DERIVATION OF LINEAR ELASTICITY
FOR A GENERAL CLASS OF ATOMISTIC ENERGIES

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ABSTRACT. The purpose of this paper is the derivation, in the framework of Gamma-convergence, of linear elastic continuum theories from a general class of atomistic models, in the regime of small deformations. Existing results are available only in the special case of one-well potentials accounting for very short interactions. We consider here the general case of multi-well potentials accounting for interactions of finite but arbitrarily long range. The extension to this setting requires a novel idea for the proof of the Gamma-convergence which is interesting in its own right and potentially relevant in other applications.

INTRODUCTION

The passage from atomistic models to continuum theories has been the object of extensive research in the last decades. In particular, many variational tools for the mathematical analysis of discrete systems have been developed, with the objective of describing the macroscopical properties of systems whose microscopical behaviour is governed by interactions between their particles.

Within this framework, in this paper we focus on the problem of deriving linear elastic continuum theories from a general class of atomistic models in the regime of small deformations. We assume that the reference configuration of a system of particles is the portion $\mathcal{L}_\eta$ of a Bravais lattice lying inside a bounded open set Ω of $\mathbb{R}^N$, where η denotes the interatomic distance. The energy associated to a deformation $v \colon \mathcal{L}_\eta \to \mathbb{R}^N$ is of the form

$$E^\eta(v) = \sum_Q \eta^N W(D'v|_Q) + \text{surface terms}, \tag{0.1}$$

where the sum runs over lattice cells $Q \subset \Omega$ of $\mathcal{L}_\eta$ of size ηM, where $M \in \mathbb{N}$ is fixed, and $D'v|_Q$ consists of all finite differences of v between points in Q. The surface terms account for interactions between particles close to $\partial\Omega$. Energies of the form (0.1) are rather general and include in particular finite range pairwise interaction energies. The pre-factor η^N corresponds to a bulk scaling; indeed, under suitable growth assumptions, the asymptotic behaviour of E^η as $\eta \to 0$ is described by a continuum limit of the form $\int_\Omega f(\nabla v)\, \mathrm{d}x$ defined on some Sobolev space [3]. The computation of f accounts in particular for oscillations at the atomic scale and is connected to the validity or failure of the so-called Cauchy-Born rule, which holds when each atom follows the macroscopic deformation Ax, implying, roughly speaking, that $f(A) = W(A)$. This problem has been studied in [13, 9], where it has been proved that for functionals of the form (0.1) minimised on a single well the Cauchy-Born rule holds for deformations close to the well.

Within the theory of Continuum Mechanics, a variational approach for the derivation of linearised models from non linear functionals of the form $\int_\Omega f(\nabla v)\, dx$ consists in looking at minimum problems for suitable scalings of the energies when the deformations are small perturbations of an equilibrium (which without loss of generality we may assume to be the identity deformation). Specifically, let us write $v(x) = x + \varepsilon u(x)$, where εu is the displacement, and assume that f is smooth. Then, for a fixed u, a Taylor expansion of $\varepsilon \mapsto f(I + \varepsilon \nabla u)$ leads to a quadratic principal part of the form $\frac{1}{2}\varepsilon^2 D^2 f(I)[\nabla u]^2$. Hence, one expects that the limit as $\varepsilon \to 0$ of the rescaled energies

$$\varepsilon^{-2} \int_\Omega f(I + \varepsilon \nabla u)\, dx \tag{0.2}$$

is given by the linear elastic functional

$$\frac{1}{2} \int_\Omega D^2 f(I)[\nabla u]^2\, dx\,,$$

which turns out to depend only on the symmetric part of the gradient, if the initial non linear energy is frame invariant. A rigorous asymptotic analysis in terms of Γ-convergence of the rescaled energies (0.2) has been first performed in [10], ensuring, through compactness properties, the convergence of related boundary value problems. In [10] f is assumed to be minimised on a single well and to grow quadratically in terms of the distance from the well. This result has been later generalised to the case of mixed growth in [2]. Further generalisations have been obtained when f is minimised on more than one well and the distance between the wells is of order ε (see [1, 20]). It is worth mentioning that, for one-well energy densities $f(x, \nabla u)$ that are periodic with respect to x, the homogenisation and the linearisation processes commute [19]; see also [14] for a generalisation to a stochastic setting. The reader is also referred to [18] for a rigorous justification in terms of Γ-convergence of the classical linearisation approach in plasticity. More recently the case of multiple wells whose relative distance is fixed has been considered in [6]; in this context linear elasticity can be derived by adding to the multi-well energy a singular higher order term which penalises jumps from one well to another. In the continuum setting, such a perturbation turns out to be crucial to guarantee good compactness properties of minimising sequences of displacements.

Similarly to the continuum approach, in the discrete setting one studies the asymptotic behaviour of

$$\varepsilon^{-2} E^\eta(x + \varepsilon u)$$

as ε, $\eta \to 0$. In contrast to the continuum setting, in the discrete analysis one has to take into account the interplay between the two parameters η and ε. Indeed, a suitable scaling of η with respect to ε is required in some cases (see [21]) . This approach has been followed in [8, 21] in very special cases. Namely, [8] studies the case of harmonic springs between nearest neighbours minimised on a single well. In [21] such analysis has been later extended to single well energies of the form (0.1) with $M = 1$, namely accounting for very short interactions, possibly including cases when individual pair interactions are not equilibrated in the reference lattice. We emphasise that the assumptions on the potentials considered in [8] and [21] ensure the validity of the Cauchy-Born rule for deformations close to the equilibria and this turns out to be crucial in their analysis. Indeed, it rules out the possibility of oscillations at the atomic scale and leads in the limit to the linearised elastic functional associated to the Hessian $D^2W(I)$ of the cell energy. This is in line with the results proved in [19] for homogenisation. We also refer to [11] for the derivation of linearised Griffith theories from pairwise interaction potentials of Lennard-Jones type in the context of fracture mechanics.

The results of [8, 21] leave open the problem of deriving linear elasticity from more general models of interest in applications, including long-range interactions and multi-well potentials. In fact, their analysis cannot be easily adapted to such cases. The aim of the present paper is to fill

this gap by considering only minimal assumptions on energies of the form (0.1). Specifically, we extend the results to the case of interactions of finite but arbitrarily long range, namely, the case when the parameter M in (0.1) is an arbitrary integer number; second, to the case of multi-well potentials, i.e., when W is minimised on the union of a finite number of disjoint wells, in the spirit of [6]. Our main assumptions on the potential W are the following: frame invariance, minimality on the wells, mixed growth with respect to the distance of the deformation gradient from the wells, and an energetic penalisation of transitions between different wells.

The multi-well structure of the potential poses some difficulties in the proof of compactness of sequences of displacements with equibounded energy. This relies on the well-known rigidity estimate of Friesecke, James, and Müller [12], which could be directly applied in [8, 21]. In contrast, in our context it is crucial to first prove a lower bound ensuring that the energy is bounded from below by the distance of the deformation gradient from a single energy well (see Theorem 3.1). The continuum counterpart of this result was proved in [6, Theorem 2.3]. The key assumption on W coming to play in this analysis is the penalisation of transitions between different wells (see assumption (H1c) in Section 1); in particular, for pairwise potentials, such penalisation is played by interactions beyond nearest neighbours (see also [5]), which to some extent represent the discrete counterpart of the singular perturbation in [6]. The reader is also referred to [16] for the compactness of discrete multi-well energies with surface scaling.

As for the proof of the Γ-convergence, the main technical problem arising in our analysis comes from the assumption that in (0.1) M be arbitrary, in particular larger than one, which leads to new difficulties, compared to [8, 21]. A standard approach in the discrete to continuum analysis amounts to identify discrete deformations with their piecewise affine interpolations with respect to a triangulation of the domain. This allows one to represent the discrete energies in an integral form depending on gradients. In fact, such approach fails in the present setting. In order to overcome such difficulty we develop a completely new strategy, which we think may be relevant for other applications. Roughly speaking, it amounts to decompose the energy into the sum of integrals depending on suitable vector fields whose components are finite differences of the discrete deformation and that are piecewise constant on lattice cells of size ηM. Despite such vector fields are not gradients, we show that the average of the limiting vector fields can be written in terms of the gradient of the limiting deformation (see Lemma 4.2). This allows us to use a convexity argument to obtain the desired lower bound.

We prove that, under a suitable scaling of η with respect to ε, which we prove to be optimal in Example 7.4, the limit functional is still determined by the Hessian $D^2W(I)$ of the cell energy. However, in the case of more than one well, the validity of the Cauchy-Born rule for deformations close to the equilibria is not guaranteed, in contrast with [8, 21]. Indeed, in the bulk scaling regime, deformations lying in different wells can be arbitrarily mixed at a mesoscale with a negligible cost, but such oscillations are strongly penalised in our scaling regime. Hence, in contrast with the one-well model, in the case of more than one well the discrete to continuum and the linearisation processes do not commute.

We stress that the most general class of discrete energies whose continuum limit is a local functional of the form $\int_\Omega f(\nabla u)\,\mathrm{d}x$ includes cases where all the particles of the system interact. Such cases are not covered by our model. However, the locality of the limiting energy is guaranteed only if the interaction potentials decay very fast in terms of the relative distance between the particles (see [3]). In this respect, the assumption that M be finite does not seem a strong restriction and our model can thus be regarded as an approximation of those potentials.

We complement the analysis with several examples of pairwise interaction energies arising in different models, including cases when individual pair interactions are not equilibrated in the reference lattice (see in particular Example 7.3). Nonetheless, the generality of our model can also cover problems involving more general multi-body interaction energies.

The paper is organised as follows. Section 1 contains the definitions and the set of assumptions on the energy functional and specifies the conditions on the boundary data and the external loading. The main results are stated in Section 2 and proved in Section 4. The main tool to prove compactness is contained in Section 3 (see Theorem 3.1). In Section 5 we discuss the case when the boundary data are prescribed only on a subset of $\partial\Omega$. In Section 6 we show that our analysis applies to a rather general class of pairwise interaction energies and we specialise the limit functional in terms of the pairwise potentials. Finally, Section 7 is devoted to examples.

Notation. For $N \geq 2$, $\mathbb{M}^{N \times N}$ denotes the set of real $N \times N$ matrices and $SO(N)$ the set of rotations. We denote by I the identity matrix and and by Id the identity map $Id \colon \mathbb{R}^N \ni x \mapsto x$. For each $s > 1$ we denote by s' its conjugate exponent, i.e., $s' := \frac{s}{s-1}$.

In the paper, the same letter C stands for positive constants whose value may change from line to line.

1. Setting of the problem

In this section we introduce the reference configuration of the system, the admissible deformations and their discrete gradients, the mechanical energy, the boundary conditions, and the energy rescaling. We remark that our analysis applies to any Bravais lattice; by an affine change of variables, we may reduce to the lattice $\mathbb{Z}^N$.

Decomposition of $\mathbb{R}^N$. We use the so-called Kuhn decomposition, which is a partition of $\mathbb{R}^N$ into N-simplices (where $N \geq 1$). We partition the unit cube $(0,1)^N$ into N-simplices in the following way: we consider simplices T whose vertices are of the type

$$\{0, e_{i_1}, e_{i_1} + e_{i_2}, \ldots, e_{i_1} + e_{i_2} + \cdots + e_{i_N}\} \quad \text{for} \quad \begin{pmatrix} 1 & 2 & \cdots & N \\ i_1 & i_2 & \cdots & i_N \end{pmatrix} \in S_N \,,$$

where S_N is the set of permutations of N elements; see Figure 1. We denote by $\mathcal{T}_0$ the partition determined by such simplices. Next, we extend $\mathcal{T}_0$ by periodicity to all of $\mathbb{R}^N$ and denote by $\mathcal{T}$ its periodic extension.

Admissible deformations. Let Ω be an open bounded Lipschitz subset of $\mathbb{R}^N$. Given $\eta > 0$ we set

$$\mathcal{L}_\eta := \eta \mathbb{Z}^N \cap \Omega_\eta \,, \tag{1.1}$$

where Ω_η is the union of all closed hypercubes of the form $\eta(x + [0,1]^N)$, $x \in \mathbb{Z}^N$, that have non-empty intersection with Ω; see Figure 2. We identify every deformation $v \colon \mathcal{L}_\eta \to \mathbb{R}^N$ by its piecewise affine interpolation with respect to the rescaled triangulation $\eta\mathcal{T}$. By a slight abuse of
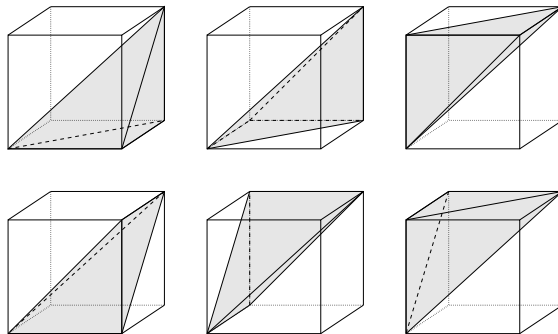

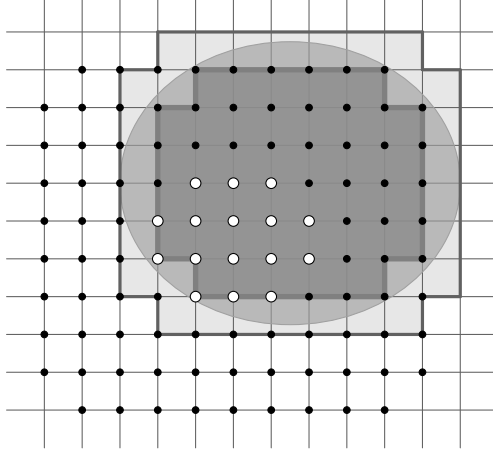Figure 1. A three-dimensional cube partitioned into six tetrahedra according to the Kuhn decomposition.

FIGURE 2. We represent some notation used in Section 1. We choose $M = 3$. The domain Ω is the open region contained inside the ellipse, displayed in grey. In light grey the (closed) set Ω_η; recall that $\mathcal{L}_\eta$ consists of all lattice points in Ω_η. In dark grey the (closed) set Ω_η^b; points in $\mathcal{L}_\eta^b$ are represented by white dots. Recall that $\mathcal{L}_\eta^b \subset \mathcal{L}_\eta^M$. The points of $\mathcal{L}_\eta^M \setminus \mathcal{L}_\eta^b$ are represented by black dots.

notation, such extension is still denoted by v. We define the domain of the functional as

$$\mathcal{A}_\eta := \big\{ v \in C^0(\Omega_\eta; \mathbb{R}^N) \colon v \text{ piecewise affine,}$$

$$\nabla v \text{ constant on } \Omega_\eta \cap \eta T \ \forall T \in \mathcal{T} \big\}.$$

We remark that all results below are independent of the choice of the interpolation. Indeed, all that follows still holds if one identifies the deformations with their piecewise constant interpolation instead of their piecewise affine interpolation, provided one uses a suitable notion of convergence; see for example [21].

Discrete gradients. Given $M \in \mathbb{N}$, let $x_1, \ldots, x_{(M+1)^N}$ be an enumeration of the set $C_M := \{0, \ldots, M\}^N$. Given $x \in \eta\mathbb{Z}^N$ and $v \colon x + \eta C_M \to \mathbb{R}^N$, we define the discrete gradient $D'_\eta v(x)$ of v in $x + \eta C_M$ as the vector composed of all the difference quotients of the function v corresponding to every two points in the cell $x + \eta C_M$. Specifically,

$$D'_\eta v(x) := \left(\frac{v(x + \eta x_l) - v(x + \eta x_k)}{\eta |x_l - x_k|} \right)_{1 \le k \ne l \le (M+1)^N}. \tag{1.2}$$

Note that $D'_\eta v(x) \in \mathbb{R}^{d(M)}$, where

$$d(M) := N(M+1)^N \Big((M+1)^N - 1 \Big).$$

We will also need a localised version of (1.2) on subsets of $x + \eta C_M$. Specifically, for $\mathcal{I} \subset \{1, \ldots, (M+1)^N\}$ we define the discrete gradient $D'_\eta|_{\mathcal{I}} v(x)$ of v in $\mathcal{I}$ as

$$D'_\eta|_{\mathcal{I}} v(x) = \left(\frac{v(x + \eta x_l) - v(x + \eta x_k)}{\eta |x_l - x_k|} \right)_{\substack{k, l \in \mathcal{I} \\ k < l}}. \tag{1.3}$$

We will employ the following notation for $1 \le k < l \le (M+1)^N$:

$$\left(D'_\eta v(x) \right)_{kl} := \frac{v(x + \eta x_l) - v(x + \eta x_k)}{\eta |x_l - x_k|}.$$

Moreover, we set, for $\zeta \in \mathbb{Z}^N$ and $x \in \mathcal{L}_\eta$,

$$D_\eta^\zeta v(x) := \frac{v(x + \eta\zeta) - v(x)}{\eta|\zeta|}\,. \tag{1.4}$$

In the case $\eta = 1$ we drop the subscript 1 and for $x = 0$ we simply write $D'v$ instead of $D_1'v(0)$ and $D'|_{\mathcal{I}}v$ instead of $D_1'|_{\mathcal{I}}v(0)$.

