepsilon(\tilde{u}, k) \simeq \int_{\Omega_k} F : (\nabla \tilde{u} \, A_\varepsilon^{-1}) \, dx$. We can then address the study of the asymptotic behaviour of the sequence

$$\mathcal{G}_\varepsilon(\tilde{u}, D, k) := \hat{\mathcal{I}}_\varepsilon^{1,1}(\tilde{u}, D, k) - \widetilde{\mathcal{F}}_\varepsilon(\tilde{u}, k)\,, \quad \tilde{u} \in \widetilde{\mathcal{A}}_\varepsilon(\Omega_k),\, D \in L^\infty(\Omega_k; \mathbb{M}^{N \times N})\,. \quad (6.5)$$

Note that in this context we cannot use the weak* convergence in $W^{1,\infty}(\Omega_k; \mathbb{R}^N)$, since this does not control $\widetilde{\mathcal{F}}_\varepsilon(\tilde{u})$, which is in fact a term depending on $D = \nabla\tilde{u}\, A_\varepsilon^{-1}$. This justifies the choice of $\hat{\mathcal{I}}_\varepsilon^{1,1}$ rather than $\mathcal{I}_\varepsilon^{1,1}$ in the definition of $\mathcal{G}_\varepsilon$: in order to control both terms in the right hand side of (6.5), we use the stronger topology provided by the weak* convergence in $W^{1,\infty}(\Omega_k; \mathbb{R}^N) \times L^\infty(\Omega_k; \mathbb{M}^{N \times N})$. The force term is indeed a continuous perturbation of $\hat{\mathcal{I}}_\varepsilon^{1,1}$ with respect to such topology. We observe that

$$\frac{C}{\varepsilon} \int_{\Omega_k} (|\nabla\tilde{u}\, A_\varepsilon^{-1}|^p - 1)\, \mathrm{d}x \leq \frac{C}{\varepsilon} \int_{\Omega_k} \mathrm{dist}^p(\nabla\tilde{u}\, A_\varepsilon^{-1}, O(N))\, \mathrm{d}x \leq \hat{\mathcal{I}}_\varepsilon^{1,1}(\tilde{u}, k)$$

and

$$\widetilde{\mathcal{F}}_\varepsilon(\tilde{u}, k) \leq C\Big(\int_{\Omega_k} |F|^{p'}\, \mathrm{d}x + \int_{\Omega_k} |\nabla\tilde{u}\, A_\varepsilon^{-1}|^p\, \mathrm{d}x \Big)\,.$$

Let now $\{(\tilde{u}_\varepsilon, D_\varepsilon)\} \in \widetilde{\mathcal{A}}_\varepsilon(\Omega_k) \times L^\infty(\Omega_k; \mathbb{M}^{N \times N})$ be a sequence such that

$$\limsup_{\varepsilon \to 0^+} \mathcal{G}_\varepsilon(\tilde{u}_\varepsilon, D_\varepsilon, k) \leq C\,.$$

The previous inequalities imply that $\|\nabla\tilde{u}\, A_\varepsilon^{-1}\|_{L^p(\Omega_k; \mathbb{M}^{N \times N})}$ is equibounded, which in turn implies that $\limsup_{\varepsilon \to 0^+} \hat{\mathcal{I}}_\varepsilon^{1,1}(\tilde{u}_\varepsilon, k) \leq C$ and thus the conclusions of Proposition 2 are still valid. (See also [16, Remark 4.2] for similar results.) Taking also into account Theorem 5.4, we derive the following result.

Theorem 6.1. *The following results hold:*

(Compactness) Let $\{(\tilde{u}_\varepsilon, D_\varepsilon)\} \in \widetilde{\mathcal{A}}_\varepsilon(\Omega_k) \times L^\infty(\Omega_k; \mathbb{M}^{N \times N})$ be a sequence such that

$$\limsup_{\varepsilon \to 0^+} \mathcal{G}_\varepsilon(\tilde{u}_\varepsilon, D_\varepsilon, k) \leq C\,.$$

Then there exists $(\tilde{u}, D) \in \hat{\mathcal{A}}^{1,1}(k)$ and a subsequence (not relabelled) such that

$$\tilde{u}_\varepsilon - \fint_{\Omega_k} \tilde{u}_\varepsilon\, \mathrm{d}x \overset{*}{\rightharpoonup} \tilde{u} \quad \text{weakly* in } W^{1,\infty}(\Omega_k; \mathbb{R}^N)\,,$$

$$\nabla\tilde{u}_\varepsilon A_\varepsilon^{-1} = (\nabla u_\varepsilon) \circ A_\varepsilon \overset{*}{\rightharpoonup} D \quad \text{weakly* in } L^\infty(\Omega_k; \mathbb{M}^{N \times N})\,.$$

