Surface energies emerging in a microscopic, two-dimensional two-well problem

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In this paper we are interested in the microscopic modelling of a two-dimensional two-well problem that arises from the square-to-rectangular transformation in (two-dimensional) shape-memory materials. In this discrete set-up, we focus on the surface energy scaling regime and further analyse the Hamiltonian that was introduced by Kitavtsev *et al*. in 2015. It turns out that this class of Hamiltonians allows for a direct control of the discrete second-order gradients and for a one-sided comparison with a two-dimensional spin system. Using this and relying on the ideas of Conti and Schweizer, which were developed for a continuous analogue of the model under consideration, we derive a (first-order) continuum limit. This shows the emergence of surface energy in the form of a sharp-interface limiting model as well the explicit structure of the minimizers to the latter.

1. Introduction

In this paper we are concerned with the modelling of a discrete, two-dimensional square-to-rectangular martensitic phase transition in the regime of surface energy scaling. Due to their interesting thermodynamical and mathematical behaviour, martensitic phase transitions, being examples of diffusionless, solid–solid phase transitions, have attracted a large amount of attention (see [6, 26] for overviews). Hence, a number of models for these phase transitions, describing them from both microscopic and macroscopic points of view, exist in the literature. In the present paper we continue to analyse the microscopic discrete model for the square-to-rectangular martensitic transition that was introduced in [20]. In particular, we

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1041

compare it with its continuous analogues, which have been considered previously in the literature.

1.1. Macroscopic continuum models

Before describing our microscopic discrete model, we recall the most commonly used features of *macroscopic continuum models* for martensitic phase transitions (see, for example, [4,12,15,21,22] and references therein). In this context, a classical modelling approach is the analysis of *purely elastic multi-well energies* of the form

$$\int_\Omega W(\nabla u)\,\mathrm{d}x. \tag{1.1}$$

Here $W\colon \mathbb{R}^{2\times 2} \to [0,\infty)$ is an SO(2) invariant, in general non-quasiconvex (bulk) *energy density* that describes the energy cost of deforming a *reference configuration* Ω into its image configuration $u(\Omega)$ by the *deformation* $u\colon \Omega \to \mathbb{R}^2$, which is considered under appropriate boundary conditions. It is assumed that the deformation u and the associated *deformation gradient* ∇u are in appropriate Sobolev spaces, which are determined by the growth conditions imposed on the energy density W.

In modelling our phase transitions, we focus on the regime in which the martensitic phase is favoured and W has multiple *energy wells*, i.e. there exist $U_1, \ldots, U_m \subset \mathbb{R}^{2\times 2}_{\mathrm{sym}}$ such that $W(M) = 0$ if and only if $M \in \bigcup_{k=1}^{m} \mathrm{SO}(2)U_k$. Deformations u that (almost everywhere) satisfy $\nabla u \in \bigcup_{k=1}^{m} \mathrm{SO}(2)U_k$ are known as *exactly stress-free states*. If there are *rank-one connections* between the energy wells, i.e. if for U_k, $U_{k'}$, with $k \neq k'$, there exist a rotation $Q \in \mathrm{SO}(2)$ and vectors $a \in \mathbb{R}^2 \setminus \{0\}$, $n \in \mathbb{S}^1$ such that

$$U_k - QU_{k'} = a \otimes n,$$

then examples of stress-free states are provided by so-called *simple laminates*. These are Lipschitz continuous deformations u that only depend on the variable $n \cdot x$ and whose gradient alternates between the two values U_k, $QU_{k'}$, for example,

$$\nabla u(x) \in \begin{cases} U_k & \text{if } x \cdot n \geqslant 0, \\ QU_{k'} & \text{if } x \cdot n < 0. \end{cases}$$

However, under general boundary conditions, due to the non-quasiconvex nature of the energy density W, exact minimizers of (1.1) do not exist. Instead, in many cases infimizing sequences display highly oscillatory behaviour.

In order to remedy this non-existence issue and the 'unphysical' infinitely fine oscillations, *higher-order regularizations* are added [12,15,21,22] leading to energies like, for instance,

$$\int_\Omega W(\nabla u)\,\mathrm{d}x + \varepsilon \int_\Omega |\nabla^2 u|^2\,\mathrm{d}x \quad \text{with } \varepsilon > 0. \tag{1.2}$$

These additional higher-order contributions are interpreted as *surface energies* since they penalize oscillations and transitions between different energy wells. Due to compactness, in general in the associated spaces minimizers to (1.2) exist and display characteristic length scales (see [12, 21, 22]).

While the basic intention of higher-order regularizations always consists of penalizing too high oscillations, their precise functional form for macroscopic models is in general not known (from experiments, for instance). Hence, a number of different possible regularizations exist, which range from various kinds of diffuse to sharp interface models. Strikingly, experiments show the presence of both diffuse and sharp interfaces around twin planes for different materials [3,5]. Hence, in order to answer the question as to which of these energies is appropriate in which situation, a first principles approach coming from microscopic considerations seems to be desirable.

1.2. The microscopic two-well problem

While the previously described models have had enormous success in predicting material patterns and microstructure, they are all continuum models. As such they are *macroscopic* and 'phenomenological'. In order to develop a more rigorous foundation for these and other macroscopic models in mathematical physics, there has been a great effort to introduce *microscopic* discrete models describing different phenomena in mathematical physics and relating them to their continuum analogues; see, for example, [8] and references therein. In these microscopic models it is assumed that the elastic sample is given as a deformation of a ground state (atomic) lattice, for example, $(n^{-1}\mathbb{Z})^2$ or subsets thereof. This deformation is energetically described by a Hamiltonian, i.e. a sum of local energies originating from interaction of the 'atoms' involved in the microscopic sample. The described discrete models have been thoroughly analysed in one dimension (for example, for elastic chains) [9]. As in the continuous analogue, vectorial problems are less well understood and various approaches have been pursued [1,7,11,18,25,27]. Moreover, a direct comparison of the scaling behaviour of a discrete and a continuous model of a two-dimensional two-well problem is given in [23, 24]. In the context of the vectorial set-up in martensitic phase transitions, a key (mathematical) difficulty that distinguishes it from the one-dimensional case is the presence of a *continuum* of energy wells, i.e. $\bigcup_{j=1}^{k} \mathrm{SO}(2)U_j$.

In what follows, we address a specific two-dimensional martensitic phase transition, the square-to-rectangular phase transition, from a microscopic point of view. In the following sections, we introduce our precise set-up based on the discrete two-well Hamiltonian (with SO(2) symmetry) and present our main results.