The energy functional. We consider energies $E^\eta \colon \mathcal{A}_\eta \mapsto [0, +\infty]$ of the form

$$E^\eta(v) := \sum_{x \in \mathcal{L}_\eta^M} \eta^N W_\eta\big(x, D_\eta'|_{\mathcal{I}_\eta(x)}v(x)\big)\,, \tag{1.5}$$

where

$$\mathcal{L}_\eta^M := \{x \in \eta\mathbb{Z}^N \colon (x + \eta C_M) \cap \Omega \neq \varnothing\}\,, \tag{1.6}$$

$$\mathcal{I}_\eta(x) = \{l \in \{1, \dots, (M+1)^N\} \colon x + \eta x_l \in \Omega\}\,, \tag{1.7}$$

and

$$W_\eta(x, D_\eta'|_{\mathcal{I}_\eta(x)}v(x)) = \begin{cases} W(D_\eta'v(x)) & \text{if } x + \eta C_M \subset \Omega\,, \\ W_{surf}(\mathcal{I}_\eta(x), D_\eta'|_{\mathcal{I}_\eta(x)}v(x)) & \text{otherwise.} \end{cases} \tag{1.8}$$

Here $W \colon \mathcal{Z}_D \subset \mathbb{R}^{d(M)} \to [0, +\infty]$ and $\mathcal{Z}_D$ is the vector subspace of $\mathbb{R}^{d(M)}$ defined by

$$\mathcal{Z}_D := \{Z \in \mathbb{R}^{d(M)} \colon Z = D'v \text{ for some } v \colon C_M \to \mathbb{R}^N\}\,, \tag{1.9}$$

while $W_{surf} \colon \mathcal{R} \to [0, +\infty]$, where $\mathcal{R} := \{(\mathcal{I}, Z) \colon \mathcal{I} \subset \{1, \dots (M+1)^N\},\ Z \in \mathcal{Z}_D(\mathcal{I})\}$ and

$$\mathcal{Z}_D(\mathcal{I}) := \{Z \in \mathbb{R}^{d(\mathcal{I})} \colon Z = D'|_{\mathcal{I}}v \text{ for some } v \colon C_M \to \mathbb{R}^N\}\,, \tag{1.10}$$

with

$$d(\mathcal{I}) := \frac{N}{2}\#(\mathcal{I})\Big(\#(\mathcal{I}) - 1\Big)\,.$$

In what follows, given $A \in \mathbb{M}^{N \times N}$ and $b \in \mathbb{R}^N$, we will denote by $v_{A,b}$ the affine function $v_{A,b} \colon \mathbb{Z}^N \to \mathbb{R}^N$ defined by

$$v_{A,b}(y) := Ay + b, \quad y \in \mathbb{Z}^N. \tag{1.11}$$

In the case when $A = I$ and $b = 0$ we simply denote it by Id. Moreover, for $Q \in SO(N)$ the symbol Qv denotes the function $x \mapsto Qv(x)$.

Let $l \in \mathbb{N}$, let $U_1, \dots, U_l$ be invertible matrices in $\mathbb{R}^{N \times N}$, and set

$$K := \bigcup_{i=1}^l K_i\,, \quad K_i := SO(N)U_i\,.$$

We assume that the sets K_i, $i = 1, \dots, l$, are all disjoint, namely, that $U_i U_j^{-1} \notin SO(N)$ for each $i \neq j$. For simplicity, we only consider the case where $U_1 = I$, the identity matrix; up to a change of variables one can recover the general case where U_1 is any invertible matrix, which is of interest, e.g., to study systems whose equilibrium configuration is an affine deformation of $\mathbb{Z}^N$.

We consider the following set of hypotheses on the interaction potential W:

(H0) (*frame invariance*) For each function $v \colon C_M \to \mathbb{R}^N$

$$W(D'v) = W(D'Qv) \quad \forall Q \in SO(N)\,.$$

(H1) (*rigidity and coercivity of the cell energy*)

  (H1a)

$$0 = \min_v W(D'v) = W(D'v_{A,b}) \quad \forall A \in K \text{ and } b \in \mathbb{R}^N;$$

(H1b) For each function $v\colon C_M \to \mathbb{R}^N$ (identified with its piecewise affine interpolation with respect to $\mathcal{T}$), it holds

$$W(D'v) \geq C \int_{(0,M)^N} \min\{\mathrm{dist}^2(\nabla v, K), \mathrm{dist}^p(\nabla v, K)\} \,\mathrm{d}x\,,$$

for some constant $C > 0$ and some $p \in (1, 2]$;

(H1c) There exist $0 < \sigma < \frac{1}{2}\min_{l_1 \neq l_2} \mathrm{dist}(K_{l_1}, K_{l_2})$ and $C_0 > 0$ such that, whenever $\mathrm{dist}(\nabla v|_S, K_{l_1}) \leq \sigma$ and $\mathrm{dist}(\nabla v|_T, K_{l_2}) \leq \sigma$ for two neighbouring simplices $S, T \subset [0, M]^N$ and two integers $l_1, l_2 \in \{1, \ldots l\}$, with $l_1 \neq l_2$, then

$$W(D'v) \geq C_0\,.$$

(H2) (C^2-regularity in a neighbourhood of the identity) W is of class C^2 in a neighbourhood of $D'\mathit{Id}$ and in such a neighbourhood the second derivatives are uniformly bounded.

Remark 1.1. *Observe that assumption* (H1c) *makes sense only in the case of two or more wells, that is when $l \geq 2$.*

Boundary conditions and external loading. We prescribe a Dirichlet boundary condition on the admissible deformations on the whole boundary $\partial\Omega$. (For Dirichlet conditions only on a subset of the boundary, see Section 5 below.) More precisely, given $\varepsilon > 0$ and $g \in W^{1,\infty}_{loc}(\mathbb{R}^N; \mathbb{R}^N)$, we assume that $v \in \mathcal{A}_\eta$ satisfies

$$v(x) = x + \varepsilon g(x) \quad \forall\, x \in \mathcal{L}_\eta \text{ such that } \mathrm{dist}(x, \Omega^c_\eta) \leq \delta_\eta\,,$$

where

$$\lim_{\eta \to 0} \delta_\eta = 0, \quad \delta_\eta \geq \sqrt{N}M\eta\,, \tag{1.12}$$

i.e., δ_η is larger than the diameter of the cell ηC_M. If we write the deformation v in terms of the displacement

$$v(x) = x + \varepsilon u(x)\,,$$

the Dirichlet boundary condition reads

$$u(x) = g(x) \quad \forall\, x \in \mathcal{L}_\eta \text{ such that } \mathrm{dist}(x, \Omega^c_\eta) \leq \delta_\eta\,. \tag{1.13}$$

We denote by $\mathcal{A}^g_\eta$ the set of such displacements, that is

$$\mathcal{A}^g_\eta := \{u \in \mathcal{A}_\eta\colon (1.13) \text{ holds}\}\,.$$

In what follows we will identify each displacement $u \in \mathcal{A}^g_\eta$ with its extension to $\eta\mathbb{Z}^N$ by assuming $u(x) = g(x)$ on $\eta\mathbb{Z}^N \setminus \mathcal{L}_\eta$. Setting

$$\mathcal{L}^b_\eta := \{x \in \mathcal{L}_\eta\colon x + \eta C_M \subset \Omega\}\,,$$

by (1.12) and (1.13) we can write for $u \in \mathcal{A}^g_\eta$

$$E^\eta(\mathit{Id} + \varepsilon u) = \sum_{x \in \mathcal{L}^b_\eta} \eta^N\, W\big(D'_\eta \mathit{Id} + \varepsilon D'_\eta u(x)\big) + E^\eta_{surf}(\mathit{Id} + \varepsilon g)\,,$$

where

$$E^\eta_{surf}(\mathit{Id} + \varepsilon g) = \sum_{x \in \mathcal{L}^M_\eta \setminus \mathcal{L}^b_\eta} \eta^N W_{surf}\big(\mathcal{I}_\eta(x), D'_\eta|_{\mathcal{I}_\eta(x)}(\mathit{Id} + \varepsilon g)(x)\big)\,, \tag{1.14}$$

see (1.6) for the definition of $\mathcal{L}^M_\eta$ and cf. Figure 2. Since the latter term does not depend on u, it can be neglected, as far as we are interested in minimising displacements.

In our analysis we also include a small loading term, assuming that the total energy of the system is $E^\eta(v) - \varepsilon \mathcal{F}^\eta(v)$, where

$$\mathcal{F}^\eta(v) := \sum_{x \in \mathcal{L}_\eta} f^\eta(x) \cdot v(x)\,,$$

with $f^\eta \colon \mathcal{L}_\eta \to \mathbb{R}^N$. We identify f^η with its piecewise constant interpolation and we assume that $f^\eta \rightharpoonup f$ in $L^q(\Omega; \mathbb{R}^N)$, as $\eta \to 0$, for some $q > 1$ which will be specified later on. We set

$$\mathcal{F}(v) := \int_\Omega f(x) \cdot v(x)\, \mathrm{d}x \quad \text{for } v \in L^2(\Omega; \mathbb{R}^N)\,.$$

Note that

$$E^\eta(Id + \varepsilon u) - \varepsilon \mathcal{F}^\eta(Id + \varepsilon u) = E^\eta(Id + \varepsilon u) - \varepsilon^2 \mathcal{F}^\eta(u) - \varepsilon \mathcal{F}^\eta(Id)\,.$$

Since the last term does not depend on u, it can be neglected in our variational analysis.

Energy rescaling. In order to study the asymptotic behaviour of the minimisers of (1.5) subject to the Dirichlet boundary condition (1.13), we then express the energies in terms of the displacement fields and properly renormalise and rescale them, by setting for $u \in \mathcal{A}_\eta^g$

$$\mathcal{E}_\varepsilon^\eta(u) := \frac{1}{\varepsilon^2}\big(E^\eta(Id + \varepsilon u) - E_{surf}^\eta(Id + \varepsilon g)\big) = \frac{1}{\varepsilon^2} \sum_{x \in \mathcal{L}_\eta^b} \eta^N\, W\big(D_\eta' Id + \varepsilon D_\eta' u(x)\big)\,. \qquad (1.15)$$

In the case of external loads, we will provide convergence results for the solutions of

$$\min_u \{\mathcal{E}_\varepsilon^{\eta(\varepsilon)}(u) - \mathcal{F}^{\eta(\varepsilon)}(u)\}\,.$$

The heuristic argument which allows one to identify the elastic energy associated with $\mathcal{E}_\varepsilon^\eta$ as ε and η go to 0, consists in computing the pointwise limit of $\mathcal{E}_\varepsilon^\eta(u)$ for a fixed smooth function u. Indeed, by a Taylor expansion of W about $D_\eta' Id$ as $\varepsilon \to 0$ we get

$$\mathcal{E}_\varepsilon^\eta(u) = \frac{1}{2} \sum_{x \in \mathcal{L}_\eta^b} \eta^N\, D_Z^2 W\big(D' Id)[D_\eta' u(x)]^2 + o(1)\,,$$

where $D_Z^2 W$ denotes the matrix of second derivatives of W with respect to the argument $Z \in \mathcal{Z}_D$, recall (1.9)–(1.10). We observe that $\mathcal{E}_\varepsilon^\eta(u)$ converges, as ε and η tend to 0, to

$$\int_\Omega \phi(\nabla u)\, \mathrm{d}x\,,$$

where

$$\phi(A) := \frac{1}{2} D_Z^2 W(D' Id)[D' v_{A,0}]^2 \quad \forall A \in \mathbb{M}^{N \times N}\,. \qquad (1.16)$$

By frame invariance, the quadratic form $A \mapsto D_Z^2 W(D' Id)[D' v_{A,0}]^2$ depends only on $\frac{1}{2}(A + A^T)$, the symmetric part of A, hence

$$\int_\Omega \phi(\nabla u)\, \mathrm{d}x = \int_\Omega \phi(e(u))\, \mathrm{d}x\,.$$

The above argument will be rigorously justified in terms of Γ-convergence [7] and complemented with a compactness result. In the case of two or more wells, that is $l \geq 2$, the compactness result will be proved under a suitable scaling of $\eta = \eta(\varepsilon)$. Precisely, given $r \in (1, p]$, the following scaling assumption on $\eta = \eta(\varepsilon)$ will ensure compactness of minimising sequences in $W^{1,r}(\Omega; \mathbb{R}^N)$:

$$\lim_{\varepsilon \to 0} \eta(\varepsilon) = 0\,, \quad \eta(\varepsilon) \geq C \varepsilon^{2 - \frac{r(N-1)}{N}}\,. \qquad (1.17)$$

In the case $l = 1$, we only assume $\lim_{\varepsilon \to 0} \eta(\varepsilon) = 0$, which yields compactness in $W^{1,p}(\Omega; \mathbb{R}^N)$. We finally define

$$\mathcal{E}_\varepsilon(u) := \begin{cases} \mathcal{E}_\varepsilon^{\eta(\varepsilon)}(u) & \text{if } u \in \mathcal{A}_{\eta(\varepsilon)}^g\,, \\ +\infty & \text{if } u \in L^1(\Omega; \mathbb{R}^N) \setminus \mathcal{A}_{\eta(\varepsilon)}^g \end{cases} \qquad (1.18)$$

and

$$E_\varepsilon(v) := \frac{1}{\varepsilon^2}\big(E^{\eta(\varepsilon)}(v) - E_{surf}^{\eta(\varepsilon)}(Id + \varepsilon g)\big)\,, \quad v \in \mathcal{A}_{\eta(\varepsilon)}\,. \qquad (1.19)$$

For later use, we introduce the set consisting of the union of all cells contained in Ω,

$$\Omega_\eta^b := \bigcup_{x \in \mathcal{L}_\eta^b} \left(x + [0, M\eta]^N \right). \tag{1.20}$$

By (H1b), it follows that

$$E_\varepsilon(v) = \mathcal{E}_\varepsilon(u) \geq C \frac{1}{\varepsilon^2} \int_{\Omega_{\eta(\varepsilon)}^b} \min\{\text{dist}^2(\nabla v, K), \text{dist}^p(\nabla v, K)\} \, dx, \tag{1.21}$$

where $v = Id + \varepsilon u$.

2. Main results

Theorem 2.1 (Compactness). *Let W satisfy* (H0) *and* (H1) *and let $g \in W_{loc}^{1,\infty}(\mathbb{R}^N; \mathbb{R}^N)$. Let $\eta(\varepsilon) \to 0$; if $l \geq 2$, assume in addition that $\eta(\varepsilon)$ satisfies* (1.17) *for a given $r \in (1, p]$. Let $s = p$ for $l = 1$ and $s = r$ for $l \geq 2$. Then there is a sequence $\alpha_\varepsilon \to 0$ such that the following hold.*

(i) *(Case of zero loading) If $\{u_\varepsilon\}$ is a sequence in $\mathcal{A}_{\eta(\varepsilon)}^g$ such that $\mathcal{E}_\varepsilon(u_\varepsilon)$ is uniformly bounded, then there exists a positive constant $C > 0$ such that*

$$\int_\Omega |\nabla u_\varepsilon|^s \, dx \leq C \left((\mathcal{E}_\varepsilon(u_\varepsilon))^{\frac{s}{2}} + \int_{\partial\Omega} |g|^s \, d\mathcal{H}^{N-1} \right) + \alpha_\varepsilon. \tag{2.1}$$

In particular,

$$\|u_\varepsilon\|_{W^{1,s}(\Omega;\mathbb{R}^N)} \leq C, \tag{2.2}$$

for some positive constant C independent of ε.

(ii) *(Case of nonzero loading with $l = 1$) Assume $l = 1$ and let $f^{\eta(\varepsilon)}$ be bounded in $L^{s'}(\Omega; \mathbb{R}^N)$. If $\{u_\varepsilon\}$ is a sequence in $\mathcal{A}_{\eta(\varepsilon)}^g$ such that $\mathcal{E}_\varepsilon(u_\varepsilon) - \mathcal{F}^{\eta(\varepsilon)}(u_\varepsilon)$ is uniformly bounded, then there exists a positive constant $C > 0$ such that*

$$\int_\Omega |\nabla u_\varepsilon|^s \, dx \leq C \left((\mathcal{E}_\varepsilon(u_\varepsilon))^{\frac{s}{2}} + \varepsilon^{2-s} \mathcal{E}_\varepsilon(u_\varepsilon) + \int_{\partial\Omega} |g|^s \, d\mathcal{H}^{N-1} \right) + \alpha_\varepsilon. \tag{2.3}$$

Moreover (2.2) *holds true and $\mathcal{E}_\varepsilon(u_\varepsilon)$ is uniformly bounded.*

(iii) *(Case of nonzero loading with $l \geq 2$) Assume $l \geq 2$ and let $f^{\eta(\varepsilon)}$ be bounded in $L^{s'}(\Omega; \mathbb{R}^N)$. If $\{u_\varepsilon\}$ is a sequence in $\mathcal{A}_{\eta(\varepsilon)}^g$ such that $\mathcal{E}_\varepsilon(u_\varepsilon) - \mathcal{F}^{\eta(\varepsilon)}(u_\varepsilon)$ is uniformly bounded, then there exists a positive constant $C > 0$ such that*

$$\int_\Omega |\nabla u_\varepsilon|^s \, dx \leq C \left((\mathcal{E}_\varepsilon(u_\varepsilon))^{\frac{s}{2}} + \varepsilon^{2-s} \mathcal{E}_\varepsilon(u_\varepsilon) + (\mathcal{E}_\varepsilon(u_\varepsilon))^{\frac{N}{N-1}} + \int_{\partial\Omega} |g|^s \, d\mathcal{H}^{N-1} \right) + \alpha_\varepsilon. \tag{2.4}$$

Moreover, if $s > \frac{N}{N-1}$ or $\eta(\varepsilon) \gg \varepsilon$, then (2.2) *holds true and $\mathcal{E}_\varepsilon(u_\varepsilon)$ is uniformly bounded.*

Theorem 2.2 (Γ-convergence). *Let W satisfy* (H0), (H1a), *and* (H2) *and let $g \in W_{loc}^{1,\infty}(\mathbb{R}^N; \mathbb{R}^N)$. Let $s \in (1, 2]$ and let $\eta = \eta(\varepsilon) \to 0$. Then, as $\varepsilon \to 0^+$ the sequence of functionals $\{\mathcal{E}_\varepsilon\}$ Γ-converges, with respect to the weak topology of $W^{1,s}(\Omega; \mathbb{R}^N)$, to the functional*

$$\mathcal{E}(u) := \begin{cases} \displaystyle\int_\Omega \phi(e(u)) \, dx & \text{if } u \in H_g^1(\Omega; \mathbb{R}^N), \\ +\infty & \text{otherwise}, \end{cases} \tag{2.5}$$

where ϕ is defined in (1.16).