(Γ-limit) The sequence of functionals $\{\mathcal{G}_\varepsilon\}$ Γ-converges, as $\varepsilon \to 0^+$, to the functional

$$\mathcal{G}(u, D, k) := \hat{\mathcal{I}}^{1,1}(u, D, k) - \widetilde{\mathcal{F}}(D, k)\,, \quad (6.6)$$

with respect to the weak convergence in $W^{1,\infty}(\Omega_k; \mathbb{R}^N) \times L^\infty(\Omega_k; \mathbb{M}^{N \times N})$, where*

$$\widetilde{\mathcal{F}}(D, k) := (2k)^{N-1} \int_{-L}^{L} \big(F_1 \cdot d_1 + \cdots + F_N \cdot d_N \big)\, \mathrm{d}x_1$$

for $D = (d_1 | \cdots | d_N)$.

As a consequence of the previous theorem and the standard properties of Γ-convergence we infer the following result about convergence of minima and minimisers.

Corollary 1. *We have that*

$$\lim_{\varepsilon \to 0} \min\{\mathcal{G}_\varepsilon(u, D) \colon (u, D) \in \widetilde{\mathcal{A}}_\varepsilon(\Omega_k) \times L^\infty(\Omega_k; \mathbb{M}^{N \times N})\}$$

$$= \min\{\mathcal{G}(u, D, k) \colon (u, D) \in \hat{\mathcal{A}}^{1,1}(k)\}\,.$$

Moreover if $(u_\varepsilon, D_\varepsilon) \in \widetilde{\mathcal{A}}_\varepsilon(\Omega_k) \times L^\infty(\Omega_k; \mathbb{M}^{N \times N})$ *is such that*

$$\lim_{\varepsilon \to 0} \mathcal{G}_\varepsilon(u_\varepsilon, D_\varepsilon) = \lim_{\varepsilon \to 0} \min\{\mathcal{G}_\varepsilon(u, D) \colon (u, D) \in \widetilde{\mathcal{A}}_\varepsilon(\Omega_k) \times L^\infty(\Omega_k; \mathbb{M}^{N \times N})\},$$

then any cluster point $(\overline{u}, \overline{D})$ *of* $(u_\varepsilon, D_\varepsilon)$ *with respect to the weak* convergence in* $W^{1,\infty}(\Omega_k; \mathbb{R}^N) \times L^\infty(\Omega_k; \mathbb{M}^{N \times N})$ *is a minimiser for* $\min\{\mathcal{G}(u, D, k) : (u, D) \in \hat{\mathcal{A}}^{1,1}(k)\}$.

We now come back to the question of the consistency of the model with the non-interpenetration condition. In this context we cannot expect that minimisers of (6.5) preserve orientation for the whole class of loads defined above. This is clarified in the following remark.

Remark 7. Minimisers of the functional defined by (6.6) may have transition points between the two wells $SO(N)$ and $O(N) \backslash SO(N)$. Suppose for instance that $F_1, \ldots, F_N$ satisfy the following properties: there exist $n_1, \ldots, n_N \in S^{N-1}$, $a \in (-L, L)$, such that $(n_1 | \cdots | n_N) \in SO(N)$, $F_i(x_1) = f_i(x_1) n_i$ for each $i = 1, \ldots, N$, $f_1 \in \mathbb{R}$, $f_i > 0$ in $(-L, L)$ for each $i = 1, \ldots, N-1$, $f_N > 0$ in $(-L, a)$, $f_N < 0$ in (a, L).

Define $\overline{D} := (n_1 | \cdots | n_N)$ if $x_1 \in (-L, a)$, and $\overline{D} := (n_1 | \cdots | n_{N-1} | - n_N)$ if $x_1 \in (a, L)$. Note that $(x_1 n_1, \overline{D}) \in \hat{\mathcal{A}}^{1,1}(k)$, and $\overline{D}$ has a transition point at $x_1 = a$. Denote by $\hat{\mathcal{A}}_0^{1,1}(k)$ the subset of $\hat{\mathcal{A}}^{1,1}(k)$ of deformations with no transitions; i.e., $\hat{\mathcal{A}}_0^{1,1}(k) := \{(u, D) \in \hat{\mathcal{A}}^{1,1}(k) \colon \hat{\mathcal{I}}^{1,1}(u, D, k) = 0\}$. It is easy to see that

$$C := \min_{(u,D) \in \hat{\mathcal{A}}_0^{1,1}(k)} -\widetilde{F}(D, k) > -\widetilde{F}(\overline{D}, k)$$

$$= -(2k)^{N-1} \left(\sum_{i=1}^{N-1} \int_{-L}^{L} f_i \, \mathrm{d}x_1 + \int_{-L}^{a} f_N \, \mathrm{d}x_1 - \int_{a}^{L} f_N \, \mathrm{d}x_1 \right).$$