1.2.1. *Setting*

In this section we describe the basic set-up of our discrete two-well problem. We define the underlying domains and function spaces and explain our explicit model Hamiltonian. In what follows, we seek to model the two-dimensional square-to-rectangular phase transition in the martensitic phase in which the variants of martensite constitute the energy wells. For this purpose we introduce the following energy wells:

$$K := \mathrm{SO}(2)U_0 \cup \mathrm{SO}(2)U_1, \quad \text{where } U_0 = \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix}, \ U_1 = \begin{pmatrix} b & 0 \\ 0 & a \end{pmatrix}, \ a \neq b. \quad (1.3)$$

Although for the mathematical treatment of our problem this is not necessary, we restrict ourselves to the most relevant physical situation of volume-preserving
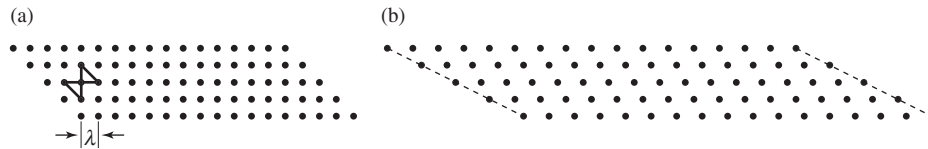
Figure 1. The set-up of our problem. (a) The reference domain Ω_n. The solid triangles correspond to two of the grid triangles $\Delta_{ij}^{n,\pm}$. (b) Ω_n is mapped into an image configuration. In the image configuration, admissibility as formulated in (1.10) has to be preserved. This includes the non-interpenetration condition but also the attainment of the correct boundary data along the dashed lines.

transformations. This corresponds to the assumption $ab = 1$. In this study, for convenience of notation, we denote by c any positive constant depending only (if not stated explicitly otherwise) on the lattice parameters a and b. Moreover, we often use the special constant

$$\bar{c} := \mathrm{dist}(\mathrm{SO}(2)U_0, \mathrm{SO}(2)U_1). \tag{1.4}$$

We recall that for every deformation $U \in \mathrm{SO}(2)U_0$ there are exactly two rank-one connected matrices in $\mathrm{SO}(2)U_1$, i.e. there exist (exactly) two rotations Q, $\tilde{Q}$ such that

$$\left.\begin{aligned} U_0 - QU_1 &= \sqrt{2}\,\frac{a^2 - b^2}{a^2 + b^2}\begin{pmatrix} a \\ -b \end{pmatrix} \otimes \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \\ U_0 - \tilde{Q}U_1 &= \sqrt{2}\,\frac{a^2 - b^2}{a^2 + b^2}\begin{pmatrix} a \\ b \end{pmatrix} \otimes \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}. \end{aligned}\right\} \tag{1.5}$$

Macroscopically, we expect that a shape memory alloy with these wells can form two variants of simple laminates (without bulk energy cost), where the normals to the jump planes are either given by $\begin{pmatrix} 1 \\ 1 \end{pmatrix}$ or $\begin{pmatrix} 1 \\ -1 \end{pmatrix}$. Our first compactness result (see proposition 2.3) shows that indeed this *macroscopic* expectation can be justified by starting from a *microscopic* point of view and passing to the corresponding continuum limit. Moreover, we note that, due to the rank-one connections between the wells, U_0 and QU_1 are both rank-one connected with their convex combinations:

$$F_\lambda := \lambda U_0 + (1 - \lambda)QU_1, \tag{1.6}$$

where Q is the rotation from (1.5) and $\lambda \in (0, 1)$.

In order to prepare the definition of our model Hamiltonian, which is formed by a sum of local energies h having the set K as the set of their local minimizers, we first define the precise set-up regarding the underlying domains and function spaces (see figure 1).

DEFINITION 1.1 (domains, deformations, admissibility). In what follows, we consider the following domains.

- For $x \in \mathbb{R}^2$, $d, l \in \mathbb{R}$, we define the translated parallelograms

$$\left.\begin{aligned} \Omega_{d,l}^+(x) &:= \mathrm{conv}\{(-d - l, l), (d - l, l), (d + l, -l), (l - d, -l)\} + x, \\ \Omega_{d,l}^-(x) &:= \mathrm{conv}\{(l - d, l), (l + d, l), (-l - d, -l), (d - l, -l)\} + x. \end{aligned}\right\} \tag{1.7}$$

If $x = (0,0)$, we also omit the point in the notation and simply write $\Omega_{d,l}^+$, $\Omega_{d,l}^-$.

- Using the previous notation, we set $\Omega := \Omega_{4,1}^+$ and $\Omega_n := \Omega \cap (n^{-1}\mathbb{Z})^2$.

- In what follows, we work on the triangles

$$\Delta_{i,j}^{n,+} := \operatorname{conv}\{(i/n, j/n), (i/n, (j+1)/n), ((i+1)/n, j/n)\},$$
$$\Delta_{i,j}^{n,-} := \operatorname{conv}\{(i/n, j/n), ((i-1)/n, j/n), (i/n, (j-1)/n)\}.$$

- $G^n(\Omega_n)$ denotes the set of all edges involved in the triangles $\Delta_{i,j}^{n,\pm} \subset \Omega_n$. With slight abuse of notation, we also refer to 'the grid Ω_n' in what follows, by which we mean the pair $(\Omega_n, \Delta_{i,j}^{n\pm})$ for $(i,j) \in n\Omega_n$.

Moreover, for any given set $M \subset \mathbb{R}^2$ and any $n \in \mathbb{N}$ we define

$$nM := \{(i,j) \colon (i/n, j/n) \in M\}.$$

In particular, this defines the sets $n\Omega$ and $n\Delta_{ij}^{n,\pm}$.

On the respective domains, we consider associated deformations $u \in C(\Omega, \mathbb{R}^2) \cap H^1(\Omega, \mathbb{R}^2)$ and denote their values on lattice points by

$$u^{i,j} := u(i/n, j/n) \quad \text{for } (i,j) \in n\Omega. \tag{1.8}$$

Additionally, we restrict ourselves to *admissible* lattice deformations u satisfying a *non-interpenetration* condition, i.e. on any domain $\Lambda \in \{\Omega_{d,l}^+, \Omega_{d,l}^-\}$ under consideration, $u \in \mathcal{A}_{n\Lambda}$, where

$$\mathcal{A}_{n\Lambda} := \{v \in C(\Lambda, \mathbb{R}^2) \cap H^1(\Lambda, \mathbb{R}^2) \colon \text{for all } n\Delta_{ij}^{n,\pm} \in \Lambda, \ \det(v^{ij} - v^{kl}, v^{rs} - v^{kl}) > 0,$$
$$\text{where } (k,l), (r,s) \in \mathbb{Z}^2 \text{ are adjacent grid vertices in } n\Delta_{ij}^{n,\pm}\}. \tag{1.9}$$

Finally, we impose *boundary conditions* prescribed by the matrices from (1.6) on admissible deformations considered on the whole domain Ω, i.e. for any admissible deformation defined on the whole domain Ω, we demand that $u \in \mathcal{A}_n^{F_\lambda}$, where

$$\mathcal{A}_n^{F_\lambda} := \{v \in \mathcal{A}_{n\Omega} \colon \text{for all } |j| \leqslant n, \ v^{ij} = F_\lambda(i/n, j/n) \text{ if } i + j \leqslant -4n,$$
$$v^{ij} = F_\lambda(i/n, j/n) + c \text{ for some } c \in \mathbb{R}^2 \text{ if } i + j \geqslant 4n\}. \tag{1.10}$$

Let us comment on these notions. We remark that we can easily switch from functions $u \colon \Omega \to \mathbb{R}^2$ to *grid functions* $u^{ij} \colon n\Omega \to \mathbb{R}^2$ using the definition given in (1.8). Conversely, starting from a discrete lattice function $u^{ij} \colon n\Omega \to \mathbb{R}^2$, we can pass to a function $u \in C(\Omega, \mathbb{R}^2)$ by piecewise affine interpolation on the triangles $n\Delta_{i,j}^{n,\pm}$. Hence, most of the functions $u \in \mathcal{A}_n^{F_\lambda}$ in our applications will be piecewise affinely interpolated lattice functions satisfying (1.10). Thus, with slight abuse of notation, in what follows we will use the phrase 'let $\{u_n\}_{n\in\mathbb{N}} \subset \mathcal{A}_n^{F_\lambda}$ be a sequence of piecewise affine functions on Ω_n' to denote a sequence of admissible functions that is affine on all of the grid triangles $\Delta_{i,j}^{n,\pm} \subset \Omega$.