The proofs of Theorems 2.1 and 2.2 will be given in Section 4. As a direct consequence of such results, we deduce the convergence of minima and minimisers stated in the following corollary.

Corollary 2.3. *Under the assumptions of Theorems 2.1 and 2.2, let $f^\eta \rightharpoonup f$ in $L^{s'}(\Omega; \mathbb{R}^N)$,*

$$m_\varepsilon := \inf\{\mathcal{E}_\varepsilon(u) - \mathcal{F}^{\eta(\varepsilon)}(u) \colon u \in \mathcal{A}^g_{\eta(\varepsilon)}\},$$

and let $u_\varepsilon \in \mathcal{A}^g_{\eta(\varepsilon)}$ be such that

$$\mathcal{E}_\varepsilon(u_\varepsilon) - \mathcal{F}^{\eta(\varepsilon)(u)} \le m_\varepsilon + o(1).$$

Then $\{u_\varepsilon\}$ weakly converges in $W^{1,s}(\Omega; \mathbb{R}^N)$ to the unique solution of

$$\min\{\mathcal{E}(u) - \mathcal{F}(u) \colon u \in H^1_g(\Omega; \mathbb{R}^N)\} =: m,$$

where $s \in (1, p]$ is as in Theorem 2.1. Moreover $m_\varepsilon \to m$.

Analogous results with Dirichlet conditions prescribed only on a subset of the boundary are presented in Section 5 below.

Remark 2.4. *It is possible to prove the optimality of the scaling (1.17) in the case $l \ge 2$, by providing examples of sequences with equibounded energy that are unbounded in $W^{1,r}(\Omega; \mathbb{R}^N)$ if $\eta(\varepsilon) \ll C\varepsilon^{2 - \frac{r(N-1)}{N}}$, see Example 7.4 below.*

In the case $r > \frac{N}{N-1}$, the scaling (1.17) implies $\eta(\varepsilon) \gg \varepsilon$. This might suggest that linearisation occurs when the scale of the displacement is much smaller than the interatomic distance. In fact, this would actually hold only if we assumed that u_ε be bounded in L^∞, which is not implied by our hypotheses. We highlight here the crucial role played by assumption (H1c) in the case of two or more wells: indeed, even in the case $\eta(\varepsilon) \gg \varepsilon$, one can provide examples of two-well nearest-neighbour interaction energies such that (H1c) is not satisfied and the compactness result stated in Theorem 2.1 does not hold; see the last remark in Example 7.1.

3. A RIGIDITY RESULT

In the present section we prove a one-well lower bound that will play a key role in the proof of the main theorems: it ensures that configurations with equibounded energy lie close to a certain energy well in most of the domain. We remark that the results of this section are independent of both the boundary condition and the external loading.

The following rigidity result provides a lower bound on the functional (1.19) in terms of the distance of the deformation gradient from a single energy well and it will be the main tool in proving Theorem 2.1.

Theorem 3.1. *Let W satisfy assumptions (H0) and (H1). For a given $\eta = \eta(\varepsilon)$, assume that $v_\varepsilon \in \mathcal{A}_{\eta(\varepsilon)}$ is a sequence such that $\lim_{\varepsilon \to 0} \varepsilon^2 E_\varepsilon(v_\varepsilon) = 0$, where E_ε is defined in (1.19). Then there exists $C > 0$ such that*

(a) *if $l = 1$, then*

$$\frac{1}{\varepsilon^p} \int_{\Omega^b_{\eta(\varepsilon)}} \operatorname{dist}^p(\nabla v_\varepsilon, SO(N)) \, \mathrm{d}x \le C\left(\left(E_\varepsilon(v_\varepsilon)\right)^{\frac{p}{2}} + \varepsilon^{2-p} E_\varepsilon(v_\varepsilon)\right); \tag{3.1}$$

(b) *if $l \ge 2$ and $r \in (1, p]$, then for ε sufficiently small there is $i_\varepsilon \in \{1, \dots, l\}$ such that*

$$\frac{1}{\varepsilon^r} \int_{\Omega^b_{\eta(\varepsilon)}} \operatorname{dist}^r(\nabla v_\varepsilon, K_{i_\varepsilon}) \, \mathrm{d}x \le C\left(\left(E_\varepsilon(v_\varepsilon)\right)^{\frac{r}{2}} + \varepsilon^{2-r} E_\varepsilon(v_\varepsilon) + \varepsilon^{-r}\left(\frac{\varepsilon^2}{\eta}\right)^{\frac{N}{N-1}} \left(E_\varepsilon(v_\varepsilon)\right)^{\frac{N}{N-1}}\right). \tag{3.2}$$

Remark 3.2. *For later use notice that, under assumption (1.17), in (3.2) $\varepsilon^{-r}\left(\frac{\varepsilon^2}{\eta}\right)^{\frac{N}{N-1}} \le C$.*

Proof. To ease notation we write Ω_ε^b in place of $\Omega_{\eta(\varepsilon)}^b$, cf. (1.20). Recalling that $\varepsilon^2 E_\varepsilon(v_\varepsilon) \to 0$, (1.21) in turn yields

$$|\Omega_\varepsilon^b \setminus \hat{\Omega}_\varepsilon| \to 0 \,, \tag{3.3}$$

where

$$\hat{\Omega}_\varepsilon := \{\mathrm{dist}(\nabla v_\varepsilon, K) < \hat{\sigma}\} \,, \tag{3.4}$$

with $\hat{\sigma} := \sigma \wedge 1$ and σ defined in assumption (H1c). Set $\Omega_\varepsilon^i := \{\mathrm{dist}(\nabla v_\varepsilon, K_i) < \hat{\sigma}\}$, $i = 1, \ldots, l$, and note that, since $\hat{\Omega}_\varepsilon = \bigcup_{i=1}^l \Omega_\varepsilon^i$, by (3.3) there exists $i_\varepsilon \in \{1, \ldots, l\}$ such that for ε sufficiently small

$$|\Omega_\varepsilon^{i_\varepsilon}| > C \,, \tag{3.5}$$

for some positive constant C independent of ε. Given $1 < s \leq 2$, we write

$$\int_{\Omega_\varepsilon^b} \mathrm{dist}^s(\nabla v_\varepsilon, K_{i_\varepsilon}) \, \mathrm{d}x = \int_{\Omega_\varepsilon^{i_\varepsilon}} \mathrm{dist}^s(\nabla v_\varepsilon, K_{i_\varepsilon}) \, \mathrm{d}x + \int_{\Omega_\varepsilon^b \setminus \Omega_\varepsilon^{i_\varepsilon}} \mathrm{dist}^s(\nabla v_\varepsilon, K_{i_\varepsilon}) \, \mathrm{d}x \,. \tag{3.6}$$

We estimate the first term in the right hand side using Hölder's inequality and the quadratic growth of the functional near the wells to obtain

$$\int_{\Omega_\varepsilon^{i_\varepsilon}} \mathrm{dist}^s(\nabla v_\varepsilon, K_{i_\varepsilon}) \, \mathrm{d}x \leq C \Big(\int_{\Omega_\varepsilon^{i_\varepsilon}} \mathrm{dist}^2(\nabla v_\varepsilon, K_{i_\varepsilon}) \, \mathrm{d}x \Big)^{\frac{s}{2}} \leq C \varepsilon^s \big(E_\varepsilon(v_\varepsilon) \big)^{\frac{s}{2}}. \tag{3.7}$$

Observe that if $l = 1$ we have $\Omega_\varepsilon^{i_\varepsilon} = \hat{\Omega}_\varepsilon$ and in $\Omega_\varepsilon^b \setminus \hat{\Omega}_\varepsilon$

$$\min\{\mathrm{dist}^2(\nabla v_\varepsilon, SO(N)), \mathrm{dist}^p(\nabla v_\varepsilon, SO(N))\} \geq C \, \mathrm{dist}^p(\nabla v_\varepsilon, SO(N)) \tag{3.8}$$

for some constant C depending on $\hat{\sigma}$. Then (3.1) follows from (1.21), (3.6), (3.7) with $s = p$, and (3.8).

In the case $l \geq 2$ we take $s = r$ in (3.6) and (3.7) and we split the integral on $\Omega_\varepsilon^b \setminus \Omega_\varepsilon^{i_\varepsilon}$ into two parts:

$$\int_{\Omega_\varepsilon^b \setminus \Omega_\varepsilon^{i_\varepsilon}} \mathrm{dist}^r(\nabla v_\varepsilon, K_{i_\varepsilon}) \, \mathrm{d}x =$$

$$\int_{(\Omega_\varepsilon^b \setminus \Omega_\varepsilon^{i_\varepsilon}) \cap \{|\nabla v_\varepsilon| \leq \rho\}} \mathrm{dist}^r(\nabla v_\varepsilon, K_{i_\varepsilon}) \, \mathrm{d}x + \int_{(\Omega_\varepsilon^b \setminus \Omega_\varepsilon^{i_\varepsilon}) \cap \{|\nabla v_\varepsilon| > \rho\}} \mathrm{dist}^r(\nabla v_\varepsilon, K_{i_\varepsilon}) \, \mathrm{d}x \,,$$

where $\rho > 0$. Choosing ρ sufficiently large, one has that $\mathrm{dist}(\nabla v_\varepsilon, K)$ is bounded away from zero whenever $|\nabla v_\varepsilon(x)| > \rho$. Hence, for ρ sufficiently large, the second term in the right hand side can be estimated as follows:

$$\int_{(\Omega_\varepsilon^b \setminus \Omega_\varepsilon^{i_\varepsilon}) \cap \{|\nabla v_\varepsilon| > \rho\}} \mathrm{dist}^r(\nabla v_\varepsilon, K_{i_\varepsilon}) \, \mathrm{d}x \leq C \int_{(\Omega_\varepsilon^b \setminus \Omega_\varepsilon^{i_\varepsilon}) \cap \{|\nabla v_\varepsilon| > \rho\}} \mathrm{dist}^p(\nabla v_\varepsilon, K) \, \mathrm{d}x \leq C \varepsilon^2 E_\varepsilon(v_\varepsilon) \,.$$

In order to estimate the first term, we provide a bound on the perimeter $\mathrm{Per}(\Omega_\varepsilon^{i_\varepsilon})$ after noticing that

$$\int_{(\Omega_\varepsilon^b \setminus \Omega_\varepsilon^{i_\varepsilon}) \cap \{|\nabla v_\varepsilon| \leq \rho\}} \mathrm{dist}^r(\nabla v_\varepsilon, K_{i_\varepsilon}) \, \mathrm{d}x \leq C \, |\Omega_\varepsilon^b \setminus \Omega_\varepsilon^{i_\varepsilon}| \,. \tag{3.9}$$

Set

$$\mathcal{T}_\varepsilon := \{T \in \eta\mathcal{T} :$$

$$T \subset \Omega_\varepsilon^{i_\varepsilon} \text{ and there exists a neighbouring simplex } S \in \eta\mathcal{T} \text{ with } S \subset \Omega_\varepsilon^b \setminus \Omega_\varepsilon^{i_\varepsilon} \} \,,$$

and notice that

$$\frac{1}{C} \, \mathrm{Per}(\Omega_\varepsilon^{i_\varepsilon}) \leq \eta^{N-1} \# \mathcal{T}_\varepsilon \leq C \, \mathrm{Per}(\Omega_\varepsilon^{i_\varepsilon}) \,. \tag{3.10}$$

Let $T \in \mathcal{T}_\varepsilon$ and let S be a neighbouring simplex lying in $\Omega_\varepsilon^b \setminus \Omega_\varepsilon^{i_\varepsilon}$. Fix $x \in \mathcal{L}_\eta$ such that $T \cup S \subset x + \eta C_M$. Then, using assumption (H1b) if $S \subset \Omega_\varepsilon^b \setminus \hat{\Omega}_\varepsilon$ and (H1c) if $S \subset \hat{\Omega}_\varepsilon \setminus \Omega_\varepsilon^{i_\varepsilon}$,

$$W(D_\eta' v_\varepsilon(x)) \geq C > 0 \,.$$

The above inequality, in combination with (3.10), yields

$$\operatorname{Per}(\Omega_\varepsilon^{i_\varepsilon}) \leq C \frac{\varepsilon^2}{\eta} E_\varepsilon(v_\varepsilon) \,, \tag{3.11}$$

where the constant C accounts for the fact that each cell contains a fixed number of simplices. In view of (3.11) and of the isoperimetric inequality we have

$$\min\{|\Omega_\varepsilon^{i_\varepsilon}|, |\Omega_\varepsilon^b \setminus \Omega_\varepsilon^{i_\varepsilon}|\} \leq C \operatorname{Per}(\Omega_\varepsilon^{i_\varepsilon})^{\frac{N}{N-1}} \leq C \left(\frac{\varepsilon^2}{\eta} E_\varepsilon(v_\varepsilon) \right)^{\frac{N}{N-1}}. \tag{3.12}$$

Suppose now that $\min\{|\Omega_\varepsilon^{i_\varepsilon}|, |\Omega_\varepsilon^b \setminus \Omega_\varepsilon^{i_\varepsilon}|\} = |\Omega_\varepsilon^b \setminus \Omega_\varepsilon^{i_\varepsilon}|$. Then, from (3.9) we deduce the following estimate

$$\int_{(\Omega_\varepsilon^b \setminus \Omega_\varepsilon^{i_\varepsilon}) \cap \{|\nabla v_\varepsilon| \leq \rho\}} \operatorname{dist}^r(\nabla v_\varepsilon, K_{i_\varepsilon}) \, \mathrm{d}x \leq C \left(\frac{\varepsilon^2}{\eta} E_\varepsilon(v_\varepsilon) \right)^{\frac{N}{N-1}}. \tag{3.13}$$

If on the contrary $\min\{|\Omega_\varepsilon^{i_\varepsilon}|, |\Omega_\varepsilon^b \setminus \Omega_\varepsilon^{i_\varepsilon}|\} = |\Omega_\varepsilon^{i_\varepsilon}|$, then from (3.5) and (3.12) we deduce that

$$\left(\frac{\varepsilon^2}{\eta} E_\varepsilon(v_\varepsilon) \right)^{\frac{N}{N-1}} \geq C$$

and therefore, since the left-hand side of (3.13) is bounded, we again find that (3.13) holds. □

4. Proof of the main results

4.1. **Proof of compactness.**

Proof of Theorem 2.1. As in the proof of Theorem 3.1, Ω_ε^b stands for $\Omega_{\eta(\varepsilon)}^b$, cf. (1.20). Let $v_\varepsilon = x + \varepsilon u_\varepsilon$ and set $g_\varepsilon := g|_{\eta(\varepsilon)\mathbb{Z}^N}$, both identified with their piecewise affine interpolations. By (1.12) and (1.13), $u_\varepsilon = g_\varepsilon$ in $\Omega \setminus \Omega_\varepsilon^b$.

In order to apply Theorem 3.1, we first show that $\varepsilon^2 E_\varepsilon(v_\varepsilon) \to 0$. This is trivial in the case of zero loading (i), since $E_\varepsilon(v_\varepsilon)$ is assumed to be equibounded in ε. In the case of nonzero loading (ii)–(iii), the proof follows the steps of the proof of [6, Theorem 1.8 (ii)], that we briefly detail here for the reader's convenience. Assuming $\mathcal{E}_\varepsilon(u_\varepsilon) - \mathcal{F}^{\eta(\varepsilon)}(u_\varepsilon) \leq M$, by Poincaré inequality we get

$$\mathcal{E}_\varepsilon(u_\varepsilon) \leq M + \mathcal{F}^{\eta(\varepsilon)}(u_\varepsilon) \leq C(1 + \|\nabla u_\varepsilon\|_{L^s(\Omega;\mathbb{R}^{d\times d})}) \leq C\left(1 + \|\nabla u_\varepsilon\|_{L^p(\Omega;\mathbb{R}^{d\times d})}\right). \tag{4.1}$$

Moreover, by assumption (H1b), see (1.21), we get

$$\int_{\Omega_\varepsilon^b \setminus \hat{\Omega}_\varepsilon} |\nabla u_\varepsilon|^p \, \mathrm{d}x \leq \frac{C}{\varepsilon^p} \int_{\Omega_\varepsilon^b \setminus \hat{\Omega}_\varepsilon} \operatorname{dist}^p(\nabla v_\varepsilon, K) \, \mathrm{d}x$$

$$\leq C \frac{1}{\varepsilon^2} \int_{\Omega_\varepsilon^b} \min\{\operatorname{dist}^2(\nabla v_\varepsilon, K), \operatorname{dist}^p(\nabla v_\varepsilon, K)\} \, \mathrm{d}x \leq C \mathcal{E}_\varepsilon(u_\varepsilon) \,,$$

where $\hat{\Omega}_\varepsilon$ is as in (3.4). On the other hand, in $\hat{\Omega}_\varepsilon$ we have $|\nabla v_\varepsilon| \leq C$, thus $|\nabla u_\varepsilon| \leq \frac{C}{\varepsilon}$, a.e.; finally, in $\Omega \setminus \Omega_\varepsilon^b$ we have $|\nabla u_\varepsilon| \sim |\nabla g| \leq C$. Therefore, for any $\kappa < 1$ there exists C_κ such that

$$\|\nabla u_\varepsilon\|_{L^p(\Omega;\mathbb{R}^{d\times d})}^p \leq \frac{C}{\varepsilon^p} + C \mathcal{E}_\varepsilon(u_\varepsilon) \leq \frac{C_\kappa}{\varepsilon^p} + \kappa \|\nabla u_\varepsilon\|_{L^p(\Omega;\mathbb{R}^{d\times d})}^p \,,$$

where in the last inequality we employed (4.1) in combination with Young's inequality. We obtain that $\|\nabla u_\varepsilon\|_{L^p(\Omega;\mathbb{R}^{d\times d})} \leq \frac{C}{\varepsilon}$ and, by using again (4.1), that $E_\varepsilon(v_\varepsilon) = \mathcal{E}_\varepsilon(u_\varepsilon) \leq \frac{C}{\varepsilon}$, in particular $\varepsilon^2 E_\varepsilon(v_\varepsilon) \to 0$.