Therefore, if $f_1, \ldots, f_N$ are such that

$$-\widetilde{F}(\overline{D}, k) + \gamma(I, J; k) < C,$$

then it is energetically preferred to have a transition at a, namely, all minimisers of $\mathcal{G}$ are given by $(x_1 n_1 + b, \overline{D})$, with b any vector in $\mathbb{R}^N$. In contrast, if f_N is always positive, then minimisers will not display any transition.

7. **Comparison with models including dislocations.** The lattice mismatch in heterostructured materials, corresponding to $\lambda \neq 1$ in the model described in this section, can be relieved by creation of dislocations; i.e., line defects of the crystal structure. We refer to [9, 13, 19] for an account of the literature on dislocations in nanowires. A model for discrete heterostructured nanowires accounting for dislocations was studied in [14, 15] under the assumption that deformations fulfil the non-interpenetration condition. In this paper we have chosen to consider only defect-free configurations in order to both simplify the exposition and to pose emphasis on the difficulties to overcome when the non-interpenetration assumption is removed. In the final part of the paper, we outline the results that can be obtained when dislocations are accounted for.

Following the ideas of [14], in dimension $N = 2$ we introduce other possible models where the reference configuration represents a lattice with dislocations. More precisely, we fix $\rho \in [\lambda, 1]$ and set

$$\mathcal{L}_\varepsilon(\rho, k) := \mathcal{L}_\varepsilon^-(1, k) \cup \mathcal{L}_\varepsilon^+(\rho, k),$$
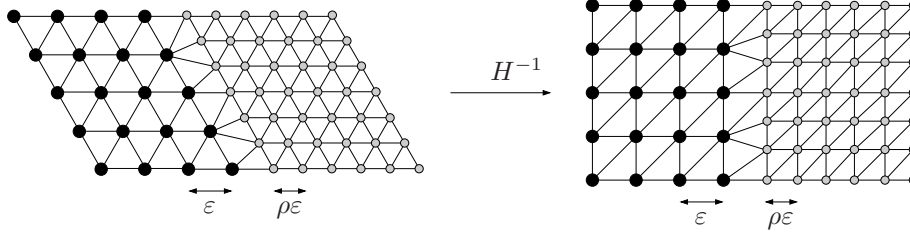
FIGURE 3. Lattices with dislocations: choice of the interfacial nearest neighbours in $\mathcal{L}_\varepsilon(\rho, k)$ and $H\mathcal{L}_\varepsilon(\rho, k)$ for a Delaunay triangulation.

where

$$\mathcal{L}_\varepsilon^-(1, k) := \varepsilon\mathbb{Z}^2 \cap \overline{\Omega}_{k\varepsilon} \cap \{x_1 < 0\},$$
$$\mathcal{L}_\varepsilon^+(\rho, k) := \rho\varepsilon\mathbb{Z}^2 \cap \overline{\Omega}_{k\varepsilon} \cap \{x_1 \geq 0\},$$

and $\overline{\Omega}_\varepsilon$ is as in (1.1). For $\rho \neq 1$, the number of atomic layers parallel to e_1 is different in the two sublattices (for sufficiently large k); this can be regarded as a system containing dislocations at the interface.

In presence of dislocations, the choice of the interactions and of the equilibria strongly depends on the lattice that one intends to model. Therefore, in this section we focus on the simplest situation of hexagonal (or equilateral triangular) Bravais lattices in dimension two and we fix

$$H := \begin{pmatrix} 1 & -\frac{1}{2} \\ 0 & \frac{\sqrt{3}}{2} \end{pmatrix}.$$

The lattice $H\mathcal{L}_\varepsilon(\rho, k)$ consists of two Bravais hexagonal sublattices with different lattice constants ε and $\rho\varepsilon$, respectively; see Figure 3.