In the context of our admissible lattice functions, the non-interpenetration condition contained in (1.9) corresponds to requiring that the labelling of the lattice triangles $n\Delta_{i,j}^{n,\pm}$ is not reversed or interchanged under the deformation u. Hence, it can be interpreted as a local invertibility constraint for piecewise affine deformations u on each of the lattice triangles $\Delta_{i,j}^{n,\pm} \subset \Omega$ (see the recent article of Braides and Gelli [10] for a criticism of this in the context of discrete-to-continuum fracture mechanics).

REMARK 1.2. By applying the conventions from definition 1.1 and, in particular, by interpreting $u \colon \Omega \to \mathbb{R}^2$ as the above described piecewise affine interpolation of the lattice deformation $u^{i,j}$, the usual spatial gradient ∇u of the deformation is well defined and satisfies $\nabla u \in \mathrm{PC}(\Omega, \mathbb{R}^{2\times 2})$. Here $\mathrm{PC}(\Omega, \mathbb{R}^{2\times 2})$ denotes the space of piecewise constant matrix-valued functions. In addition, we further agree on working with the following Lebesgue representative for the equivalence class of our deformation gradient ∇u: on the edges of the lattice triangles $\partial(\Delta_{i,j}^{n,\pm})$ we define the gradient of u to be equal to its value in the interior of the corresponding triangle $\Delta_{k,l}^{n,+}$ that contains the considered edge. Also, at the lattice point $(i/n, j/n) \in \Omega_n$ the gradient is identified with the one on $\Delta_{i,j}^{n,+}$. Using this convention, the abbreviations

$$\nabla u^{i,j} := \nabla u(i/n, j/n), \quad \partial_s u^{i,j} := \partial_s u(i/n, j/n) \quad \text{for } s = 1, 2,$$

which are used in what follows, are properly defined.

Propositions 2.4 and 3.7 will deal with functions ϕ_u^{ij} of $\nabla u \in \mathrm{PC}(\Omega, \mathbb{R}^{2\times 2})$, which are compositions of Lipschitz functions ϕ and ∇u. Consequently, these are piecewise constant themselves. In this context, we will work with discrete gradients, which we denote by $\nabla_n \phi_u^{ij}$. Here, for any lattice function $f^{ij} \colon \Omega_n \to \mathbb{R}$ we set

$$\nabla_n f^{ij} = (n(f^{i+1,j} - f^{i,j}), n(f^{i,j+1} - f^{i,j}))^{\mathrm{T}}. \tag{1.11}$$

REMARK 1.3. Note that in order to avoid additional technicalities connected with boundary effects and in order to keep the leading order of the bulk elastic energy zero in all considerations below, we define our reference domain Ω as the parallelogram from definition 1.1 (with sides orthogonal to one of the normals of the rank-one connections from (1.5)).

Keeping these conventions in mind, we proceed with the definition of our model Hamiltonian, which was previously introduced in [20].

DEFINITION 1.4 (model Hamiltonian, I). Let $u \in C(\Omega, \mathbb{R}^2) \cap H^1(\Omega, \mathbb{R}^2)$. Then the *model Hamiltonian* on the lattice $n\Omega$ is defined as

$$\begin{aligned}
\tilde{H}_n(u) &= \sum_{(i,j)\in n\Omega} \tilde{h}_u^{i,j} \\
&:= \sum_{i,j\in n\Omega} \lambda_n^2 \tilde{h}\left(\frac{u^{ij} - u^{i\pm 1j}}{\lambda_n}, \frac{u^{ij} - u^{ij\pm 1}}{\lambda_n}\right)
\end{aligned}$$

$$
:= \sum_{(i,j)\in n\Omega} \lambda_n^2 \Bigg[\sum_{\ell\in\{j+1,j-1\}} \left(\left(\frac{u^{i\ell}-u^{ij}}{\lambda_n} \right)^2 - a^2 \right)^2
$$

$$
+ \sum_{k\in\{i+1,i-1\}} \left(\left(\frac{u^{kj}-u^{ij}}{\lambda_n} \right)^2 - b^2 \right)^2
$$

$$
+ \sum_{\substack{\ell\in\{j+1,j-1\},\\ k\in\{i+1,i-1\}}} \left| \left(\frac{u^{i\ell}-u^{ij}}{\lambda_n}, \frac{u^{kj}-u^{ij}}{\lambda_n} \right) \right| \Bigg]
$$

$$
\times \Bigg[\sum_{\ell\in\{j+1,j-1\}} \left(\left(\frac{u^{i\ell}-u^{ij}}{\lambda_n} \right)^2 - b^2 \right)^2
$$

$$
+ \sum_{k\in\{i+1,i-1\}} \left(\left(\frac{u^{kj}-u^{ij}}{\lambda_n} \right)^2 - a^2 \right)^2
$$

$$
+ \sum_{\substack{\ell\in\{j+1,j-1\},\\ k\in\{i+1,i-1\}}} \left| \left(\frac{u^{i\ell}-u^{ij}}{\lambda_n}, \frac{u^{kj}-u^{ij}}{\lambda_n} \right) \right| \Bigg], \qquad (1.12)
$$

where $\lambda_n := n^{-1}$ and $(\cdot,\cdot)$ denotes the scalar product in $\mathbb{R}^2$.

REMARK 1.5 (boundary conditions). We stress that in our model we impose 'hard' boundary conditions in the form of (1.10). Already at this stage we emphasize that they are 'seen' by our Hamiltonian, as for points (i,j) on the layers with $i+j=-4n$, $i+j=4n$ the Hamiltonian still takes the left and right neighbours of these into account. On these the boundary conditions have already been prescribed. This will give rise to boundary layer energies (see theorem 1.11).

The Hamiltonian in definition 1.4 is constructed in such a way that the matrices from (1.3) indeed form its energy wells, i.e. $\tilde{H}_n(u) \geqslant 0$ for all admissible u and $\tilde{H}_n(u) = 0$ if and only if $\nabla u \in \mathrm{SO}(2)U_0$ or $\nabla u \in \mathrm{SO}(2)U_1$ on the whole of Ω. On the level of the local energies $\tilde{h}_u^{i,j}$ the deviation from the wells is measured by penalizing deformations that do not map horizontal and vertical unit line segments onto line segments of either the lengths a or b. Physically, this corresponds to two-body interactions between the five neighbouring atoms $(i/n, j/n)$, $(i\pm 1/n, j/n)$ and $(i/n, j\pm 1/n)$. Moreover, the local energy $\tilde{h}_u^{ij}$ favours deformations that enforce that orthogonal line segments are mapped to orthogonal line segments, i.e. deviations from orthogonality of the pairs $(i \pm 1/n, j/n)$ and $(i/n, j \pm 1/n)$ are penalized. The latter is physically achieved by three-body interactions measuring the angles between the vectors $u^{i\pm 1,j}$ and $u^{i,j\pm 1}$. We emphasize that the condition on the angles is necessary in modelling the deformation of an elastic body, as otherwise no shear resistance would be present.