In all cases (i)–(iii), we may now apply Theorem 3.1, hence there is $i_\varepsilon \in \{1, \ldots, l\}$ such that

$$\int_\Omega \text{dist}^s(\nabla v_\varepsilon, K_{i_\varepsilon}) \, dx = \int_{\Omega_\varepsilon^b} \text{dist}^s(\nabla v_\varepsilon, K_{i_\varepsilon}) \, dx + \int_{\Omega \setminus \Omega_\varepsilon^b} \text{dist}^s(I + \varepsilon \nabla g_\varepsilon, K_{i_\varepsilon}) \, dx$$
$$\leq C \, \varepsilon^s \Big(\big(E_\varepsilon(v_\varepsilon)\big)^{\frac{s}{2}} + \varepsilon^{2-s} E_\varepsilon(v_\varepsilon) + \tau_\varepsilon \big(E_\varepsilon(v_\varepsilon)\big)^{\frac{N}{N-1}} \Big) + C \, |\Omega \setminus \Omega_\varepsilon^b| \,, \tag{4.2}$$

where $\tau_\varepsilon = 0$ if $l = 1$ and $\tau_\varepsilon = \varepsilon^{-s}(\frac{\varepsilon^2}{\eta})^{\frac{N}{N-1}}$ if $l \geq 2$. Observe that $|\Omega \setminus \Omega_\varepsilon^b| \to 0$. We next prove that $\text{dist}(\nabla v_\varepsilon, K_{i_\varepsilon}) \to 0$ in $L^s(\Omega)$. This follows in case (i) because $E_\varepsilon(v_\varepsilon)$ is equibounded and $\tau_\varepsilon \leq C$, cf. (1.17) if $l \geq 2$, so the right-hand side of (4.2) tends to zero. In cases (ii)–(iii) we have already proved that $E_\varepsilon(v_\varepsilon) \leq \frac{C}{\varepsilon}$. Hence, in case (ii), or in case (iii) if $s > \frac{N}{N-1}$, the conclusion follows as in case (i). In case (iii) with $s = \frac{N}{N-1}$, by the assumption $\eta(\varepsilon) \gg \varepsilon$ one has $\tau_\varepsilon \to 0$, so again the right-hand side of (4.2) tends to zero. In particular this implies $\text{dist}(\nabla v_\varepsilon, K_{i_\varepsilon}) \to 0$ in $L^s(\Omega)$ also for $s < \frac{N}{N-1}$.

We now show that $i_\varepsilon = 1$ for ε sufficiently small. Suppose on the contrary that there is $\bar{\imath} \in \{2, \ldots, l\}$ such that $i_\varepsilon = \bar{\imath}$ for a subsequence $\varepsilon \to 0$ (not relabelled). Recall the sets $\Omega_\varepsilon^i = \{\text{dist}(\nabla v_\varepsilon, K_i) < \hat{\sigma}\}$ defined in the proof of Theorem 3.1, with $\hat{\sigma} = \sigma \wedge 1$ and σ as in (H1c). By (1.13), $\Omega_\varepsilon^1 \supset \{\text{dist}(x, \Omega_\eta^c) \leq \delta_\eta\}$ for ε sufficiently small. Let $\widetilde{\Omega}_\varepsilon$ be the connected component of $\Omega \setminus \Omega_\varepsilon^{\bar{\imath}}$ containing $\{\text{dist}(x, \Omega_\eta^c) \leq \delta_\eta\}$ and observe that $\text{Per}(\{\text{dist}(x, \Omega_\eta^c) \leq \delta_\eta\}) \geq C$ for some $C > 0$. Since $\text{dist}(\nabla v_\varepsilon, K_{\bar{\imath}}) \to 0$ in $L^s(\Omega)$, we deduce that $|\Omega \setminus \Omega_\varepsilon^{\bar{\imath}}| \to 0$ and in particular $|\widetilde{\Omega}_\varepsilon| \to 0$, which yields $\text{Per}(\widetilde{\Omega}_\varepsilon) \geq C$. On the other hand, by (3.11) we have $\text{Per}(\Omega_\varepsilon^{i_\varepsilon}) \leq C\frac{\varepsilon^2}{\eta} E_\varepsilon(v_\varepsilon) \to 0$, giving a contradiction since $\text{Per}(\Omega_\varepsilon^{i_\varepsilon}) \geq \text{Per}(\widetilde{\Omega}_\varepsilon)$.

We then proceed as in the proof of [10, Proposition 3.4], cf. also the proof of [6, Theorem 1.8 (i)]: by means of the rigidity estimate [12, Theorem 3.1] we obtain

$$\frac{1}{\varepsilon^s} \int_\Omega |\nabla v_\varepsilon - I|^s \, dx \leq C \Big(\big(E_\varepsilon(v_\varepsilon)\big)^{\frac{s}{2}} + \varepsilon^{2-s} E_\varepsilon(v_\varepsilon) + \tau_\varepsilon \big(E_\varepsilon(v_\varepsilon)\big)^{\frac{N}{N-1}} + \int_{\partial\Omega} |g|^s \, d\mathcal{H}^{N-1} \Big) + \alpha_\varepsilon \,, \tag{4.3}$$

where $\alpha_\varepsilon = C \int_{\Omega \setminus \Omega_\varepsilon^b} |\nabla g_\varepsilon|^s \, dx \to 0$. Hence (2.1), (2.3) and (2.4) follow; we obtain also (2.2) in case (i). Finally, by (4.1) and (4.3) we have

$$\|\nabla u_\varepsilon\|_{L^s}^s \leq C \Big(\|\nabla u_\varepsilon\|_{L^s}^{\frac{s}{2}} + \varepsilon^{2-s} \|\nabla u_\varepsilon\|_{L^s} + \tau_\varepsilon \|\nabla u_\varepsilon\|_{L^s}^{\frac{N}{N-1}} + 1 \Big) .$$

This readily implies that (2.2) holds also in cases (ii)–(iii). (Notice that in case (iii) with $s \leq \frac{N}{N-1}$ we use the assumption $\eta(\varepsilon) \gg \varepsilon$ to get $\tau_\varepsilon \to 0$, as above.) The uniform boundedness of $\mathcal{E}_\varepsilon(u_\varepsilon)$ follows from (4.1). $\qquad\square$

4.2. **Proof of Γ-convergence.** For a fixed a sequence $\varepsilon_j \to 0^+$, we introduce the functionals

$$\mathcal{E}'(u) := \Gamma\text{-}\liminf \mathcal{E}_{\varepsilon_j} = \inf \Big\{ \liminf_{j \to +\infty} \mathcal{E}_{\varepsilon_j}(u_j) \colon u_j \rightharpoonup u \text{ in } W^{1,s}(\Omega; \mathbb{R}^N) \Big\},$$

$$\mathcal{E}''(u) := \Gamma\text{-}\limsup \mathcal{E}_{\varepsilon_j} = \inf \Big\{ \limsup_{j \to +\infty} \mathcal{E}_{\varepsilon_j}(u_j) \colon u_j \rightharpoonup u \text{ in } W^{1,s}(\Omega; \mathbb{R}^N) \Big\}.$$

In order to prove Theorem 2.2, we will show that $\mathcal{E}''(u) \leq \mathcal{E}(u) \leq \mathcal{E}'(u)$ for every function $u \in W^{1,s}(\Omega; \mathbb{R}^N)$. We set $\eta_j := \eta(\varepsilon_j)$.

Strategy of the proof of the Γ-liminf inequality. Before providing the proof of the Γ-liminf inequality we first comment on the strategy. A standard approach in discrete-to-continuum analysis amounts to give an optimal lower bound on discrete energies by integrals depending on gradients of suitable affine interpolations of the discrete fields. Such approach cannot be followed in the case $M > 1$ due to the nontrivial dependence of the cell energy W on difference quotients of the discrete fields, see also Remark 6.3.

We adopt a different strategy. The idea is to partition the lattice $\eta_j \mathbb{Z}^N$ into sublattices $\mathcal{L}_j^m$, $m = 1, \ldots, M^N$, with elementary lattice cells of size $\eta_j M$, and identify $D'_{\eta_j} u$ with a set of vector fields $U_j^1, \ldots, U_j^{M^N}$ that are piecewise constant on each cell of the corresponding sublattice. Accordingly, the total interaction energy is decomposed into a sum of discrete energies $\mathcal{E}_j^m$, where, for every m, $\mathcal{E}_j^m$ can be written as an integral depending on U_j^m, see (4.13) below.

If $u_j \to u$ in $W^{1,s}$, the corresponding vector fields U_j^m, converge to limits that may be singularly not related to ∇u. In contrast, in the crucial Lemma 4.2 we prove that, for a.e. x, the *average* of the limiting vector fields, evaluated at x, is uniquely determined by $\nabla u(x)$, see (4.7). Finally, the previous decomposition of the energy, Jensen's inequality, and a lower semicontinuity argument allow us to obtain the desired lower bound by applying the linearisation process to each of the integrals $\mathcal{E}_j^m$.

In order to clarify the construction of the vector fields U_j^m and the result of Lemma 4.2 we provide the following one-dimensional example.

Example 4.1. *Let $N = 1$, $\Omega = (0,1)$, $M = 2$, and $u(x) = zx$ with $z \in \mathbb{R}$. Given $z_1, z_2 \in \mathbb{R}$ such that $\frac{1}{2}(z_1 + z_2) = z$, let w be the 1-periodic function defined by $w(x) = z_1$ if $x \in (0, \frac{1}{2})$ and $w(x) = z_2$ if $x \in (\frac{1}{2}, 1)$. Then let $u_j \in \mathcal{A}_{\eta_j}$ (identified with its piecewise affine interpolation) be determined by the following conditions: $u_j(0) = 0$, $u_j'(x) = w(\frac{x}{2\eta_j})$. Clearly $u_j \overset{*}{\rightharpoonup} u$ weakly* in $W^{1,\infty}(0,1)$. Then one has, for every j and x, $U_j^1(x) \equiv (z_1, z_2, z)$, $U_j^2(x) \equiv (z_2, z_1, z)$, $\frac{1}{2}(U_j^1(x) + U_j^2(x)) \equiv (z, z, z) = D'(v_{z,0}) = D'(v_{u'(x),0})$ (recall (1.11) for the notation $v_{z,0}$). Therefore $\frac{1}{2}(U_j^1(x) + U_j^2(x))$ is uniquely determined by $z = \nabla u(x)$, while neither $U_j^1(x)$ nor $U_j^2(x)$ is.*

Before stating Lemma 4.2 we introduce some notation. Recall the integer $M \in \mathbb{N}$ introduced in the definition of E^η; see (1.5)–(1.10). Notice that we may partition $\mathbb{Z}^N$ as

$$\mathbb{Z}^N = \bigcup_{m=1}^{M^N} \left(y_m + M\mathbb{Z}^N \right),$$

where

$$\{y_1, \ldots, y_{M^N}\} = \mathbb{Z}^N \cap [0, M)^N. \tag{4.4}$$

Set

$$\mathcal{L}_j^m := \eta_j (y_m + M\mathbb{Z}^N). \tag{4.5}$$

Given $u \in \mathcal{A}_{\eta_j}$, for every $m \in \{1, \ldots, M^N\}$ we introduce the piecewise constant vector fields $U^m : \Omega_{\eta_j}^b \to \mathbb{R}^{d(M)}$ defined by

$$U^m(y) := D'_{\eta_j} u(x), \quad \text{where } x \in \mathcal{L}_j^m \text{ is the only point such that } y \in x + \eta_j[0, M)^N. \tag{4.6}$$

Lemma 4.2. *Let $u_j \in \mathcal{A}_{\eta_j}$ be a sequence such that $u_j \rightharpoonup u$ in $W^{1,s}(\Omega; \mathbb{R}^N)$ and let U_j^m be the associated sequence of vector fields defined by (4.6) for $m \in \{1, \ldots, M^N\}$. Given $\Omega' \subset\subset \Omega$, if $U_j^m \rightharpoonup U^m$ in $L^s(\Omega'; \mathbb{R}^{d(m)})$ for every $m \in \{1, \ldots, M^N\}$, then*

$$\frac{1}{M^N} \sum_{m=1}^{M^N} U^m(y) = D'(v_{\nabla u(y),0}) \quad \text{for a.e. } y \in \Omega', \tag{4.7}$$

where $v_{\nabla u(y),0}$ is as in (1.11).

Proof. One can easily see that

$$\frac{1}{M^N} \sum_{m=1}^{M^N} U_j^m(\cdot + \eta_j y_m) \rightharpoonup \frac{1}{M^N} \sum_{m=1}^{M^N} U^m \quad \text{weakly in } L^s(\Omega'; \mathbb{R}^{d(M)}). \tag{4.8}$$
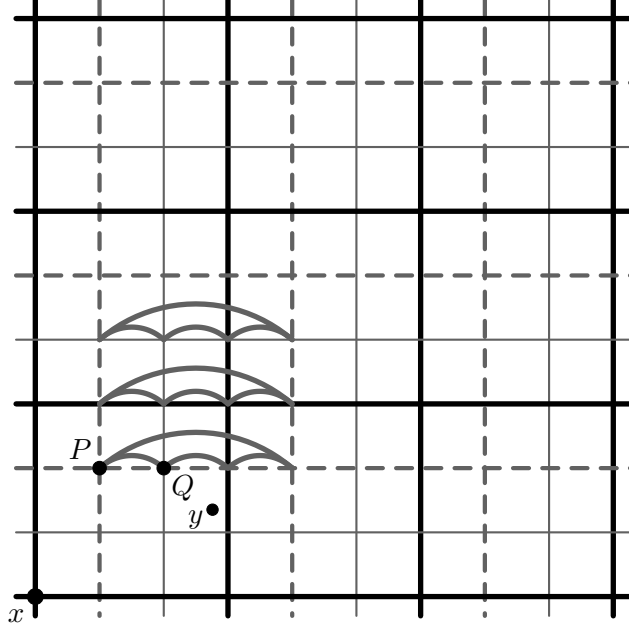
FIGURE 3. Idea of the proof of (4.17) for $N = 2$, $M = 3$. Given y, the point x is chosen as in (4.9). The lattice $\mathcal{L}_j^1$ is represented by the intersections of the bold lines. The nine short arches displayed in the picture connect the pairs of points involved in the finite differences appearing in (4.10) for $i = 1$, $x_k = (1, 2)$, $x_l = (2, 2)$, y' varying in the set $\{(0, 0), (0, 1), (0, 2)\}$, and $h = 0, 1, 2$. The finite difference between the points $P = x + \eta_j x_k$ and $Q = x + \eta_j x_l$ is obtained for $y' = (0, 0)$ and $h = 0$. For each $y' \in \{(0, 0), (0, 1), (0, 2)\}$, the sum of the corresponding three finite differences divided by 3 gives the finite difference corresponding to the long arch. The sum in (4.10) is the average of the three finite differences corresponding to the three long arches. Each of such finite differences is regarded as the derivative with respect to the vector $3e_1$ of the piecewise affine interpolation of u_j with respect to the Kuhn decomposition of the lattice $(y_1 + y' + x_k) + M\mathbb{Z}^N$ (with y_1 defined by (4.4)). Dashed lines represent the lattice $(y_1 + x_k) + M\mathbb{Z}^N$.