The bonds between nearest and next-to-nearest neighbours are defined first in the lattice $H\mathcal{L}_\varepsilon(\rho, k)$. To this end, one chooses a Delaunay triangulation of $H\mathcal{L}_\varepsilon(\rho, k)$ as defined in [14, Section 1]. Two points x, y of the lattice are said to be nearest neighbours if there is a lattice point z such that the triangle $[x, y, z]$ is an element of the triangulation. Two points x, y are next-to-nearest neighbours if there are z_1, z_2 such that $[x, z_1, z_2]$ and $[y, z_1, z_2]$ are elements of the triangulation. These definitions coincide with the usual notions of nearest and next-to-nearest neighbours away from the interface. We underline that other choices of interfacial bonds are possible to derive our main results. Indeed, one may start from any triangulation of the lattice satisfying the following properties: the number of nearest neighbours of each point has to be uniformly bounded by a constant independent of ε, while the length of the bonds in $H\mathcal{L}_\varepsilon(\rho, k)$ has to be uniformly bounded by a constant $C_\varepsilon = C\varepsilon$.

Once the bonds in the lattice $H\mathcal{L}_\varepsilon(\rho, k)$ are defined, we define the bonds of a point $x \in \mathcal{L}_\varepsilon(\rho, k)$ as follows:

$B_1(x) := \{\xi \in \mathbb{R}^N : Hx, \ H(x+\xi) \in H\mathcal{L}_\varepsilon(\rho, k) \text{ are nearest neighbours}\}$,

$B_2(x) := \{\xi \in \mathbb{R}^N : Hx, \ H(x+\xi) \in H\mathcal{L}_\varepsilon(\rho, k) \text{ are next-to-nearest neighbours}\}$.

We remark that if $x_1 \leq -2\varepsilon$, then $B_1(x) = B_1$ and $B_2(x) = B_2$, while if $x_1 \geq \rho\varepsilon$, then $B_1(x) = \rho B_1$ and $B_2(x) = \rho B_2$, where B_1, B_2 are as in (1.2)–(1.3). The total

interaction energy is

$$\mathcal{E}_\varepsilon^{1,\lambda}(u,\rho,k) :=$$

$$\sum_{\substack{x\in\mathcal{L}_\varepsilon^-(\rho,k)\\\xi\in B_1(x)}} c_1 \left|\left|\frac{|u(x+\xi)-u(x)|}{\varepsilon}\right| - 1\right|^p + \sum_{\substack{x\in\mathcal{L}_\varepsilon^+(\rho,k)\\\xi\in B_1(x)}} c_1 \left|\left|\frac{|u(x+\xi)-u(x)|}{\varepsilon}\right| - \lambda\right|^p$$

$$+ \sum_{\substack{x\in\mathcal{L}_\varepsilon^-(\rho,k)\\\xi\in B_2(x)}} c_2 \left|\frac{|u(x+\xi)-u(x)|}{\varepsilon} - \sqrt{3}\right|^p + \sum_{\substack{x\in\mathcal{L}_\varepsilon^+(\rho,k)\\\xi\in B_2(x)}} c_2 \left|\frac{|u(x+\xi)-u(x)|}{\varepsilon} - \sqrt{3}\lambda\right|^p.$$

Notice that away from the interface all bonds in the reference configuration are in equilibrium if $\rho = \lambda$; instead, interfacial bonds are never in equilibrium. The equilibrium distance of two atoms at the interface is in fact an average of the equilibrium distances of the two sublattices. Generalisations of this energy can be considered as described in [14, Section 4].

The results shown in detail in this paper for the defect-free case (corresponding to $\rho = 1$) can be extended to models with dislocations ($\rho \neq 1$) without significant changes in the proof. Thus we obtain a Γ-convergence result for the rescaled functionals $\mathcal{I}_\varepsilon^{1,\lambda}(\cdot,\rho,k)$ defined as in (1.7). (Notice that the definition of the admissible functions is given as in the dislocation-free case, with the only variant that the gradients are constant on the elements of the triangulation introduced to define the interfacial bonds.) Before stating the theorem we introduce the lattices

$$\mathcal{L}_\infty(\rho,k) := \mathcal{L}_\infty^-(1,k) \cup \mathcal{L}_\infty^+(\rho,k),$$
$$\mathcal{L}_\infty^-(1,k) := \mathbb{Z}^2 \cap \overline{\Omega}_{k,\infty} \cap \{x_1 < 0\},$$
$$\mathcal{L}_\infty^+(\rho,k) := \rho\mathbb{Z}^2 \cap \overline{\Omega}_{k,\infty} \cap \{x_1 \geq 0\},$$

where the triangulation is chosen in analogy with the one for $\mathcal{L}_\varepsilon(\rho,k)$. We also set