REMARK 1.6. Using the notation from definition 1.1, we can rewrite the brackets in the definition of the Hamiltonian (1.12) in terms of lengths and angles of the horizontal and vertical derivatives of the deformations. For instance, the first bracket

in (1.12) turns into

$$
\begin{aligned}
\bar{h}_{U_0}(\partial_1 u^{i,j}, \partial_1 u^{i-1,j}, \partial_2 u^{i,j}, \partial_2 u^{i,j-1}) := (|\partial_1 u^{i,j}|^2 - a^2)^2 + (|\partial_1 u^{i-1,j}|^2 - a^2)^2 \\
+ (|\partial_2 u^{i,j}|^2 - b^2)^2 + (|\partial_2 u^{i,j-1}|^2 - b^2)^2 \\
+ \sum_{\substack{k \in \{i+1, i-1\}, \\ \ell \in \{j+1, j-1\}}} |(\partial_1 u^{k,j}, \partial_2 u^{i,\ell})|. \quad (1.13)
\end{aligned}
$$

Hence, the local energy density $\tilde{h} \colon \mathbb{R}^2 \times \mathbb{R}^2 \times \mathbb{R}^2 \times \mathbb{R}^2 \to \mathbb{R}$,

$$
\begin{aligned}
(\partial_1 u^{i,j}, \partial_1 u^{i-1,j}, \partial_2 u^{i,j}, \partial_2 u^{i,j-1}) \mapsto \tilde{h}(\partial_1 u^{i,j}, \partial_1 u^{i-1,j}, \partial_2 u^{i,j}, \partial_2 u^{i,j-1}) \\
:= \bar{h}_{U_0}(\partial_1 u^{i,j}, \partial_1 u^{i-1,j}, \partial_2 u^{i,j}, \partial_2 u^{i,j-1}) \\
\times \bar{h}_{U_1}(\partial_1 u^{i,j}, \partial_1 u^{i-1,j}, \partial_2 u^{i,j}, \partial_2 u^{i,j-1}),
\end{aligned}
$$

can also be regarded as a function of the lengths and angles formed by the corresponding partial derivatives of the deformation. Here

$$
\bar{h}_{U_1}(\partial_1 u^{i,j}, \partial_1 u^{i-1,j}, \partial_2 u^{i,j}, \partial_2 u^{i,j-1}) := \bar{h}_{U_0}(\partial_2 u^{i,j}, \partial_2 u^{i,j-1}, \partial_1 u^{i,j}, \partial_1 u^{i-1,j}).
$$

This also serves as a guiding intuition in defining a more general class of Hamiltonians for which our results are valid (see definition 1.10).

In this sense the density $\tilde{h}$ in the Hamiltonian from definition 1.4 (and later also the ones from definitions 1.8 and 1.10) can be viewed as a Lipschitz continuous function. The Hamiltonian can be considered as a function of u^{ij} or ∇u.

For the individual brackets of the Hamiltonian from definition 1.4 we introduce the notation

$$
\begin{aligned}
\bar{h}^{ij}_{u,U_0} &:= \bar{h}_{U_0}(\partial_1 u^{i,j}, \partial_1 u^{i-1,j}, \partial_2 u^{i,j}, \partial_2 u^{i,j-1}), \\
\bar{h}^{ij}_{u,U_1} &:= \bar{h}_{U_1}(\partial_1 u^{i,j}, \partial_1 u^{i-1,j}, \partial_2 u^{i,j}, \partial_2 u^{i,j-1}).
\end{aligned}
$$

This notation is used in step 2 of the proof of the Γ-convergence result in § 3.3.

As well as this geometric interpretation of the energy density, the definition of $\tilde{h}$ also implies the following pointwise control on the distance of ∇u to the energy wells K.

LEMMA 1.7 (lower bound). *Let $u \in \mathcal{A}^{F\lambda}_n$. Then for each $(i,j) \in n\Omega$ the following bound holds:*

$$
\tilde{h}^{i,j}_u \geqslant c \operatorname{dist}(\nabla u^{i,j}, K)^2.
$$

In particular,

$$
H_n(u) \geqslant c \int_\Omega \operatorname{dist}(\nabla u, K)^2 \, \mathrm{d}x.
$$

Proof. The proof follows immediately from noticing that, for $\nabla u^{i,j} \in \mathrm{GL}(2,\mathbb{R})_+$,

$$
\min\{||\partial_1 u^{i,j}| - a| + ||\partial_2 u^{i,j}| - b|, ||\partial_1 u^{i,j}| - b| + ||\partial_2 u^{i,j}| - a|\}^2 + |(\partial_1 u^{i,j}, \partial_2 u^{i,j})|
$$
$$
\geqslant c \operatorname{dist}(\nabla u^{i,j}, K)^2. \quad \square
$$

We further remark that the Hamiltonian defined in definition 1.4 is of mixed L^2–L^8 growth: if on $\Delta_{ij}^{n,\pm}$ the gradient ∇u is close to the wells, the local energy h is comparable to $\mathrm{dist}^2(\nabla u_n, \mathrm{SO}(2)U_0 \cup \mathrm{SO}(2)U_1)$, while if ∇u is at a finite distance from the wells, the energy controls the L^8-norm of ∇u. Hence, in total

$$\tilde{H}_n(u_n) \geqslant c \int_\Omega \max\{\mathrm{dist}^8(\nabla u, K), \mathrm{dist}^2(\nabla u, K)\}.$$

In order to avoid technical difficulties with the mixed growth behaviour at infinity, we truncate the energy density for large gradient values.

DEFINITION 1.8 (model Hamiltonian, II). Let $u \in \mathcal{A}_n^{F_\lambda}$. Let $k \colon (\mathbb{R}^2)^4 \to \mathbb{R}$ be a Lipschitz continuous function satisfying the bound

$$c_1|F|^2 \leqslant k(F) \leqslant c_2|F|^2$$

for any $F \in (\mathbb{R}^2)^4$ and for some universal constants $c_1, c_2 > 0$. Using this function, we define a modified energy density as

$$h_u^{i,j} := \gamma(|U^{i,j}|)\tilde{h}_u^{i,j} + (1-\gamma)(|U^{i,j}|)k(U^{ij}), \tag{1.14}$$

with $U^{i,j} := (\partial_1 u^{i,j}, \partial_1 u^{i-1,j}, \partial_2 u^{i,j}, \partial_2 u^{i,j-1})$ and a cut-off function $\gamma \in C^\infty(\mathbb{R}, \mathbb{R})$ that is chosen such that $\gamma(F) = 1$ for all $|F| \leqslant 10(\bar{c}+1)$ and $\gamma(F) = 0$ for $|F| \geqslant 20(\bar{c}+1)$. Here the constant $\bar{c}$ is the one from (1.4). Using this, we define the *(final) model Hamiltonian* as

$$H_n(u) := \sum_{(i,j) \in n\Omega} \lambda_n^2 h_u^{i,j}.$$

REMARK 1.9. We remark that the energy density from definition 1.8 in particular satisfies L^2-bounds at infinity, and for each $(i,j) \in n\Omega$ the global estimate

$$\mathrm{dist}^2(\nabla u^{i,j}, \mathrm{SO}(2)U_0 \cup \mathrm{SO}(2)U_1) \lesssim h_u^{i,j} \lesssim \mathrm{dist}^2(\nabla u^{i,j}, \mathrm{SO}(2)U_0 \cup \mathrm{SO}(2)U_1) \tag{1.15}$$

holds.

In concluding this section we stress that the following results are not only valid for our model Hamiltonian from definition 1.8, but hold for the following more general class of discrete Hamiltonians.