Note that, by definition (4.6), for a fixed $x \in \mathcal{L}_j^1$ each summand in the left-hand side above is constant on $x + \eta_j[0, M)^N$. Next we rewrite such sum in a more convenient form. To this end, for any $i \in \{1, \dots, N\}$, let Π_M^i be the facet of the discrete cell $\mathbb{Z}^N \cap [0, M)^N$ orthogonal to e_i, that is

$$\Pi_M^i := \mathbb{Z}^N \cap [0, M)^N \cap \{x \in \mathbb{R}^N \colon x \cdot e_i = 0\}.$$

We have $\#\Pi_M^i = M^{N-1}$. Observe that

$$\{y_m \colon m = 1, \dots, M^N\} = \{y' + he_i \colon y' \in \Pi_M^i, \ h = 0, \dots, M - 1\}.$$

For any $i \in \{1, \dots, N\}$ we can thus regroup the sum in the left-hand side of (4.8) as

$$\frac{1}{M^N} \sum_{m=1}^{M^N} U_j^m(y + \eta_j y_m) = \frac{1}{M^{N-1}} \sum_{y' \in \Pi_M^i} \frac{1}{M} \sum_{h=0}^{M-1} D'_{\eta_j} u_j(x + \eta_j(y' + he_i)), \qquad (4.9)$$

where $x \in \mathcal{L}_j^1$ is the only point such that $y \in x + \eta_j[0, M)$ (see Figure 3). Next fix k, l in (1.2) such that $x_l = x_k + e_i$ for some $i = 1, \ldots, N$. We explicitly write the kl-th component of (4.9):

$$\left(\frac{1}{M^N} \sum_{m=1}^{M^N} U_j^m(y + \eta_j y_m) \right)_{kl} = \frac{1}{M^{N-1}} \sum_{y' \in \Pi_M^i} \frac{1}{M} \sum_{h=0}^{M-1} \left(D'_{\eta_j} u_j(x + \eta_j(y' + he_i)) \right)_{kl}$$

$$= \frac{1}{M^{N-1}} \sum_{y' \in \Pi_M^i} \frac{1}{M} \sum_{h=0}^{M-1} \frac{u_j(x + \eta_j(y' + x_k + (h+1)e_i)) - u_j(x + \eta_j(y' + x_k + he_i))}{\eta_j}$$

$$= \frac{1}{M^{N-1}} \sum_{y' \in \Pi_M^i} D_{\eta_j}^{Me_i} u_j\left(x + \eta_j(y' + x_k) \right), \tag{4.10}$$

where we have employed the notation (1.4). Denote by $\mathcal{T}'$ the triangulation of the lattice $(y_1 + y' + x_k) + M\mathbb{Z}^N$ associated to the Kuhn decomposition of the elementary cells of the lattice; then the sequence of the piecewise affine interpolations of u_j on $\eta_j \mathcal{T}'$ still converges to u weakly in $W^{1,s}(\Omega; \mathbb{R}^N)$, see [4, Appendix A]. Therefore, for any y' fixed,

$$\sum_{x \in \mathcal{L}_j^1 \cap \Omega} D_{\eta_j}^{Me_i} u_j\left(\cdot + \eta_j(y' + x_k) \right) \chi_{x + \eta_j[0,M)^N} \rightharpoonup \nabla u \cdot e_i \quad \text{weakly in } L^s(\Omega'; \mathbb{R}^N). \tag{4.11}$$

Finally, notice that all the other components of $\frac{1}{M^N} \sum_{m=1}^{M^N} U_j^m(y + \eta_j y_m)$ are linear combinations of those considered in (4.10). The thesis then follows from (4.8), (4.10), and (4.11). □

We are now in a position to prove the Γ-liminf inequality, which is the first step of the proof of Theorem 2.2. The second step is the proof of the Γ-limsup inequality, which follows from the discretisation argument detailed below.

Proof of Theorem 2.2. Step 1: $\mathcal{E}(u) \leq \mathcal{E}'(u)$. Let $u_j \rightharpoonup u$ in $W^{1,s}(\Omega; \mathbb{R}^N)$. Upon passing to a subsequence, it is not restrictive to assume that $\mathcal{E}_{\varepsilon_j}(u_j)$ is uniformly bounded. Recall (4.5) and notice that

$$\mathcal{E}_{\varepsilon_j}(u_j) = \sum_{m=1}^{M^N} \mathcal{E}_{\varepsilon_j}^m(u_j), \tag{4.12}$$

where

$$\mathcal{E}_{\varepsilon_j}^m(u_j) = \frac{1}{\varepsilon_j^2} \sum_{\substack{x \in \mathcal{L}_j^m \\ x + \eta_j C_M \subset \mathcal{L}_{\eta_j}}} \eta_j^N W\left(D'_{\eta_j} Id + \varepsilon_j D'_{\eta_j} u_j(x) \right).$$

For every $m \in \{1, \ldots, M^N\}$ let U_j^m be the sequence of piecewise constant vector fields defined by (4.6) associated to u_j. Fix $\Omega' \subset\subset \Omega$. From the boundedness in $W^{1,s}(\Omega; \mathbb{R}^N)$ of $(u_j)_j$ (see Theorem 2.1) we deduce that $(U_j^m)_j$ is bounded in $L^s(\Omega'; \mathbb{R}^{d(M)})$ for every $m \in \{1, \ldots, M^N\}$. Indeed, all finite differences contained in $U_j^m(y)$ can be bounded in terms of finite differences of u_j between nearest neighbours. Hence, up to passing to a further subsequence (not relabelled), we may assume that, for every $m \in \{1, \ldots, M^N\}$, $U_j^m \rightharpoonup U^m$ weakly in $L^s(\Omega'; \mathbb{R}^{d(M)})$ for some $U^m \in L^s(\Omega'; \mathbb{R}^{d(M)})$. Note that, if $x \in \mathcal{L}_j^m$ and $x + \eta_j[0, M)^N \subset \Omega$, then

$$\eta_j^N W\left(D'_{\eta_j} Id + \varepsilon_j D'_{\eta_j} u_j(x) \right) = \frac{1}{M^N} \int_{x + \eta_j[0,M)^N} W(D' Id + \varepsilon_j U_j^m(y)) \, dy.$$

In particular, we have for j sufficiently large

$$\mathcal{E}_{\varepsilon_j}^m(u_j) \geq \frac{1}{\varepsilon_j^2} \frac{1}{M^N} \int_{\Omega'} W(D' Id + \varepsilon_j U_j^m(y)) \, dy. \tag{4.13}$$

By a Taylor expansion of W about $D'Id$ with Lagrange remainder, we get

$$\frac{1}{\varepsilon_j^2} \int_{\Omega'} W(D'Id + \varepsilon_j U_j^m(y))\, \mathrm{d}y = \frac{1}{2} \int_{\Omega'} D_Z^2 W(D'Id + t_j \varepsilon_j U_j^m(y))[U_j^m(y)]^2\, \mathrm{d}y\,, \qquad (4.14)$$

for some $t_j \in (0, 1)$. For $\delta > 0$, let

$$\omega(\delta) := \sup_{\|Z\| \le \delta} \|D_Z^2 W(D'Id + Z) - D_Z^2 W(D'Id)\|\,.$$

By the regularity assumption (H2), we know that $\lim_{\delta \to 0^+} \omega(\delta) = 0$. Let $\gamma_j \to +\infty$ such that

$$\lim_{j \to +\infty} \omega(\varepsilon_j \gamma_j)\gamma_j^2 = 0 \qquad (4.15)$$

and set

$$B_j^m := \{y \in \Omega' \colon \|U_j^m(y)\| \le \gamma_j\}\,, \quad \hat{U}_j^m = \chi_{B_j^m} U_j^m\,.$$

By the Chebyshev inequality and the L^s-boundedness of U_j^m we get that

$$|\Omega' \setminus B_j^m| \le \frac{C}{\gamma_j^s} \to 0\,,$$

hence $\hat{U}_j^m \rightharpoonup U^m$ weakly in $L^s(\Omega'; \mathbb{R}^{d(M)})$. By (4.14), we then get

$$\frac{1}{\varepsilon_j^2} \int_{\Omega'} W(D'Id + \varepsilon_j U_j^m(y))\, \mathrm{d}y \ge \frac{1}{2} \int_{\Omega'} D_Z^2 W(D'Id)[\hat{U}_j^m(y)]^2\, \mathrm{d}y - C\omega(\varepsilon_j \gamma_j)\gamma_j^2\,.$$

By (4.15) and the convexity of $\mathcal{Z}_D \ni Z \mapsto D_Z^2 W(D'Id)[Z]^2$ we have

$$\liminf_{j \to +\infty} \frac{1}{\varepsilon_j^2} \int_{\Omega'} W(D'Id + \varepsilon_j U_j^m(y))\, \mathrm{d}y \ge \frac{1}{2} \int_{\Omega'} D_Z^2 W(D'Id)[U^m(y)]^2\, \mathrm{d}y\,. \qquad (4.16)$$

By Lemma 4.2 we find that

$$\frac{1}{M^N} \sum_{m=1}^{M^N} U^m(y) = D'(v_{\nabla u(y),0}) \quad \text{for a.e. } y \in \Omega'\,. \qquad (4.17)$$

Then, by (4.12), (4.13), (4.17), (4.16), and again by the convexity of $\mathcal{Z}_D \ni Z \mapsto D_Z^2 W(D'Id)[Z]^2$ we infer that

$$\liminf_{j} \mathcal{E}_{\varepsilon_j}(u_j) \ge \frac{1}{2} \int_{\Omega'} \sum_{m=1}^{M^N} \frac{1}{M^N} D_Z^2 W(D'Id)[U^m(y)]^2\, \mathrm{d}y$$

$$\ge \frac{1}{2} \int_{\Omega'} D_Z^2 W(D'Id)[D'(v_{\nabla u(y),0})]^2\, \mathrm{d}y = \int_{\Omega'} \phi(e(u))\, \mathrm{d}y\,.$$

This concludes the proof of $\mathcal{E}(u) \le \mathcal{E}'(u)$ upon letting $\Omega' \nearrow \Omega$ and noticing that, by the continuity of the trace, $u \in H_g^1(\Omega; \mathbb{R}^N)$.

Step 2: $\mathcal{E}''(u) \le \mathcal{E}(u)$. Assume first that $u \in g + C_c^\infty(\Omega; \mathbb{R}^N)$. By a convolution and a cut-off argument, we can find a sequence $(u^n)_n$ such that $u^n \to u$ strongly in $H^1(\Omega; \mathbb{R}^N)$ and $u^n \in (g + C_c^\infty(\Omega; \mathbb{R}^N)) \cap C^\infty(\Omega \setminus S_n; \mathbb{R}^N)$, where $S_n := \{x \in \Omega \colon \mathrm{dist}(x, \Omega^c) < \delta_n\}$, with $\delta_n \to 0$. Define $u_j^n = u^n|_{\mathcal{L}_{\eta_j}}$. For every $x \in \mathcal{L}_{\eta_j}$ set

$$U_j^n(y) := D'_{\eta_j} u_j^n(x), \quad y \in x + \eta_j[0, M)^N\,.$$

Then, using the C^2 regularity of W, a Taylor expansion about $D'Id$ gives

$$\frac{\eta_j^N}{\varepsilon_j^2} W\big(D'Id + \varepsilon_j D'_{\eta_j} u_j^n(x)\big) = \frac{1}{M^N} \frac{1}{\varepsilon_j^2} \int_{x+\eta_j[0,M)^N} W\big(D'Id + \varepsilon_j U_j^n(y)\big)\,\mathrm{d}y$$

$$= \frac{1}{M^N} \int_{x+\eta_j[0,M)^N} \frac{1}{2} D_Z^2 W(D'Id)[U_j^n(y)]^2\,\mathrm{d}y + \eta_j^N o(1)\,. \tag{4.18}$$

If $x + \eta_j[0,M)^N \subset \Omega \setminus S_n$, from (4.18) it follows

$$\frac{\eta_j^N}{\varepsilon_j^2} W\big(D'Id + \varepsilon_j D'_{\eta_j} u_j^n(x)\big) = \frac{1}{M^N} \int_{x+\eta_j[0,M)^N} \frac{1}{2} D_Z^2 W(D'Id)[D'(v_{\nabla u^n(y)},0)]^2\,\mathrm{d}y + \eta_j^N o(1)\,, \tag{4.19}$$

where we used the Lipschitz regularity of ∇u^n in $\Omega \setminus S_n$. If instead $(x + \eta_j[0,M)^N) \cap S_n \neq \emptyset$, we use the Lipschitz regularity of u_n and get from (4.18)

$$\frac{\eta_j^N}{\varepsilon_j^2} W\big(D'Id + \varepsilon_j D'_{\eta_j} u_j^n(x)\big) \leq \eta_j^N C + \eta_j^N o(1)\,. \tag{4.20}$$

Summing over $x \in \mathcal{L}_{\eta_j}$ and combining (4.19) and (4.20), we obtain

$$\mathcal{E}''(u^n) \leq \limsup_{j \to +\infty} \mathcal{E}_{\varepsilon_j}(u_j^n) \leq \int_\Omega \frac{1}{2} D_Z^2 W(D'Id)[D'(v_{\nabla u^n(y)},0)]^2\,\mathrm{d}y + C\delta_n = \mathcal{E}(u^n) + C\delta_n\,.$$

Hence, upon letting $n \to +\infty$, by the lower semicontinuity of $\mathcal{E}''$ and the strong H^1-convergence of u^n to u, we get

$$\mathcal{E}''(u) \leq \mathcal{E}(u)\,. \tag{4.21}$$

In the general case $u \in H_g^1(\Omega;\mathbb{R}^N)$, we can find a sequence $(u_k)_k$ in $g + C_c^\infty(\Omega;\mathbb{R}^N)$ such that $u_k \to u$ strongly in $H^1(\Omega;\mathbb{R}^N)$, so that $\lim_{k \to +\infty} \mathcal{E}(u_k) = \mathcal{E}(u)$. Then, we conclude by (4.21) with u_k in place of u and again by the lower semicontinuity of $\mathcal{E}''$. □

5. Partial Dirichlet boundary data

The aim of the present section is to briefly discuss the case of Dirichlet boundary conditions assigned only on a subset of $\partial\Omega$. We will see that in such a case the surface term appearing in (1.5)–(1.8) cannot be neglected and that its presence will in fact affect the choice of the scaling. We assume that Ω is a connected open bounded set of $\mathbb{R}^N$ with Lipschitz boundary and consider an open subset $\gamma \subset \partial\Omega$ such that $\mathcal{H}^{N-1}(\gamma) > 0$ where the Dirichlet condition is prescribed. The derivation of linear elasticity for pure traction problems, corresponding to $\gamma = \emptyset$, has been recently considered in continuum settings e.g. in [17]. We assume that γ has Lipschitz boundary in $\partial\Omega$ according to [2, Definition 2.1]. Such assumption is needed for a density result employed in the proof of the Γ-limsup inequality in Theorem 5.6, but weaker regularity conditions may be required as done in [6].

Given $\varepsilon > 0$ and $g \in W_{loc}^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)$, we assume that $v \in \mathcal{A}_\eta$ satisfies

$$v(x) = x + \varepsilon g(x) \quad \forall\, x \in \mathcal{L}_\eta \text{ such that } \mathrm{dist}(x,\gamma) \leq \delta_\eta\,,$$

where δ_η satisfies (1.12). We denote by $\mathcal{A}_\eta^g(\gamma)$ the set of corresponding displacements, that is

$$\mathcal{A}_\eta^g(\gamma) := \{u \in \mathcal{A}_\eta : u(x) = g(x)\ \forall\, x \in \mathcal{L}_\eta \text{ such that } \mathrm{dist}(x,\gamma) \leq \delta_\eta\}\,. \tag{5.1}$$

In contrast with the case of boundary conditions assigned on the whole boundary, here the surface energy (1.14) depends on u and not only on g and therefore the total energy cannot

be renormalised as in (1.15). We will then study the following rescaled functionals defined for $u \in \mathcal{A}_\eta^g(\gamma)$ by

$$\mathcal{E}_\varepsilon^\eta(u) := \frac{1}{\varepsilon^2}\big(E^\eta(Id + \varepsilon u)\big)$$
$$= \frac{1}{\varepsilon^2} \sum_{x \in \mathcal{L}_\eta^b} \eta^N W\big(D_\eta' Id + \varepsilon D_\eta' u(x)\big) + \frac{1}{\varepsilon^2} \sum_{x \in \mathcal{L}_\eta^M \setminus \mathcal{L}_\eta^b} \eta^N W_{surf}\big(\mathcal{I}_\eta(x), D_\eta'|_{\mathcal{I}_\eta(x)}(Id + \varepsilon u)(x)\big)\,.$$

The surface term in the above sum will play a role in the choice of $\eta(\varepsilon)$; with such a choice the Γ-limit will be only determined by the bulk term. The scaling of $\eta = \eta(\varepsilon)$ will depend on a compatibility condition according to the following definition.

Definition 5.1. *We say that W_{surf} is compatible with W if there exists $\sigma > 0$ such that*

$$W_{surf}\big(\mathcal{I}, D'|_{\mathcal{I}}(v)\big) \leq CW(D'v) \tag{5.2}$$

for each $\mathcal{I} \subset \{1, \dots, (M+1)^N\}$, and for each $v\colon C_M \to \mathbb{R}^N$ such that $\mathrm{dist}(\nabla v, K) \leq \sigma$ (where ∇v denotes the gradient of the piecewise affine interpolation of v).

Remark 5.2. *Note that in the case of pairwise interactions, the compatibility of W_{surf} with W holds if the system is not frustrated (see Remark 6.3).*

In the case of compatibility the scaling assumptions on $\eta(\varepsilon)$ will be the same as in Sections 1–2, while in the case of incompatibility our analysis applies only to the case of a single well under the more restrictive assumption that $\eta(\varepsilon) \ll \varepsilon^2$. Indeed in the case of multiple wells the latter assumption is incompatible with (1.17). Set

$$\mathcal{E}_\varepsilon(u, \gamma) := \begin{cases} \mathcal{E}_\varepsilon^{\eta(\varepsilon)}(u) & \text{if } u \in \mathcal{A}_{\eta(\varepsilon)}^g(\gamma)\,, \\ +\infty & \text{if } u \in W^{1,r}(\Omega; \mathbb{R}^N) \setminus \mathcal{A}_{\eta(\varepsilon)}^g(\gamma)\,. \end{cases}$$

In this section, we assume for simplicity that there is no volume force, that is $f_\eta \equiv 0$. In fact, the difficulties related to partial boundary data affect the proofs of Theorems 5.4 and 5.6, which extend Theorems 3.1 and 2.2 and are independent of the presence of forces. Recall the definition (1.20) for the set $\Omega_{\eta(\varepsilon)}^b$.