$$\gamma(P_1,\lambda P_2;\rho,k) := \inf\left\{\mathcal{E}_\infty^{1,\lambda}(v,\rho,k)\colon M>0,\ v\in\mathcal{A}_\infty(\Omega_{k,\infty}),\right.$$
$$\nabla v = P_1 H \text{ for } x_1 \in (-\infty,-M),$$
$$\left.\nabla v = \tfrac{\lambda}{\rho}P_2 H \text{ for } x_1 \in (M,+\infty)\right\},$$

with

$$\mathcal{E}_\infty^{1,\lambda}(u,\rho,k) :=$$

$$\sum_{\substack{x\in\mathcal{L}_\infty^-(\rho,k)\\\xi\in B_1(x)}} c_1 \Big||u(x+\xi)-u(x)| - 1\Big|^p + \sum_{\substack{x\in\mathcal{L}_\infty^+(\rho,k)\\\xi\in B_1(x)}} c_1 \Big||u(x+\xi)-u(x)| - \lambda\Big|^p$$

$$+ \sum_{\substack{x\in\mathcal{L}_\infty^-(\rho,k)\\\xi\in B_2(x)}} c_2 \Big||u(x+\xi)-u(x)| - \sqrt{3}\Big|^p + \sum_{\substack{x\in\mathcal{L}_\infty^+(\rho,k)\\\xi\in B_2(x)}} c_2 \Big||u(x+\xi)-u(x)| - \sqrt{3}\lambda\Big|^p.$$

Theorem 7.1. *The sequence of functionals $\{\mathcal{I}_\varepsilon^{1,\lambda}(\cdot,\rho,k)\}$ Γ-converges, as $\varepsilon \to 0^+$, to the functional*

$$\mathcal{I}^{1,\lambda}(u,\rho,k) = \begin{cases} \gamma(\rho,k) & \textit{if } u \in \mathcal{A}^{1,\lambda}(\rho,k), \\ +\infty & \textit{otherwise,} \end{cases}$$

with respect to the weak* convergence in $W^{1,\infty}(\Omega_k; \mathbb{R}^N)$, where

$$\mathcal{A}^{1,\lambda}(\rho, k) := \big\{ u \in W^{1,\infty}(\Omega_k; \mathbb{R}^N) \colon \partial_2 u = 0 \text{ a.e. in } \Omega_k \,,$$
$$|\partial_1 u| \le 1 \text{ a.e. in } \Omega_k^- \,, \ |\partial_1 u| \le \tfrac{\lambda}{\rho} \text{ a.e. in } \Omega_k^+ \big\}$$

and

$$\gamma(\rho, k) := \min \big\{ \gamma(I, \lambda I; \rho, k), \gamma(I, \lambda J; \rho, k) \big\}.$$

The stronger topology introduced in Theorem 5.4 allows us to take into account the cost of "folding" the lattice using rotoreflections, giving deeper insight into deformations that bridge different equilibria. Indeed, it is possible to combine Theorems 5.4 and 7.1 giving the Γ-convergence in the stronger topology for models with dislocations; we omit the full statement for brevity.

Remark 8. It is easy to see that for $\rho = \lambda$

$$C_1 k \le \gamma(\lambda, k) \le C_2 k$$

for some constants $C_1, C_2 > 0$. To obtain the estimate from above it is sufficient to consider the identical deformation and recall that the maximal length of a bond and the maximal number of bonds per atom in the lattice $\mathcal{L}_\infty(\rho, k)$ are uniformly bounded. This configuration corresponds to the case when dislocations are uniformly distributed along the interface between the two sublattices. (Recall that here $N = 2$ and that the length of the interface is $2k$.) In contrast, the cost of a defect-free configuration ($\rho = 1$) is superlinear as already shown in Theorem 2.2. In fact, following the same proof it is possible to conclude that whenever $\rho \ne \lambda$ one has

$$\gamma(\rho, k) \le C_\rho \, k^2 \quad \text{and} \quad \lim_{k \to \infty} \frac{\gamma(\rho, k)}{k} = +\infty \,.$$

This gives a mathematical proof of the experimentally observed fact that dislocations are preferred in order to relieve the lattice mismatch when the thickness of the specimen is sufficiently large. We recall that a similar result was proven in [14, 15] (under the non-interpenetration assumption), see also Remark 1.

The results sketched here for hexagonal lattices can be obtained also for other lattices by adapting the technique to each specific case. In particular, we refer to [15] for details on the rigidity of face-centred and body-centred cubic lattices in dimension three.

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