DEFINITION 1.10 (general class of Hamiltonians). For $u \in \mathcal{A}_n^{F_\lambda}$ let h_u^{ij} be the density from definition 1.8 and let $\hat{h}. \in C^{0,1}((\mathbb{R}^2)^4, \mathbb{R})$ be such that (1.15) is satisfied and the lower bound

$$\hat{h}_u^{i,j} \geqslant c_1 h_u^{i,j} \tag{1.16}$$

holds for each $(i,j) \in n\Omega$ and some positive constant c_1. Here the abbreviation $\hat{h}_u^{ij}$ is used as above to denote the pointwise evaluation $\hat{h}_u(i/n, j/n)$ at $(i,j) \in n\Omega$ (analogously to the evaluations defined in remark 1.6). We set

$$H_n(u) := \sum_{(i,j) \in n\Omega} n^{-2} \hat{h}_u^{i,j}.$$

We emphasize two important properties of this class of Hamiltonians: these are the lower bound from lemma 1.7 (which follows from that for h_u^{ij}) and the lower bound (1.16), which allows us to invoke the comparison arguments from appendix A. The lower bound (1.16) contains the origin of the surface energies, which are more closely analysed in §3.

As there are only small modifications in the proofs of the following results, we always carry them out for our model Hamiltonian H_n from definition 1.8 and leave the corresponding modifications for the general class to the reader.

1.2.2. *Main results*

Our main objective in this paper is an analysis of the discrete square-to-rectangular phase transition in the regime of surface energy scaling. In this context we will analyse the microscopic Hamiltonians from definitions 1.8 and 1.10 on 'low energy deformations'. More precisely, as in [20], in what follows we study sequences of admissible deformations $\{u_n\}_{n \in \mathbb{N}}$ for which

$$H_n(u_n) \leqslant \frac{C}{n}, \tag{1.17}$$

for some uniform (in n) constant $0 < C < \infty$. As an immediate property of this scaling, we observe that, since the Hamiltonian controls the distance of ∇u to the wells, we in particular obtain that $\operatorname{dist}(\nabla u, \mathrm{SO}(2)U_0 \cup \mathrm{SO}(2)U_1) \to 0$ in measure for deformations satisfying (1.17).

As in the case of atomic chains, which were investigated in [20], we expect that this scaling in n (in combination with the boundary conditions given by (1.6)) yields deformations that are locally simple laminates in the limit $n \to \infty$ (see proposition 2.3).

In this context our main interest is driven by the modelling side of the problem and by the question of whether the discrete problem can be regarded as an 'equivalent' of the continuous regularization. Mathematically, our analysis is strongly based on the fundamental ideas introduced in the treatment of the continuum version of the two-well problem by Conti and Schweizer [13–15]. Let us also mention that these methods differ substantially from the ones introduced in our preceding paper [20], where, after a special reduction of the Hamiltonian from definition 1.4 onto one-dimensional chains, low energy deformations were treated both analytically and numerically. Due to the presence of 'atomic chains', additional structural conditions had been exploited in that context.

As the main result of this paper, we prove that in the surface energy scaling regime and in the continuum limit, i.e. as $n \to \infty$, there exists a limiting surface energy that resembles the analogous limiting energy from the continuous set-up [15]. This result is formulated precisely in the following theorem.

THEOREM 1.11. *Let $H_n(u)$ be as in definition 1.8. Then, in the sense of Γ-limits with respect to the L^1 topology on $\mathcal{A}_n^{F_\lambda}$,*

$$nH_n \to E_{\mathrm{surf}},$$

where

$$E_{\text{surf}}(u_0) := \begin{cases} \displaystyle\int_{J_{\nabla u_0}} \bar{C}(\nabla u_0(x-,0), \nabla u_0(x+,0)) \,\mathrm{d}\mathcal{H}^1 \\ \qquad \textit{if } u_0 \textit{ is a piecewise affine deformation} \\ \qquad \textit{satisfying the boundary condition} \\ \qquad \nabla u_0(x) = F_\lambda \textit{ for } x_1 + x_2 \leqslant -4, \ |x_2| \leqslant 1, \\ \qquad \nabla u_0(x) = F_\lambda \textit{ for } x_1 + x_2 \geqslant 4, \ |x_2| \leqslant 1, \\ \qquad \textit{and } \nabla u_0 \in \mathrm{BV}_{\text{loc}}(\mathbb{R} \times [-1,1]) \textit{ such that} \\ \qquad \nabla u_0 \in \mathrm{SO}(2)U_0 \cup \mathrm{SO}(2)U_1 \textit{ almost everywhere} \\ \qquad \textit{in } \Omega, \\ \infty \qquad \textit{otherwise.} \end{cases}$$

Here $J_{\nabla u_0}$ denotes the jump set of ∇u_0 and

$$u(x-) := \lim_{\substack{y=(y_1,y_2)\to x=(x_1,x_2), \\ y_1 \leqslant x_1}} u(y).$$

The function $\bar{C}(\cdot, \cdot)\colon (\mathrm{SO}(2)U_0 \cup \mathrm{SO}(2)U_1)^2 \to \mathbb{R}$ is the limiting energy density obtained indirectly by minimizing among all deformations with the correct boundary conditions (see definition 3.3).

Let us comment on the result of theorem 1.11 and its relation to [24]. Similarly to [24], our analysis is motivated by understanding the relation between the discrete and continuous regularizations of the square-to-rectangular phase transition. In this context we are particularly interested in studying the origins of surface energies. The article [24] compared the scaling of infimizers of a functional of type (1.2) with a discretization of (1.1) and showed that the corresponding scaling behaviours coincide. In particular, (for infimizers) this allows one to switch between the discrete and continuum functional (up to giving up constants) and to transfer bounds from the discrete to the analogous continuum model. In principle, this would permit us to establish compactness properties for sequences for the discrete (minimizing) sequences from the compactness properties of their continuous analogues. However, due to the loss of the constants, [24] does *not* imply our Γ-convergence result. Instead of exploiting the result of [24], we give an independent proof of the compactness properties, since in our discrete setting this step is simplified by a comparison with a spin system (due to the presence of next-to-nearest neighbour interactions). Having established compactness, our proof then follows the ideas outlined by Conti and Schweizer [13–15] adapted to our discrete set-up.

Let us further note that while theorem 1.11 does not explain the different diffuse and sharp interface features observed in experiments, it does show that, as in the one-dimensional case and as in [23, 24], discrete two-well energies such as in definitions 1.8 and 1.10 naturally lead to higher-order regularizations. If understood on the level of finite but large sample sizes, they might even give indications for the experimentally observed behaviour. The analogy between the discrete and the continuous setting is highlighted in table 1. It provides a natural correspondence

Table 1. *Comparison of the relevant continuous and discrete quantities.*

	continuum, macroscopic	discrete, microscopic
energies	$\int_{\Omega} \frac{1}{\varepsilon} W(\nabla u) + \varepsilon \lvert \nabla^2 u \rvert^2 \, dx \leqslant C,$ $\varepsilon \to 0$	$\sum_{i=-n}^{n} \sum_{j=-n}^{n} \frac{1}{n^2} h_{u_n}^{ij} \leqslant \frac{C}{n},$ $n \to \infty$
regularity of the deformation	$u \in W^{2,2}(\Omega, \mathbb{R}^2)$	$u \in C^{0,1}(\Omega, \mathbb{R}^2)$ is piecewise affine on the underlying lattice (after interpolation)
surface energies	$\int_{\Omega} \varepsilon \lvert \nabla^2 u \rvert^2 \, dx \leqslant C$	$\sum_{i=-n}^{n} \sum_{j=-n}^{n} \frac{1}{n^2} \lvert \nabla_n^2 u \rvert^2 \leqslant Cn$
scaling parameter	ε	$\dfrac{1}{n}$

between continuum objects considered by Conti and Schweizer [13–15] and our discrete setting introduced in the previous paragraph.