Theorem 5.3 (Compactness). *Let W satisfy (H0) and (H1) and let $g \in W_{loc}^{1,\infty}(\mathbb{R}^N; \mathbb{R}^N)$. Let $\eta(\varepsilon) \to 0$; if $l \geq 2$, assume in addition that $\eta(\varepsilon)$ satisfies (1.17) for a given $r \in (1, p]$. Let $s = p$ for $l = 1$ and $s = r$ for $l \geq 2$. Then there is a sequence $\alpha_\varepsilon \to 0$ such that, if $\{u_\varepsilon\}$ is a sequence in $\mathcal{A}_{\eta(\varepsilon)}^g(\gamma)$ with $\mathcal{E}_\varepsilon(u_\varepsilon, \gamma)$ uniformly bounded, then there exist a positive constant C and a sequence $\hat{u}_\varepsilon$ satisfying $\hat{u}_\varepsilon = u_\varepsilon$ in $\Omega_{\eta(\varepsilon)}^b$ and*

$$\int_\Omega |\nabla \hat{u}_\varepsilon|^s \, \mathrm{d}x \leq C \left((\mathcal{E}_\varepsilon(u_\varepsilon))^{\frac{s}{2}} + \int_\gamma |g|^s \, \mathrm{d}\mathcal{H}^{N-1} \right) + \alpha_\varepsilon\,. \tag{5.3}$$

In particular,

$$\|\hat{u}_\varepsilon\|_{W^{1,s}(\Omega; \mathbb{R}^N)} \leq C\,, \tag{5.4}$$

for some positive constant C independent of ε.

The proof of Theorem 5.3 follows from Theorem 5.4 exactly as Theorem 2.1 follows from Theorem 3.1.

Theorem 5.4. *Let W satisfy (H0) and (H1). For a given $\eta = \eta(\varepsilon)$, assume that $v_\varepsilon \in \mathcal{A}_{\eta(\varepsilon)}$ is a sequence such that $\lim_{\varepsilon \to 0} \varepsilon^2 E_\varepsilon(v_\varepsilon) = 0$, where E_ε is defined in (1.19). Then there exist $C > 0$ and a sequence $\hat{v}_\varepsilon$ such that $\hat{v}_\varepsilon = v_\varepsilon$ in the set $\Omega_{\eta(\varepsilon)}^b$ and*

(a) *if $l = 1$, then*

$$\frac{1}{\varepsilon^p} \int_\Omega \mathrm{dist}^p(\nabla \hat{v}_\varepsilon, SO(N)) \, \mathrm{d}x \leq C\left(\left(E_\varepsilon(\hat{v}_\varepsilon) \right)^{\frac{p}{2}} + \varepsilon^{2-p} E_\varepsilon(\hat{v}_\varepsilon) \right); \tag{5.5}$$

(b) *if $l \geq 2$, then for ε sufficiently small there is $i_\varepsilon \in \{1, \ldots, l\}$ such that*

$$\frac{1}{\varepsilon^r} \int_\Omega \mathrm{dist}^r(\nabla \hat{v}_\varepsilon, K_{i_\varepsilon}) \, \mathrm{d}x \leq C\left(\left(E_\varepsilon(\hat{v}_\varepsilon) \right)^{\frac{r}{2}} + \varepsilon^{2-r} E_\varepsilon(\hat{v}_\varepsilon) + \varepsilon^{-r} \left(\frac{\varepsilon^2}{\eta} \right)^{\frac{N}{N-1}} \left(E_\varepsilon(\hat{v}_\varepsilon) \right)^{\frac{N}{N-1}} \right). \tag{5.6}$$

Proof. Neglecting the surface term in the functional, one can argue as in the proof of Theorem 3.1 and prove estimates (5.5)-(5.6) with Ω replaced by $\Omega^b_{\eta(\varepsilon)}$. The conclusion follows from Lemma 5.5 below. $\qquad \square$

The next lemma is a slight generalisation of [21, Lemma 3.2] and we refer the reader to [21] for its proof.

Lemma 5.5. *Let $q > 1$ and $i \in \{1, \ldots, l\}$. There exists $C > 0$ such that for each $v \in \mathcal{A}_{\eta(\varepsilon)}$ one can find $\hat{v} \in \mathcal{A}_{\eta(\varepsilon)}$ that satisfies the following conditions:*

(i) $\hat{v} = v$ *in* $\Omega^b_{\eta(\varepsilon)}$;

(ii) $\displaystyle \int_\Omega \mathrm{dist}^q(\nabla \hat{v}, K_i) \, \mathrm{d}x \leq C \int_{\Omega^b_{\eta(\varepsilon)}} \mathrm{dist}^q(\nabla v, K_i) \, \mathrm{d}x$.

The existence of the Γ-limit depends on the validity of the compatibility condition (5.2). Precisely, in the case when (5.2) is satisfied, Theorem 2.2 still holds. If (5.2) is not satisfied, then Theorem 2.2 holds only in the case $l = 1$ and under the additional assumption that $\eta(\varepsilon) \ll \varepsilon^2$. This is formalised in the next theorem, where we use the notation

$$H^1_{g,\gamma}(\Omega; \mathbb{R}^N) := \{ u \in H^1(\Omega; \mathbb{R}^N) : u = g \ \mathcal{H}^{N-1}\text{-a.e. on } \gamma \} \,.$$

Theorem 5.6 (Γ-convergence). *Let W satisfy* (H0), (H1a), *and* (H2) *and let $g \in W^{1,\infty}_{loc}(\mathbb{R}^N; \mathbb{R}^N)$. Let $s \in (1, 2]$ and let $\eta = \eta(\varepsilon) \to 0$. Suppose that (5.2) is satisfied, or $l = 1$ and $\eta(\varepsilon) \ll \varepsilon^2$. Then, as $\varepsilon \to 0^+$, the sequence of functionals $\{ \mathcal{E}_\varepsilon(\cdot, \gamma) \}$ Γ-converges, with respect to the weak topology of $W^{1,s}(\Omega; \mathbb{R}^N)$, to the functional*

$$\mathcal{E}(u, \gamma) := \begin{cases} \displaystyle \int_\Omega \phi(e(u)) \, \mathrm{d}x & \text{if } u \in H^1_{g,\gamma}(\Omega; \mathbb{R}^N), \\ +\infty & \text{otherwise,} \end{cases} \tag{5.7}$$

where ϕ is defined in (1.16).

Proof. The proof of the Γ-liminf inequality is exactly as in Theorem 2.2, since it involves only the bulk term of the energies. As long as the Γ-limsup inequality is concerned, it suffices to prove it for a dense subset of $H^1_{g,\gamma}(\Omega; \mathbb{R}^N)$, specifically, for the set of functions $u \in g + C^\infty_c(\mathbb{R}^N \backslash \gamma; \mathbb{R}^N)$; by the regularity assumption on γ, the density is guaranteed by [2, Proposition A.2] or [6, Lemma A.2]. As in *Step 2* in the proof of Theorem 2.2, by a convolution and a cut-off argument, for a given u in such a class we can find a sequence $(u^n)_n$ such that $u^n \to u$ strongly in $H^1(\Omega; \mathbb{R}^N)$ and $u^n \in (g + C^\infty_c(\mathbb{R}^N \backslash \gamma; \mathbb{R}^N)) \cap C^\infty(\overline{\Omega} \backslash S_n; \mathbb{R}^N)$, where $S_n := \{ x \in \mathbb{R}^N : \mathrm{dist}(x, \gamma) < \delta_n \}$, with $\delta_n \to 0$. Let, then, $u^n_j = u^n|_{\mathcal{L}_{\eta_j}}$. We estimate the bulk term of $\mathcal{E}_{\varepsilon_j}(u^n_j, \gamma)$ as in the proof of Theorem 2.2. Therefore, it suffices to show that the surface contribution vanishes in the limit as $\varepsilon_j \to 0$. In the case when the compatibility condition (5.2) is satisfied, a Taylor expansion of W

about the identity yields

$$\frac{1}{\varepsilon_j^2} \sum_{x \in \mathcal{L}_{\eta_j}^M \setminus \mathcal{L}_{\eta_j}^b} \eta_j^N W_{surf}\big(\mathcal{I}_{\eta_j}(x), D'_{\eta_j}|_{\mathcal{I}_{\eta_j}(x)}(Id + \varepsilon_j u_j^n)(x)\big) \leq C \frac{1}{\varepsilon_j^2} \sum_{x \in \mathcal{L}_{\eta_j}^M \setminus \mathcal{L}_{\eta_j}^b} \eta_j^N W\big(D'_{\eta_j}(Id + \varepsilon_j u_j^n)(x)\big)$$

$$\leq C \frac{1}{\varepsilon_j^2} \varepsilon_j^2 \eta_j^N \sharp(\mathcal{L}_{\eta_j}^M \setminus \mathcal{L}_{\eta_j}^b) \leq C \eta_j \to 0 \,.$$

In the case when $l = 1$ and $\eta(\varepsilon) \ll \varepsilon^2$, using that W_{surf} is bounded in a neighbourhood of the identity, we get

$$\frac{1}{\varepsilon_j^2} \sum_{x \in \mathcal{L}_{\eta_j}^M \setminus \mathcal{L}_{\eta_j}^b} \eta_j^N W_{surf}\big(\mathcal{I}_{\eta_j}(x), D'_{\eta_j}|_{\mathcal{I}_{\eta_j}(x)}(Id + \varepsilon_j u_j^n)(x)\big) \leq C \frac{\eta_j^N}{\varepsilon_j^2} \sharp(\mathcal{L}_{\eta_j}^M \setminus \mathcal{L}_{\eta_j}^b) \leq C \frac{\eta_j}{\varepsilon_j^2} \to 0 \,.$$

This concludes the proof. $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad$ $\square$

Remark 5.7 (Convergence of minima and minimisers). *Observe that the analogue of Theorem 2.3 still holds up to replacing the sequence of almost minimisers u_ε by $\frac{1}{\varepsilon}(\hat{v}_\varepsilon - x)$, where $v_\varepsilon = x + \varepsilon u_\varepsilon$ and $\hat{v}_\varepsilon$ is the modification introduced in Theorem 5.3. This is a consequence of Theorems 5.3 and 5.6 and of the fact that the Γ-liminf inequality involves only the bulk term of the energies.*

6. Pairwise interactions

In this section we show how the analysis and the results established so far apply in particular to the class of pairwise discrete energies. Namely, we consider energies $(\hat{E}_{pw})^\eta \colon \mathcal{A}_\eta \mapsto [0, +\infty]$ of the form

$$(\hat{E}_{pw})^\eta(v) := \sum_{\xi \in \mathbb{Z}^N} \sum_{\substack{x \in \mathcal{L}_\eta \\ x + \eta\xi \in \mathcal{L}_\eta}} \eta^N \psi\Big(\xi, \frac{|v(x + \eta\xi) - v(x)|}{\eta}\Big), \tag{6.1}$$

where $\psi \colon \mathbb{Z}^N \times \mathbb{R}^n \to \mathbb{R}$ and we assume that there exists $R > 0$ such that

$$\psi(\xi, \rho) = 0 \quad \text{if } |\xi| > R \,.$$

By introducing a cell energy that suitably weights the interactions in a fixed periodic cell of the lattice, we can rewrite such energies in the form (1.5) up to an additive constant. Precisely, given $M \in \mathbb{N}$ with $M \geq R$, define for a function $v \colon C_M \to \mathbb{R}^N$

$$\hat{W}(D'v) := \sum_{\xi \in \mathbb{Z}^N} \sum_{\substack{y \in C_M \\ y + \xi \in C_M}} \lambda_M(y, \xi) \psi\Big(\xi, |v(y + \xi) - v(y)|\Big), \tag{6.2}$$

where $D'v = D'_1 v(0)$ is defined in (1.2) and $\lambda_M \colon C_M \times \mathbb{Z}^N \to [0, +\infty)$ satisfies

$$\sum_{\substack{y \in C_M \\ y + \xi \in C_M}} \lambda_M(y, \xi) = 1 \quad \forall \, \xi \in \mathbb{Z}^N. \tag{6.3}$$

Moreover, given $\mathcal{I} \subset \{1, \ldots, (M+1)^N\}$ and recalling that $x_1, \ldots, x_{(M+1)^N}$ is an enumeration of C_M, let $A(\mathcal{I}) := \{x_l \colon l \in \mathcal{I}\}$ and set

$$\hat{W}_{surf}(\mathcal{I}, D'|_{\mathcal{I}}v) := \sum_{\xi \in \mathbb{Z}^N} \sum_{\substack{y \in A(\mathcal{I}) \\ y + \xi \in A(\mathcal{I})}} \lambda_M(y, \xi) \psi\Big(\xi, |v(y + \xi) - v(y)|\Big),$$

where $D'|_{\mathcal{I}}v$ is defined in (1.3). Abusing notation, we set for $v \in \mathcal{A}_\eta$ and $x \in \mathcal{L}_\eta$

$$\hat{W}(D'_\eta v(x)) := \hat{W}\left(D'\frac{1}{\eta}v(\eta \cdot +x)\right),$$

$$\hat{W}_{surf}(\mathcal{I}, D'_\eta|_{\mathcal{I}}v(x)) := \hat{W}_{surf}\left(\mathcal{I}, D'|_{\mathcal{I}}\frac{1}{\eta}v(\eta \cdot +x)\right).$$

Finally, define $\mathcal{L}_\eta^M$ and $\mathcal{I}_\eta(x)$ by (1.6) and (1.7), respectively, and

$$\hat{W}_\eta(x, D'_\eta|_{\mathcal{I}_\eta(x)}v(x)) = \begin{cases} \hat{W}(D'_\eta v(x)) & \text{if } \mathcal{I}_\eta(x) = \{1, \ldots, (M+1)^N\}, \\ \hat{W}_{surf}(\mathcal{I}_\eta(x), D'_\eta|_{\mathcal{I}_\eta(x)}v(x)) & \text{otherwise.} \end{cases}$$

Hence, we can see that

$$(\hat{E}_{pw})^\eta(v) = \sum_{x \in \mathcal{L}_\eta^M} \eta^N \hat{W}_\eta\big(x, D'_\eta|_{\mathcal{I}_\eta(x)}v(x)\big). \tag{6.4}$$

Note that the coefficients λ_M are chosen in such a way that, in the final sum, boundary interactions and internal interactions have the same weight.

Setting

$$m_\eta(x) := \min_v \hat{W}_\eta(x, D'_\eta|_{\mathcal{I}_\eta(x)}v(x)),$$

we renormalise the functionals $(\hat{E}_{pw})^\eta$ by setting

$$(E_{pw})^\eta(v) := (\hat{E}_{pw})^\eta - \sum_{x \in \mathcal{L}_\eta^M} \eta^N m_\eta(x) = \sum_{x \in \mathcal{L}_\eta^M} \eta^N \left(\hat{W}_\eta\big(x, D'_\eta|_{\mathcal{I}_\eta(x)}v(x)\big) - m_\eta(x)\right),$$

which is of the form (1.5) with

$$W_\eta\big(x, D'_\eta|_{\mathcal{I}_\eta(x)}v(x)\big) := \hat{W}_\eta\big(x, D'_\eta|_{\mathcal{I}_\eta(x)}v(x)\big) - m_\eta(x).$$

Note that $m_\eta(x)$ does not depend on x if $x + \eta C_M \subset \Omega$. We can thus set

$$\overline{m} := \min_v \hat{W}_\eta(x, D'_\eta|_{\mathcal{I}_\eta(x)}v(x)) = \min_v \hat{W}\big(D'v\big) \quad \text{for every } x \text{ s.t. } x + \eta C_M \subset \Omega \tag{6.5}$$

and

$$W\big(D'(x)v(x)\big) := \hat{W}\big(D'v(x)\big) - \overline{m}. \tag{6.6}$$

Then, if assumptions (H0)–(H2) are satisfied by the cell energy W defined by (6.6), we can apply Theorem 2.2 to derive the linear elastic energy associated to the family of scaled and renormalised functionals defined as in (1.15) by

$$(\mathcal{E}_{pw})^\eta_\varepsilon = \frac{1}{\varepsilon^2} \sum_{x \in \mathcal{L}_\eta^b} \eta^N W\big(D'_\eta Id + \varepsilon D'_\eta u(x)\big), \quad u \in \mathcal{A}_\eta^g.$$

Remark 6.1. *Note that* (H0) *is always satisfied by any cell energy W defined by* (6.2)–(6.6), *since the pair potential ψ depends on the distance between points in the deformed configuration. Moreover,* (H1)–(H2) *are satisfied whenever the following hold:*

- *W is minimised exactly on K,*
- *(H1c) holds with $\sigma = 0$,*
- *$\rho \mapsto \psi(\xi, \rho)$ is smooth for every ξ,*
- *$\psi(\xi, \rho) \geq C(\rho - |U_i\xi|)^2$ for every $i = 1, \ldots, l$ and every ρ in a neighbourhood of $|U_i\xi|$,*
- *there is $p > 1$ such that $\psi(\xi, \rho) \geq C\rho^p$ for every $\xi \in \{e_1, \ldots, e_n\}$ and for ρ sufficiently large.*

Finally, we underline that the validity of (H1c) *is usually implied by the energetic penalisation due to the interactions beyond nearest neighbours (see the examples in Section 7).*

For the reader's convenience we restate Theorem 2.2 in this specific case, providing an explicit formula for the Γ-limit.