1.3. Organization of the paper

The remainder of the paper is organized as follows. In § 2 we derive compactness (proposition 2.2) and rigidity (propositions 2.3 and 2.4) properties of the sequences of deformations u_n obeying the surface energy scaling (1.17). In § 3 we describe the limiting surface energies and prove theorem 1.11. Important auxiliary results are proved in the appendices. In appendix A we provide a mapping of our discrete two-well problem to a spin system. This yields a one-sided estimate of the original Hamiltonian from below. These results are crucially used in our proof of the compactness results of propositions 2.2 and 2.3. In appendix B we show that our discrete Hamiltonian H_n provides upper bounds of the discrete second derivatives of admissible deformations u. While the latter bounds are not actually necessary for our argument, they are included as an illustration of the comparability of our discrete model and the continuous model from [15]. Last but not least, in appendix C and appendix D we give sketches of the proofs of the discrete coarea formula and the well-definedness of the algorithm yielding the perturbed grid in the proof of proposition 3.7, step 4(a).

2. Rigidity

In this section we prove various rigidity estimates. On the one hand they yield compactness properties (see propositions 2.2 and 2.3) for admissible sequences $\{u_n\}_{n \in \mathbb{N}}$ that obey the energy bound (1.17). On the other hand, adapting to our discrete setting the ideas of Conti and Schweizer [13–15], we show finer rigidity estimates for sequences, which, in addition to (1.17), also satisfy the smallness condition (2.4) for a local *one-well* energy (see proposition 2.4). The latter estimate plays a crucial role for the cutting mechanism that is used for the construction of the recovery sequence in the Γ-lim sup inequality (see § 3.3).

2.1. Compactness

In this section we exploit the information from appendix A in order to prove rigidity of the limiting deformation fields (see propositions 2.2 and 2.3). We begin with the following auxiliary result.

LEMMA 2.1. *Let $\{u_n\}_{n\in\mathbb{N}} \subset \mathcal{A}_n^{F_\lambda}$ be a sequence of piecewise affine functions on the grid Ω_n satisfying (1.17). Then there exist (up to zero sets) disjoint Caccioppoli sets Ω_0 and Ω_1 such that*

$$\left.\begin{aligned}
\Omega_0 \cup \Omega_1 &= \Omega, \\
\operatorname{dist}(\nabla u_n, \mathrm{SO}(2)U_0) \to 0 \quad &\textit{in } L^2(\Omega_0), \\
\operatorname{dist}(\nabla u_n, \mathrm{SO}(2)U_1) \to 0 \quad &\textit{in } L^2(\Omega_1).
\end{aligned}\right\} \tag{2.1}$$

Proof. The proof is based on a comparison argument with a spin-Hamiltonian and is given in propositions A.4 and A.5. □

In general the L^2-convergence (2.1) can be arbitrarily slow; see remark A.6.

PROPOSITION 2.2. *Let $\{u_n\}_{n\in\mathbb{N}} \subset \mathcal{A}_n^{F_\lambda}$ be a sequence of piecewise affine functions on the grid Ω_n satisfying the energy bound (1.17). Then there exist a subsequence $\{n_j\}_{j\in\mathbb{N}} \subset \mathbb{N}$ and a limiting deformation $u \in W^{1,\infty}(\Omega, \mathbb{R}^2)$ such that*

(a) $\nabla u_{n_j} \to \nabla u$ *in* $L^2(\Omega_0)$,

(b) $\nabla u \in \mathrm{SO}(2)U_0$ *in* Ω_0.

An analogous statement holds in Ω_1.

In order to show this, we follow an argument of Kinderlehrer (see also [26, theorem 2.4]) in which the function $\operatorname{dist}(\cdot, \mathrm{SO}(2)U_0)$ is replaced by a lower semi-continuous analogue.

Proof.

STEP 1 (set-up). We set $f(F) := |FU_0^{-1}|^2 - 2\det(FU_0^{-1})$ and remark that $f(F) \geqslant 0$ and $f(F) = 0 \iff F = \lambda Q U_0$ with $\lambda \geqslant 0$ and $Q \in \mathrm{SO}(2)$. Moreover, we recall the truncation argument from [19], which allows us to replace u_n by a sequence $v_n \in W^{1,\infty}(\Omega)$ with the following properties:

$$\|\nabla v_n\|_{L^\infty(\Omega)} \leqslant c_1,$$

$$\|\nabla u_n - \nabla v_n\|_{L^2(\Omega)} \leqslant \int_{\{|\nabla u_n| \geqslant c_2\}} |\nabla u_n|^2 \,\mathrm{d}x$$
$$\leqslant \frac{c}{n}.$$

Here $c_1, c_2 > 0$ are universal constants (independent of n). The last estimate follows from the energy bounds (1.17) and (1.15). As a consequence of the comparability of ∇u_n and ∇v_n, the two functions have the same weak limit ∇u. Therefore, it suffices to prove the strong convergence of ∇v_n to ∇u.

STEP 2 (convergence of $f(\nabla v_n)$). We claim that

$$\lim_{n\to\infty} \int_{\Omega_0} f(\nabla v_n)\,\mathrm{d}x = 0. \tag{2.2}$$

Indeed, this is a direct consequence of the second estimate in (2.1) in lemma 2.1: as L^2-convergence implies convergence in measure, for any given $\varepsilon, \delta > 0$ there exists $N_0 = N_0(\varepsilon, \delta)$ such that for $\Omega_\delta := \{x \in \Omega_0 \mid \operatorname{dist}(\nabla v_n, \mathrm{SO}(2)U_0) < \delta\}$ it holds that

$$|\Omega_\delta| \geqslant (1 - \varepsilon)|\Omega_0| \quad \text{for all } n \geqslant N_0.$$

Thus,

$$
\begin{aligned}
\int_{\Omega_0} f(\nabla v_n)\,\mathrm{d}x &= \int_{\Omega_0 \cap \Omega_\delta^c} f(\nabla v_n)\,\mathrm{d}x + \int_{\Omega_0 \cap \Omega_\delta} f(\nabla v_n)\,\mathrm{d}x \\
&\leqslant |\Omega_0 \cap \Omega_\delta^c| f(c_1) + C|\Omega|\delta^2 \\
&\leqslant C|\Omega|(\varepsilon + \delta^2).
\end{aligned}
$$

STEP 3. Using the convergence from step 2 leads to

$$
\begin{aligned}
0 &= \liminf_{n\to\infty} \int_{\Omega_0} f(\nabla v_n)\,\mathrm{d}x \\
&= \liminf_{n\to\infty} \left(\int_{\Omega_0} |\nabla v_n U_0^{-1}|^2\,\mathrm{d}x - 2\int_{\Omega_0} \det(\nabla v_n U_0^{-1})\,\mathrm{d}x \right) \\
&\geqslant \int_{\Omega_0} |\nabla u U_0^{-1}|^2\,\mathrm{d}x - 2\int_{\Omega_0} \det(\nabla u U_0^{-1})\,\mathrm{d}x \\
&= \int_{\Omega_0} f(\nabla u)\,\mathrm{d}x \\
&\geqslant 0. \tag{2.3}
\end{aligned}
$$

Here the first equality follows from step 2. The fourth estimate is a consequence of the lower semi-continuity of the norm together with the weak continuity of the determinant (see [26, theorem 2.3(ii)] and references therein) and the fact that $\nabla v_n \rightharpoonup \nabla u$ in $L^2(\Omega)$ as $n \to \infty$. Hence, we have equalities everywhere in (2.3), and therefore

$$f(\nabla u) = 0 \quad \text{and} \quad \|\nabla v_n\|_{L^2(\Omega_0)} \to \|\nabla u\|_{L^2(\Omega_0)}$$

along a subsequence. As a consequence, along a subsequence, $\nabla u_n \to \nabla u$ in $L^2(\Omega_0)$ and $\nabla u(x) \in \mathrm{SO}(2)U_0$ (we remark that $\lambda = 1$ due to the closeness of ∇v_n to $\mathrm{SO}(2)U_0$, which follows from lemma A.5). $\qquad\square$

With these results in hand, we can now invoke the two-well rigidity result of Dolzmann and Müller [16]. This yields a structure result for the sets Ω_0, Ω_1. More precisely, the associated liming deformation u has to be a simple laminate, which (by virtue of the energy bound (1.17)) implies that $\Omega_{0,1}$ consists of a union of finitely many stripes (and triangles); see figure 2.
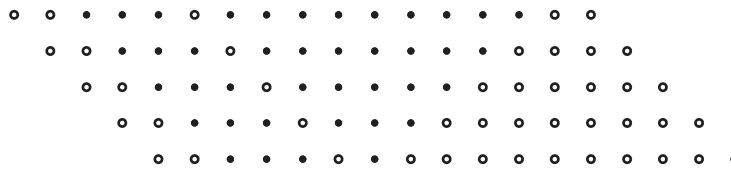
Figure 2. A simple laminate depicted in the reference configuration. The figure shows the reference configuration and the domains, in which $\nabla u \in \mathrm{SO}(2)U_0$ (open circles) and $\nabla u \in \mathrm{SO}(2)U_1$ (filled circles). In particular, the configuration need only locally be a simple laminate. It is also possible that there are intersections of the twinning planes at the boundary.

PROPOSITION 2.3 (rigidity). *Let $\{u_n\}_{n\in\mathbb{N}} \subset \mathcal{A}_n^{F_\lambda}$ be a sequence of piecewise affine functions on the grid Ω_n satisfying the energy bound (1.17). Then there exist a subsequence $\{n_j\}_{j\in\mathbb{N}} \subset \mathbb{N}$ and a limiting deformation $u \in W^{1,\infty}(\Omega, \mathbb{R}^2)$ such that the following hold.*

(a) *$\nabla u_{n_j} \to \nabla u$ in $L^2(\Omega)$, where $\nabla u \in K$ almost everywhere is a piecewise constant $\mathrm{BV}(\Omega, \mathbb{R}^{2\times 2})$ function.*

(b) *The associated domains Ω_0 and Ω_1 that were defined in lemma 2.1 consist of a union of finitely many polygonal domains that extend up to the boundary of Ω. The interfaces of the polygonal domains are either given by lines with the normals $(-1, 1)$ or $(1, 1)$ (which are determined by the rank-one connections from (1.5)) or by the boundary of Ω.*

(c) *There exists a constant $c \in \mathbb{R}^2$ with*

$$u(x_1, x_2) = F_\lambda(x_1, x_2), \qquad x_1 + x_2 \leqslant -4,$$
$$u(x_1, x_2) = F_\lambda(x_1, x_2) + c, \quad x_1 + x_2 \geqslant 4,$$

for all $|x_2| \leqslant 1$.

Proof. By proposition 2.2 there exists a subsequence $n_j \in \mathbb{N}$ such that $\nabla u_{n_j} \to \nabla u$ and $\nabla u \in \mathrm{SO}(2)U_0$ (respectively, $\nabla u \in \mathrm{SO}(2)U_1$) in Ω_0 (respectively, Ω_1). As Ω_0 and Ω_1 have finite perimeter, ∇u satisfies the conditions of [16, theorem 5.3] and the limiting deformation ∇u locally is a laminate. As $\mathrm{Per}(\Omega_1) \leqslant C < \infty$, there can only be a finite number of phase transitions between $\mathrm{SO}(2)U_0$ and $\mathrm{SO}(2)U_1$. The remaining parts of statements (a) and (b) follow from [16, theorem 5.3].

The boundary conditions that are stated in (c) are a consequence of the $H^1(\Omega)$-convergence of u and the prescribed boundary data (1.10). The finiteness of $c \in \mathbb{R}^2$ follows from the energy bound (1.17). $\square$

The compactness result of proposition 2.3 is a first important step for the formulation and derivation of the limiting surface energy (see definition 3.3, (3.2) and theorem 3.4) and the proof of theorem 1.11.

2.2. Two-well rigidity

In this section we derive an analogue of the two-well rigidity result of Conti and Schweizer [13–15] in our discrete framework.

PROPOSITION 2.4 (two-well rigidity). *Let $\alpha \in (0, 1/8)$, $x_0, y_0 \in \Omega$ with $|x_0 - y_0| = r > 0$ and $B_{2\alpha r}(x_0) \cup B_{2\alpha r}(y_0) \subset \Omega$. Define $M := \operatorname{conv}(B_{2\alpha r}(x_0) \cup B_{2\alpha r}(y_0))$ and suppose that $u \in \mathcal{A}_n$ is piecewise affine on the grid Ω_n and satisfies*

$$\sum_{(i,j)\in nM} \frac{1}{n^2}(r^{-2}\phi_u^{ij} + r^{-1}|\nabla_n \phi_u^{ij}|) \leqslant \eta, \tag{2.4}$$

where $\phi \in C^{0,1}((\mathbb{R}^2)^4, \mathbb{R})$, $\phi(\cdot) \geqslant 0$;

$$(\partial_1 u^{i,j}, \partial_1 u^{i-1,j}, \partial_2 u^{i,j}, \partial_2 u^{i,j-1}) \mapsto \phi(\partial_1 u^{i,j}, \partial_1 u^{i-1,j}, \partial_2 u^{i,j}, \partial_2 u^{i,j-1}) =: \phi_u^{ij}$$

denotes a one-well energy density with energy well $\mathrm{SO}(2)U_0$ and two-growth behaviour, i.e. there exist positive constants $c_1, c_2 > 0$ such that

$$c_1 \operatorname{dist}^2(\nabla u^{ij}, \mathrm{SO}(2)U_0) \leqslant \phi_u^{ij} \leqslant c_2 \operatorname{dist}^2(\nabla u^{ij}, \mathrm{SO}(2)U_0). \tag{2.5}$$

Let $\theta \in (0, 1)$. If $\eta = \eta(\theta, \alpha) > 0$ is chosen sufficiently small, then there exist a constant $c = c(\alpha, \theta)$ and a subset $U \subset B_{\alpha r}(x_0) \times B_{\alpha r}(y_0)$ with measure $|U| \geqslant (1-\theta)|B_{\alpha r}(x_0) \times B_{\alpha r}(y_0)|$ such that, for all $(x, y) \in U$,

$$1 - c\mu \leqslant \frac{|u(x) - u(y)|}{|U_0(x - y)|} \leqslant 1 + c\mu, \tag{2.6}$$

where

$$\mu := \frac{1}{r^2} \sum_{(i,j)\in nM} \frac{1}{n^2} \operatorname{dist}(\nabla u^{ij}, K).$$

REMARK 2.5. We recall that the symbol ∇_n in (2.4) denotes the discrete gradient as defined in (1.11).

REMARK 2.6. In what follows we call a line segment $[x, y]$ with endpoints $x, y \in \Omega$ that satisfies (2.6) *rigid*. This convention will, for instance, be used in step 4(a) in the proof of proposition 3.7.

REMARK 2.7. In the proof of proposition 2.4 we closely follow the ideas of Conti and Schweizer [14], though taking into account our discrete set-up. In particular, *a priori* we do not have enough regularity to apply C^1 degree theory. However, as our maps are piecewise affine, the weaker *almost everywhere* results, which follow from degree theory, can be upgraded to hold *everywhere*.