Theorem 6.2 (Γ-convergence)**.** *Let the function W defined in* (6.6) *satisfy* (H0)*,* (H1a)*, and* (H2) *and let $g \in W_{loc}^{1,\infty}(\mathbb{R}^N; \mathbb{R}^N)$. Let $s \in (1, 2]$ and let $\eta = \eta(\varepsilon) \to 0$. Then, as $\varepsilon \to 0^+$ the sequence of functionals $\{\mathcal{E}_\varepsilon\}$ defined by* (1.18) *with $\mathcal{E}_\varepsilon^{\eta(\varepsilon)} = (\mathcal{E}_{pw})_\varepsilon^{\eta(\varepsilon)}$, Γ-converges, with respect to the weak topology of $W^{1,s}(\Omega; \mathbb{R}^N)$, to the functional*

$$\mathcal{E}_{pw}(u) := \begin{cases} \displaystyle\iint_\Omega \phi_{pw}(e(u)) \,\mathrm{d}x & \text{if } u \in H_g^1(\Omega; \mathbb{R}^N), \\ +\infty & \text{otherwise,} \end{cases} \tag{6.7}$$

where ϕ_{pw} is defined by

$$\phi_{pw}(A) := \frac{1}{2} \sum_{\xi \in \mathbb{Z}^N} \left(D_\rho^2 \psi(\xi, |\xi|) - \frac{D_\rho \psi(\xi, |\xi|)}{|\xi|} \right) \left(\frac{\xi \cdot A\xi}{|\xi|} \right)^2 \quad \text{for every } A \in \mathbb{R}^{N \times N}. \tag{6.8}$$

Proof. By Theorem 2.2, the conclusion of the Theorem holds true with ϕ_{pw} given by (1.16) and W defined by (6.6). Hence, it only remains to prove that (6.8) holds true. To this end, observe that, given $A \in \mathbb{M}^{N \times N}$ and setting

$$h(t) := \frac{1}{2} W(D'Id + tD'u_{A,0}),$$

where $u_{A,0}$ is defined by (1.11), we have

$$\phi_{pw}(A) = h''(0). \tag{6.9}$$

Note, moreover, that

$$h(t) = \frac{1}{2} \sum_{\xi \in \mathbb{Z}^N} g_\xi(t), \tag{6.10}$$

where

$$g_\xi(t) := \psi(\xi, |\xi + tA\xi|).$$

Using the regularity assumption (H2), for sufficiently small t one finds

$$g_\xi'(t) = D_\rho \psi(\xi, |\xi + tA\xi|) \frac{(\xi + tA\xi) \cdot A\xi}{|\xi + tA\xi|}$$

and

$$\begin{aligned} g_\xi''(t) = {} & D_\rho^2 \psi(\xi, |\xi + tA\xi|) \left(\frac{(\xi + tA\xi) \cdot A\xi}{|\xi + tA\xi|} \right)^2 \\ & + D_\rho \psi(\xi, |\xi + tA\xi|) \frac{|A\xi|^2 |\xi + tA\xi|^2 - ((\xi + tA\xi) \cdot A\xi)^2}{|\xi + tA\xi|^3}. \end{aligned} \tag{6.11}$$

In particular,

$$g_\xi'(0) = D_\rho \psi(\xi, |\xi|) \frac{\xi \cdot A\xi}{|\xi|}$$

and

$$g_\xi''(0) = D_\rho^2 \psi(\xi, |\xi|) \left(\frac{\xi \cdot A\xi}{|\xi|} \right)^2 + D_\rho \psi(\xi, |\xi|) \frac{|A\xi|^2 |\xi|^2 - (\xi \cdot A\xi)^2}{|\xi|^3}.$$

Assumption (H1a) yields the following equilibrium condition:

$$\sum_{\xi \in \mathbb{Z}^N} D_\rho \psi(\xi, |\xi|) \frac{\xi \cdot A\xi}{|\xi|} = 0 \quad \text{for every } A \in \mathbb{M}^{N \times N}.$$

In particular, replacing A with $A^T A$, the equilibrium condition reads

$$\sum_{\xi \in \mathbb{Z}^N} D_\rho \psi(\xi, |\xi|) \frac{|A\xi|^2}{|\xi|} = 0 \quad \text{for every } A \in \mathbb{M}^{N \times N}. \tag{6.12}$$

From (6.10) and (6.11) we infer that

$$h''(0) = \frac{1}{2} \sum_{\xi \in \mathbb{Z}^N} \left(D_\rho^2 \psi(\xi, |\xi|) \left(\frac{\xi \cdot A\xi}{|\xi|} \right)^2 + D_\rho \psi(\xi, |\xi|) \frac{|A\xi|^2 |\xi|^2 - (\xi \cdot A\xi)^2}{|\xi|^3} \right). \tag{6.13}$$

Plugging equation (6.12) into (6.13) yields

$$h''(0) = \frac{1}{2} \sum_{\xi \in \mathbb{Z}^N} \left(D_\rho^2 \psi(\xi, |\xi|) \left(\frac{\xi \cdot A\xi}{|\xi|} \right)^2 - D_\rho \psi(\xi, |\xi|) \frac{(\xi \cdot A\xi)^2}{|\xi|^3} \right)$$

$$= \frac{1}{2} \sum_{\xi \in \mathbb{Z}^N} \left(D_\rho^2 \psi(\xi, |\xi|) - \frac{D_\rho \psi(\xi, |\xi|)}{|\xi|} \right) \left(\frac{\xi \cdot A\xi}{|\xi|} \right)^2,$$

which in turn, combined with (6.9), yields the conclusion. $\square$

Remark 6.3 (Frustrated systems). *We say that the system is not frustrated if the identity configuration Id minimises each interaction, otherwise we say that the system is frustated. Notice that, in the first case, the term $D_\rho \psi(\xi, |\xi|)$ in (6.8) is zero for every ξ.*

Remark 6.4 (Orientation-preserving constraint). *In some models, pairwise discrete energies are restricted to admissibile deformation subject to additional constraints. For instance it is possible to enforce an orientation-preserving constraint by requiring that the deformation determinant (i.e., the Jacobian determinant of the piecewise affine interpolation of the discrete deformation) is a.e. positive. Our analysis applies also to this case.*

Specifically, let $\mathcal{A}_\eta^+ := \{v \in \mathcal{A}_\eta \colon \det \nabla v > 0 \text{ a.e.}\}$ and $(\hat{E}_{pw}^+)^\eta(v)$ be defined by (6.1) if $v \in \mathcal{A}_\eta^+$, $(\hat{E}_{pw}^+)^\eta(v) = +\infty$ otherwise. Then, the cell energy $\hat{W}(D'v)$ is defined as in (6.2) if $v \colon C_M \to \mathbb{R}^N$ is such that $\det \nabla v > 0$ a.e., $\hat{W}(D'v) = +\infty$ otherwise. For such a choice of $\hat{W}$, if the function W defined in (6.6) satisfies (H0), (H1a), and (H2), then the conclusion of Theorem 6.2 still holds.

7. Examples

The present section is devoted to examples. In the first three we exhibit pairwise potentials to which our analysis applies. The last example shows the optimality of the scaling (1.17).

Example 7.1. *We present a two-dimensional example showing that our assumptions include a model for laminates. We refer to [15] for another discrete model for laminates.*

Here it will be convenient to use a triangular reference lattice, namely the Bravais lattice $\mathcal{T}^2 = \operatorname{span}_{\mathbb{Z}}\{w_1, w_2\}$ generated by the vectors

$$w_1 := (1, 0) \quad \text{and} \quad w_2 = \left(\tfrac{1}{2}, \tfrac{\sqrt{3}}{2}\right).$$

Let

$$w_3 := w_2 - w_1 = \left(-\tfrac{1}{2}, \tfrac{\sqrt{3}}{2}\right).$$

By an affine change of variables we could map $\mathcal{T}^2$ to $\mathbb{Z}^2$ so as to conform to the notation of Section 1; however we choose to work directly on $\mathcal{T}^2$ to ease notation, in particular we are going to define an energy minimised at the identity map and linearise around the identity as in the previous sections. For each point in the lattice, its nearest neighbours are those at distance 1, while its next-to-nearest neighbours are those at distance $\sqrt{3}$. See Figure 4.
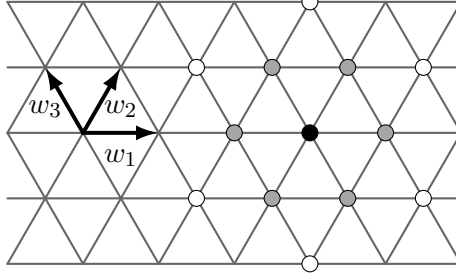
FIGURE 4. A portion of triangular lattice. The vectors w_1, w_2, w_3 are displayed. The point marked with the black dot has six nearest and six next-to-nearest neighbours, marked with grey and white dots, respectively. See Example 7.1.

In the triangular lattice we will define an interaction energy minimised on $SO(2) \cup SO(2)U$, where

$$U := \begin{pmatrix} 1 & 0 \\ 0 & b \end{pmatrix}, \quad \text{with } b \geq \sqrt{5}.$$

It turns out that in the deformed configuration $U\mathcal{T}^2$ nearest neighbours are mapped into points whose mutual distance is either 1 or $\ell_b := \frac{1}{2}\sqrt{1 + 3b^2}$, while next-to-nearest neighbours are mapped into points whose mutual distance is either $\sqrt{3}b$ or $\frac{1}{2}\sqrt{9 + 3b^2}$. See Figure 5.

We now define a pairwise interaction energy $(\hat{E}_{pw})^\eta$ as in (6.1), where we replace the square lattice $\mathbb{Z}^2$ with the triangular lattice $\mathcal{T}^2$; the set $\mathcal{L}_\eta$ is redefined accordingly. Specifically, we consider the sets of nearest and next-to-nearest neighbour bonds

$$B_1 := \{\xi \in \mathcal{T}^2 \colon |\xi| = 1\}, \quad B_2 := \{\xi \in \mathcal{T}^2 \colon |\xi| = \sqrt{3}\}.$$
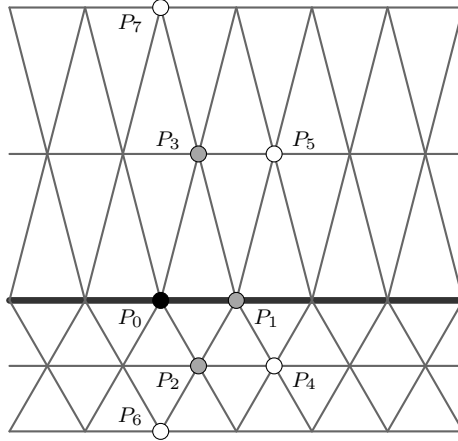

FIGURE 5. A deformation of the triangular lattice displayed in Figure 4. In the deformed configuration, the distances between the displayed points are the following: $|P_0 - P_1| = |P_0 - P_2| = 1$, $|P_0 - P_3| = \ell_b$, $|P_0 - P_4| = |P_0 - P_6| = \sqrt{3}$, $|P_0 - P_5| = \frac{1}{2}\sqrt{9 + 3b^2}$, $|P_0 - P_7| = \sqrt{3}b$. All nearest-neighbour interactions are at equilibrium. Next-to-nearest neighbour interactions across the interface (bold line) are not at equilibrium (for example P_2, P_3), which results into an energy contribution proportional to the length of the interface. See Example 7.1.

As in (6.1) *we define*

$$(\hat{E}_{pw})^\eta(v) := \sum_{\substack{\xi \in B_1 \cup B_2}} \sum_{\substack{x \in \mathcal{L}_\eta \\ x+\eta\xi \in \mathcal{L}_\eta}} \eta^N \, \psi\Big(\xi, \frac{|v(x+\eta\xi) - v(x)|}{\eta}\Big) \quad \text{for } v \in \mathcal{A}_\eta^+, \tag{7.1}$$

setting $(\hat{E}_{pw})^\eta(v) = +\infty$ *otherwise, where* $\mathcal{A}_\eta^+$ *denotes the deformations* $v \in \mathcal{A}_\eta$ *with* $\det \nabla v > 0$ *a.e., see Remark 6.4. The pairwise interaction is defined as follows:*

$$\psi(\xi, \rho) = \begin{cases} (\rho - 1)^2 & \text{if } \xi = \pm w_1, \\ (\rho - 1)^2 \wedge (\rho - \ell_b)^2 & \text{if } \xi \in B_1 \setminus \{\pm w_1\}, \\ (\rho - \sqrt{3})^2 \wedge (\rho - \sqrt{3}b)^2 & \text{if } \xi = \pm(0, \sqrt{3}), \\ (\rho - \sqrt{3})^2 \wedge \big(\rho - \frac{1}{2}\sqrt{9 + 3b^2}\big)^2 & \text{if } \xi \in B_2 \setminus \{\pm(0, \sqrt{3})\}. \end{cases}$$

Notice that the resulting energy depends both on the elongation of the bonds in the deformed configuration and on their direction in the reference configuration.

Under the previous assumptions, if a deformation has zero total interaction energy, then its gradient is a constant matrix belonging to $SO(2) \cup SO(2)U$. *Indeed, assume that a triangular cell in* $\mathcal{T}^2$ *with sides of length 1 is deformed in such a way that the nearest-neighbour energy is zero. Then the deformed triangle may have either three sides of length one (so, up to a rotation it is a cell of* $\mathcal{T}^2$) *or one side of length one and two sides of length* ℓ_b *(so, up to a rotation it is a cell of* $U\mathcal{T}^2$); *the third possibility, i.e. two sides of length one and one side of length* ℓ_b, *is ruled out by the triangle inequality if* $b > \sqrt{5}$, *and by the positive determinant constraint in the case* $b = \sqrt{5}$: *in fact,* $\ell_{\sqrt{5}} = 2$. *Next, assuming that all next-to-nearest neighbour interactions are at equilibrium, one sees that the gradient has to be constant.*

We may then apply the analysis of Section 6 by defining a cell energy as in (6.2), *but taking into account that we are working directly in* $\mathcal{T}^2$. *Specifically, we choose* $M = 2$ *and replace the unit cell* C_2 *with the rhomboid discrete cell, defined as* $\{2t_1 w_1 + 2t_2 w_2 : t_1, t_2 \in [0,1]\} \cap \mathcal{T}^2$. *In this case, the coefficients* $\lambda_2(y, \xi)$ *in* (6.2) *can be defined by any choice such that the sum* (6.3) *holds. Notice that the minimum cell energy* $\overline{m}$ *defined in* (6.5) *is zero and is attained for instance by the identity deformation. Recalling Remark 6.1, it can be seen that:*

- *Assumptions* (H0) *and* (H1a) *are satisfied by construction.*
- *Assumptions* (H1b) *and* (H2) *are satisfied by the regularity and the quadratic growth of* $\rho \mapsto \psi(\xi, \rho)$.
- *If* S, T *are two neighbouring simplices in* $\mathcal{T}^2$ *such that* $\nabla v|_S \in SO(2)$ *and* $\nabla v|_T \in SO(2)U$, *then the distance between the next-to-nearest neighbours contained in* $S \cup T$ *is not in equilibrium. By continuity,* (H1c) *holds.*

Therefore, the conclusion of Theorem 6.2 holds. Since $D_\rho^2 \psi(\xi, |\xi|) = 2$ *and* $D_\rho \psi(\xi, |\xi|) = 0$ *for every* $\xi \in B_1 \cup B_2$, *an explicit computation shows that the limiting energy density* (6.8) *is*

$$\phi_{pw}(A) = \frac{2}{\sqrt{3}} \sum_{\xi \in B_1 \cup B_2} \left(\frac{\xi \cdot A\xi}{|\xi|}\right)^2 \quad \text{for every } A \in \mathbb{R}^{2 \times 2}, \tag{7.2}$$

where the factor $\frac{2}{\sqrt{3}}$ *takes into account that the measure of the elementary cell of the lattice* T^2 *is* $\frac{\sqrt{3}}{2}$.

Remark that if in (7.1) *we remove interactions between next-to-nearest neighbours, namely the sum runs only over* $\xi \in B_1$, *then assumption* (H1c) *does not hold. In this case, since we can mix gradients lying in the two wells at zero cost (see Figure 5), one can readily see that the compactness result given in Theorem 2.1 does not hold.*
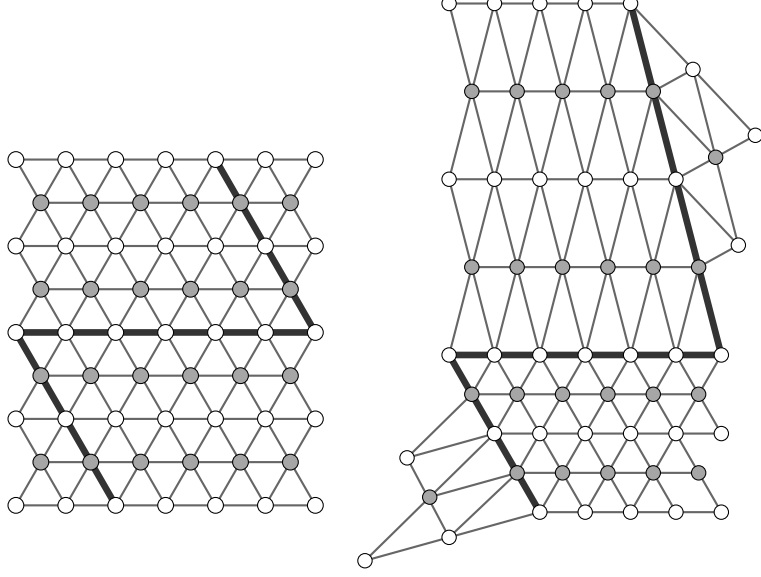
FIGURE 6. A deformation whose gradient lies in the wells of Example 7.2: left, a portion of the lattice in the reference configuration; right, deformed configuration. Atoms have been displayed in different colours in order to highlight their position in the deformed configuration. The (piecewise constant) deformation gradient takes four values: the bold line separates the corresponding phases. Next-to-nearest neighbour interactions across the interface are out of equilibrium, which amounts to an energy penalisation depending on the length of the interface and on the wells that are connected across the interface.

Example 7.2. *We modify the previous example by defining an interaction energy on nearest and next-to-nearest neighbours that depends only on their distance in the deformed configuration, regardless of the direction of the bonds in the reference configuration. We employ the notation above and refer again to the total interaction energy defined as in (7.1), with the pairwise interaction energy given by*

$$\psi(\xi, \rho) = \begin{cases} (\rho - 1)^2 \wedge (\rho - \ell_b)^2 & \text{if } \xi \in B_1 \,, \\ (\rho - \sqrt{3})^2 \wedge (\rho - \sqrt{3}b)^2 \wedge \left(\rho - \frac{1}{2}\sqrt{9 + 3b^2}\right)^2 & \text{if } \xi \in B_2 \,. \end{cases}$$

As in the previous example we assume that $b \geq \sqrt{5}$. Since $(\hat{E}_{pw})^\eta$ only depends on distances in the deformed configuration, then using the symmetries of $\mathcal{T}_2$ we see that

$$(\hat{E}_{pw})^\eta(v) = (\hat{E}_{pw})^\eta(v \circ H_j) \quad \text{for } j = 0, \ldots, 5 \,,$$

where H_j is the rotation of angle $\frac{1}{3}j\pi$. Therefore, the matrices UH_j are in the set of wells. Since $H_j = -H_{j+3}$, we have $SO(2)UH_j = SO(2)UH_{j+3}$. Arguing as in Example 7.1 it follows that, if a deformation has total interaction energy zero, then its gradient is a constant matrix belonging to

$$SO(2) \cup SO(2)U \cup SO(2)UH_1 \cup SO(2)UH_2 \,.$$

Notice that the four energy wells are mutually rank-one connected, see Figure 6. We can now repeat the steps of the previous example in order to define a cell energy as in (6.2) and show that it still satisfies assumptions (H0)–(H2). The conclusion of Theorem 6.2 holds also in this case. Since the energy agrees with the energy of Example 7.1 for small perturbation of the equilibria, the limiting energy density is given again by (7.2).
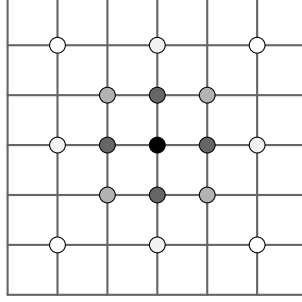
Figure 7. Square lattice displaying the interactions active in Example 7.3: the point in the centre of the picture (black dot) is bonded with its first, second, third, and fifth neighbours (represented with dark grey, grey, light grey, and white dots, respectively). Notice that interactions between third and fifth neighbours can be regarded as interactions between nearest and next-to-nearest neighbours in a sublattice with lattice distance 2.

Example 7.3. *We construct an example of frustrated model in dimension two. We employ a square lattice as in Section 1 and we assume a positive-determinant constraint as in the examples above. The interaction energy is the sum of two contributions,*

$$(\hat{E}_{pw})^{\eta}(v) := (\hat{E}_{pw})_1^{\eta}(v) + (\hat{E}_{pw})_2^{\eta}(v) \quad \text{for } v \in \mathcal{A}_{\eta}^+ \,,$$

and $(\hat{E}_{pw})^{\eta}(v) = +\infty$ otherwise. The first contribution includes nearest and next-to-nearest neighbour interactions and is given by

$$(\hat{E}_{pw})_1^{\eta}(v) := \frac{1}{2} \sum_{\substack{\xi \in \mathbb{Z}^2 \\ |\xi|=1}} \sum_{\substack{x \in \mathcal{L}_{\eta} \\ x+\eta\xi \in \mathcal{L}_{\eta}}} K_1 \, \eta^2 \left(\frac{|v(x+\eta\xi) - v(x)|}{\eta} - a_1 \right)^2$$
$$+ \frac{1}{2} \sum_{\substack{\xi \in \mathbb{Z}^2 \\ |\xi|=\sqrt{2}}} \sum_{\substack{x \in \mathcal{L}_{\eta} \\ x+\eta\xi \in \mathcal{L}_{\eta}}} K_2 \, \eta^2 \left(\frac{|v(x+\eta\xi) - v(x)|}{\eta} - a_2 \right)^2,$$

where $a_{1,2}$, $K_{1,2}$ are fixed positive numbers, see (1.1) for the definition of $\mathcal{L}_{\eta}$. The second contribution with longer range interactions is

$$(\hat{E}_{pw})_2^{\eta}(v) := \frac{1}{2} \sum_{\substack{\xi \in \mathbb{Z}^2 \\ |\xi|=2}} \sum_{\substack{x \in \mathcal{L}_{\eta} \\ x+\eta\xi \in \mathcal{L}_{\eta}}} K_3 \, \eta^2 \left(\frac{|v(x+\eta\xi) - v(x)|}{\eta} - a_3 \right)^2$$
$$+ \frac{1}{2} \sum_{\substack{\xi \in \mathbb{Z}^2 \\ |\xi|=2\sqrt{2}}} \sum_{\substack{x \in \mathcal{L}_{\eta} \\ x+\eta\xi \in \mathcal{L}_{\eta}}} K_4 \, \eta^2 \left(\frac{|v(x+\eta\xi) - v(x)|}{\eta} - a_4 \right)^2,$$

where a_i, K_i, $i = 3, 4$, are fixed positive numbers. Note that $(\hat{E}_{pw})^{\eta}$ includes interactions over first, second, third, and fifth neighbours (Figure 7); due to the geometry of the square lattice, one can recast $(\hat{E}_{pw})^{\eta}$ into the form (6.4) choosing cells with size $M = 2$. Precisely, we choose a cell energy of the form (6.2) as follows:

$$\hat{W}(D'v) = W_{(0,0)}^1 + W_{(1,0)}^1 + W_{(1,1)}^1 + W_{(0,1)}^1 + W^2,$$

where

$$W_{(i,j)}^1 = \frac{1}{4} E_{cell}(v(i,j), v(i+1,j), v(i+1,j+1), v(i,j+1); 1) \,,$$

$$W^2 = E_{cell}(v(0,0), v(2,0), v(2,2), v(0,2); 3),$$

$$E_{cell}(y_1, y_2, y_3, y_4; m) = \frac{1}{2}\sum_{h=1}^{4} K_m(|y_{h+1} - y_h| - a_m)^2 + \sum_{h=1}^{2} K_{m+1}(|y_{h+2} - y_h| - a_{m+1})^2,$$

where we use the convention that $y_5 = y_1$. The terms $W^2_{(i,j)}$ contribute to $(\hat{E}_{pw})^\eta_1$ and contain interactions over first and second neighbours; the term W^2 contributes to $(\hat{E}_{pw})^\eta_2(v)$ and contains interactions over third and fifth neighbours, corresponding to interactions over first and second neighbours in a square lattice with lattice distance 2.

By choosing $a_1 = 1$, $a_2 = \sqrt{2}$, $a_3 = 2$, and $a_4 = 2\sqrt{2}$, it turns out that the minimal energy is zero and the only energy well is $SO(2)$, independently of the choice of K_i. In contrast, by choosing different values for the parameters, one may observe frustration, i.e., there is no deformation such that the total interaction energy is zero; equivalently, there is no deformation such that all interactions are simultaneously at equilibrium.

On the other hand, it is possible to find an open range $\mathcal{U} \subset \mathbb{R}^8$ of values for a_i and K_i, $i = 1, 2, 3, 4$, such that the only minimising well of $\hat{W}$ is still $SO(2)$. This follows by an application of the results of [13]. Indeed, $E_{cell}(y_1, y_2, y_3, y_4; m)$ is of the form [13, formula (3.3)] and is minimised only by affine maps of the form $y_i = Rx_i + c$ with $R \in SO(2)$ and $c \in \mathbb{R}^2$. This property corresponds to assumption (i) in [13, Theorem 5.1], which is satisfied by E_{cell} as proved in [13, Section 6]. It is now easy to see that, when the parameters are in the range $\mathcal{U}$, then conditions (H0)–(H2) are satisfied and, if $(a_1, a_2, a_3, a_4) \neq (1, \sqrt{2}, 2, 2\sqrt{2})$, the system is frustrated.

If the positive-determinant constraint $v \in \mathcal{A}^+_\eta$ is removed, the lattice may be folded, e.g. along the sides of the bonds. However, folding is penalised by interactions beyond nearest neighbours. Indeed, it can be easily checked that in such a case the energy is bounded from below by a positive constant (see for example [5, Lemma 3.3]). Moreover, by continuity, if the parameters $(a_i, K_i) \in \mathcal{U}$ and (a_1, a_2, a_3, a_4) is sufficiently close to $(1, \sqrt{2}, 2, 2\sqrt{2})$, then the minimum value of the energy is close to zero. It turns out that global minimisers are affine maps with gradients in the set of orthogonal matrices $O(2) = SO(2) \cup (O(2) \setminus SO(2))$. This shows that our results apply to a frustrated model with two wells. Applying Theorem 6.2 we can explicitly compute the limiting energy density, which is given by

$$\phi_{pw}(A) = \frac{1}{2}\sum_{i=1}^{4}\sum_{\xi \in B_i} K_i \frac{a_i}{\ell_i}\left(\frac{\xi \cdot A\xi}{\ell_i}\right)^2 \quad \text{for every } A \in \mathbb{R}^{2\times 2},$$

where $(\ell_1, \ell_2, \ell_3, \ell_4) := (1, \sqrt{2}, 2, 2\sqrt{2})$ and $B_i := \{\xi \in \mathbb{Z}^2 : |\xi| = \ell_i\}$.

Example 7.4. *The following example shows that the scaling in (1.17) is optimal, in a model with two wells and zero volume forces. For similar examples with a Dirichlet condition on the whole boundary and with external loading, one may argue as done in [6, Examples 3.2 and 3.3] in the continuum setting.*

Let $U = I + e \otimes (1, \dots 1)$, where $e \in \mathbb{R}^N$. Assume that $K = SO(N) \cup SO(N)U$. Let $\Omega = (0,1)^N$. For every $\nu \in (0,1]$ let $\Omega^\nu = \Omega \cap \{x \in \mathbb{R}^N : x \cdot (1, \dots, 1) \leq \nu\}$ and set $\gamma = \partial\Omega \setminus \overline{\Omega}_{\bar\nu}$ for some $\bar\nu \in (0,1)$. Let $v^\nu \in W^{1,\infty}(\Omega; \mathbb{R}^d)$ be the piecewise affine deformation such that $v^\nu(x) = x$ in $\Omega \setminus \Omega^\nu$ and $\nabla v^\nu = U$ in Ω^ν. We identify v^ν with its restriction on $\mathcal{L}_\eta$. We may also assume that $E^\eta(v^\nu)$ is uniformly bounded, where E^η is defined in (1.5). (Note that all previous examples satisfy this property.) For $\varepsilon > 0$ let $u^\nu_\varepsilon := \frac{1}{\varepsilon}(v^\nu - Id)$. Observe that for every $\nu \leq \bar\nu$ the Dirichlet condition is satisfied in a neighbourhood of γ with $g = 0$, cf. (5.1).

For any $r \in (1, 2]$, we show that for $\eta = \eta(\varepsilon) \ll \varepsilon^{2 - \frac{r(N-1)}{N}}$ there is a choice of $\nu = \nu(\varepsilon)$ such that $\mathcal{E}_\varepsilon(u^\nu_\varepsilon)$ is uniformly bounded but $\|u^\nu_\varepsilon\|_{W^{1,r}(\Omega; \mathbb{R}^N)} \to \infty$ as $\varepsilon \to 0$. Since $\nabla u^\nu_\varepsilon = 0$ in $\Omega \setminus \Omega^\nu$

and $\nabla u_\varepsilon^\nu = \frac{1}{\varepsilon}(U - I)$ in Ω^ν, whose volume has the same order as ν^N, it turns out that

$$\|u_\varepsilon^\nu\|_{W^{1,r}(\Omega;\mathbb{R}^N)} \geq C \frac{\nu^N}{\varepsilon^r} \,.$$

This diverges for $\nu \gg \varepsilon^{\frac{r}{N}}$. On the other hand, the only cells where the cell energy is different from zero are those that intersect the interface $\partial\Omega^\nu \setminus \partial\Omega$. Their number has the same order as $\left(\frac{\nu}{\eta}\right)^{N-1}$, therefore

$$\mathcal{E}_\varepsilon(u_\varepsilon^\nu) \leq C \frac{\eta^N}{\varepsilon^2}\left(\frac{\nu}{\eta}\right)^{N-1} = \frac{\eta\nu^{N-1}}{\varepsilon^2} \,.$$

This is bounded if $\nu \leq C\left(\frac{\varepsilon^2}{\eta}\right)^{\frac{1}{N-1}}$. We then set $\nu(\varepsilon) := \left(\frac{\varepsilon^2}{\eta(\varepsilon)}\right)^{\frac{1}{N-1}} \wedge 1$. For $\eta \leq C\varepsilon^2$, ν has order one, $\mathcal{E}_\varepsilon(u_\varepsilon^\nu)$ is uniformly bounded and $\|u_\varepsilon^\nu\|_{W^{1,r}(\Omega;\mathbb{R}^N)} \to \infty$ as $\varepsilon \to 0$. For $\varepsilon^2 \ll \eta \ll \varepsilon^{2-\frac{r(N-1)}{N}}$ we get $\nu(\varepsilon) \to 0$ and $\varepsilon^{\frac{r}{N}} \ll \left(\frac{\varepsilon^2}{\eta}\right)^{\frac{1}{N-1}}$, thus again $\mathcal{E}_\varepsilon(u_\varepsilon^\nu)$ is uniformly bounded and $\|u_\varepsilon^\nu\|_{W^{1,r}(\Omega;\mathbb{R}^N)} \to \infty$ as $\varepsilon \to 0$. This proves the optimality of (1.17).

References

[1] Agostiniani V., Blass T., Koumatos K.: From nonlinear to linearized elasticity via Γ-convergence: The case of multiwell energies satisfying weak coercivity conditions. *Math. Models Methods Appl. Sci.* **25** 1–38 (2015).

[2] Agostiniani V., Dal Maso G., DeSimone A.: Linearized elasticity obtained from finite elasticity by Γ-convergence under weak coerciveness conditions. *Ann. Inst. H. Poincaré Anal. Non Linéaire* **29** 715–735 (2012).

[3] Alicandro R., Cicalese M.: A general integral representation result for the continuum limits of discrete energies with superlinear growth. *SIAM J. Math. Anal.* **36** 1–37 (2004).

[4] Alicandro R., Focardi M., Gelli M.S.: Finite-difference approximation of energies in fracture mechanics. *Ann. Scuola Norm. Sup. Pisa Cl. Sci. (4)* **29** 671–709 (2000).

[5] Alicandro R., Lazzaroni G., Palombaro M.: On the effect of interactions beyond nearest neighbours on non-convex lattice systems. *Calc. Var. Partial Differential Equations* **56** Art. 42 (2017).

[6] Alicandro R., Dal Maso G., Lazzaroni G., Palombaro M.: Derivation of a linearised elasticity model from singularly perturbed multiwell energy functionals. *Arch. Ration. Mech. Anal.* **230** 1–45 (2018).

[7] Braides A.: Γ-convergence for beginners. Oxford University Press, Oxford (2002).

[8] Braides A., Solci M., Vitali E.: A derivation of linear elastic energies from pair-interaction atomistic systems. *Netw. Heterog. Media* **2** 551–567 (2007).

[9] Conti S., Dolzmann G., Kirchheim B., Müller S.: Sufficient conditions for the validity of the Cauchy-Born rule close to $SO(n)$. *J. Eur. Math. Soc. (JEMS)* **8** 515–530 (2006).

[10] Dal Maso G., Negri M., Percivale D.: Linearized elasticity as Γ-limit of finite elasticity. *Set-Valued Analysis* **10** 165–183 (2002).

[11] Friedrich M., Schmidt B.: On a discrete-to-continuum convergence result for a two dimensional brittle material in the small displacement regime. *Netw. Heterog. Media* **10** 321–342 (2015).

[12] Friesecke G., James R.D., Müller S.: A theorem on geometric rigidity and the derivation of nonlinear plate theory from three-dimensional elasticity. *Comm. Pure Appl. Math.* **55** 1461–1506 (2002).

[13] Friesecke G., Theil F.: Validity and failure of the Cauchy-Born Hypothesis in a two-dimensional mass-spring lattice. *J. Nonlinear Sci.* **12** 445–478 (2002).

[14] Gloria A., Neukamm S.: Commutability of homogenization and linearization at identity in finite elasticity and applications. *Ann. Inst. H. Poincaré Anal. Non Linéaire* **28** 941–964 (2011).

[15] Kitavtsev G., Luckhaus S., Rüland A.: Surface energies emerging in a microscopic, two-dimensional two-well problem. *Proc. Roy. Soc. Edinburgh Sect. A* **147** 1041–1089 (2017).

[16] Kitavtsev G., Lauteri G., Luckhaus S., Rüland A.: A compactness and structure result for a discrete multi-well problem with $SO(n)$ symmetry in arbitrary dimension. *Arch. Ration. Mech. Anal.* **232** 531–555 (2019).

[17] Maddalena F., Percivale D., Tomarelli F.: The gap between linear elasticity and the variational limit of finite elasticity in pure traction problems. *Arch. Ration. Mech. Anal.* **234** 1091–1120 (2019).

[18] Mielke A., Stefanelli U.: Linearized plasticity is the evolutionary Γ-limit of finite plasticity. *J. Eur. Math. Soc. (JEMS)* **15** 923–948 (2013).

[19] Müller S., Neukamm S.: On the Commutability of Homogenization and Linearization in Finite Elasticity. *Arch. Ration. Mech. Anal.* **201** 465–500 (2011).

[20] Schmidt B.: Linear Γ-limits of multiwell energies in nonlinear elasticity theory. *Continuum Mech. Thermodyn.* **20** 375–396 (2008).

[21] Schmidt B.: On the derivation of linear elasticity from atomistic models. *Networks and Heterogeneous Media* **4** 789–812 (2009).

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