REMARK 2.8 (scaling). We remark that for $r \sim 1/n$ the smallness condition (2.4) turns into a pointwise condition. In what follows, by scaling we will assume that $r = 1$.

Proof.

STEP 1 (preliminaries: definition and estimates for the bad set). We note that by (2.4), U_0 is the majority phase in M. For

$$0 < \tilde{c}_1 := \tfrac{1}{4}\min\{\bar{c}, \bar{c}^2\},$$

with $\bar{c}$ as in (1.4), we consider sets of the form

$$\Omega_{\mathrm{b}}^{\tilde{c}_1} := \overline{\{x \in \Omega \cap M \colon \phi_u^{ij} \geqslant \tilde{c}_1\}}.$$

Here $\bar{\ }$ denotes the closure of a set. Since u is a piecewise affine function, it is immediate that $\Omega_{\mathrm{b}}^{\tilde{c}_1}$ consists of a finite union of grid triangles $\Delta_{ij}^n \subset \Omega_n$:

$$\Omega_{\mathrm{b}}^{\tilde{c}_1} = \bigcup_{ij} \Delta_{ij}^n \quad \text{and} \quad \partial\Omega_{\mathrm{b}}^{\tilde{c}_1} = \bigcup_{ij} \partial\Delta_{ij}^n. \tag{2.7}$$

By the discrete coarea formula (see appendix C, in particular (C 1))

$$\int_0^\infty \mathrm{Per}_M(\{(i,j)\colon \phi_u^{ij} \geqslant t\})\,\mathrm{d}t \leqslant C \sum_{(i,j)\in nM} \frac{1}{n^2}|\nabla_n \phi_u^{ij}|, \tag{2.8}$$

we infer that for each $\tilde{c}_1 > 0$ there exists $c_1 \in (\tilde{c}_1, 2\tilde{c}_1)$ such that, for $\Omega_{\mathrm{b}} := \Omega_{\mathrm{b}}^{c_1}$, it holds that

$$\mathrm{Per}_M(\Omega_{\mathrm{b}}) \leqslant C \frac{\eta}{\tilde{c}_1}.$$

Hence, by the isoperimetric inequality and by the assumption that U_0 is the majority phase in our sample M, we infer that

$$|\Omega_{\mathrm{b}}| \leqslant C \frac{\eta}{\tilde{c}_1}. \tag{2.9}$$

By definition of the 'bad set' Ω_{b}, on its complement, i.e. on $M \setminus \Omega_{\mathrm{b}}$, ∇u_n is c_1-close to $\mathrm{SO}(2)U_0$. On the boundary, however, this is not necessarily true. Setting

$$(M \cap \partial\Omega_{\mathrm{b}})_\varepsilon := \{x \in M \setminus \Omega_{\mathrm{b}}\colon \mathrm{dist}(x, \Omega_{\mathrm{b}}) = \varepsilon\} \quad \text{for any } \varepsilon \in \left(0, \frac{1}{10n}\right),$$

and recalling the continuity of u and the structure of $\partial\Omega_{\mathrm{b}}$, we obtain

$$\mathcal{H}^1(u(M \cap \partial\Omega_{\mathrm{b}})) = \lim_{\varepsilon \to 0} \mathcal{H}^1(u(M \cap \partial\Omega_{\mathrm{b}})_\varepsilon),$$
$$\mathcal{H}^1(M \cap \partial\Omega_{\mathrm{b}}) = \lim_{\varepsilon \to 0} \mathcal{H}^1((M \cap \partial\Omega_{\mathrm{b}})_\varepsilon).$$

Using these observations and the fact that $u(M \cap \partial\Omega_{\mathrm{b}})$ and $u((M \cap \Omega_{\mathrm{b}})_\varepsilon)$ are rectifiable (as the images of Lipschitz sets under a Lipschitz function), we therefore obtain

$$\begin{aligned}
\mathcal{H}^1(u(M \cap \partial\Omega_{\mathrm{b}})) &\leqslant 2\mathcal{H}^1(u(M \cap \partial\Omega_{\mathrm{b}})_\varepsilon) \\
&\leqslant 2 \int_{(M \cap \partial\Omega_{\mathrm{b}})_\varepsilon} |\nabla u|\,\mathrm{d}\mathcal{H}^1 \\
&\leqslant 2(1 + c_1)\mathcal{H}^1((M \cap \partial\Omega_{\mathrm{b}})_\varepsilon) \\
&\leqslant 4(1 + c_1)\mathcal{H}^1(M \cap \partial\Omega_{\mathrm{b}}) \\
&\leqslant 4C\eta
\end{aligned} \tag{2.10}$$

for all sufficiently small ε. Here we invoked the area formula and used that ∇u is c_1-close to $\mathrm{SO}(2)U_0$ in $(M \cap \partial \Omega_\mathrm{b})_\varepsilon$. Moreover,

$$
\begin{aligned}
|u(\Omega_\mathrm{b})| \leqslant \int_{\Omega_\mathrm{b}} |\det(\nabla u)| \, \mathrm{d}x &\leqslant C \int_{\Omega_\mathrm{b}} (1 + \mathrm{dist}^2(\nabla u, \mathrm{SO}(2)U_0)) \, \mathrm{d}x \\
&\leqslant C|\Omega_\mathrm{b}| + C \sum_{(i,j) \in nM} \frac{1}{n^2} \phi_u^{ij} \\
&\leqslant C\eta,
\end{aligned}
\tag{2.11}
$$

where we exploited the two-growth (2.5) and estimated

$$
|\det(\nabla u)| \leqslant
\begin{cases}
1 & \text{if } |\nabla u| \leqslant 20c_1/\tilde{c}_1, \\
C \, \mathrm{dist}(\nabla u, \mathrm{SO}(2)U_0)^2 & \text{if } |\nabla u| \geqslant 20c_1/\tilde{c}_1.
\end{cases}
$$

Thus, this argument yields control on the size of the measure of the bad points in the reference configuration. As in [14], this results in a one-sided control of type (2.6), which for completeness is presented in step 2.

STEP 2 (the upper bound). In this step we consider integrals on segments $[x, y] \subset M$ of certain functions f of $\nabla u \in \mathrm{PC}(\Omega, \mathbb{R}^2)$. We will use that for any direction $(x - y)/|x - y|$ that is not parallel to the grid edges and for almost any point x, the restrictions $\nabla u|_{[x,y]}$ and $f(\nabla u)|_{[x,y]}$ are well-defined $L^1([x, y])$ functions. However, the grid edges constitute a zero set in $B_\alpha(x_0) \times B_\alpha(y_0)$, and thus we will exclude this set from our consideration. Additionally, we use the convention of saying that certain statements are valid *for most pairs* (x, y) belonging to a certain set. This will mean that the Lebesgue measure of such pairs (x, y) constitutes at least $(1 - \theta)$ total measure of the latter set. Obtaining such a statement will in particular lead to a θ dependence in the relevant constants. Often, several properties have to be satisfied on a set of size $(1 - \theta)$ of the total measure, which leads to additional losses in the constants.

With these preliminaries and as in [14] we claim that the following hold.

(i) For most pairs $(x, y) \in (B_\alpha(x_0) \setminus \Omega_b) \times (B_\alpha(y_0) \setminus \Omega_b)$ it holds that

$$
[x, y] \cap \Omega_\mathrm{b} = \emptyset.
$$

(ii) For most pairs $(x, y) \in (B_\alpha(x_0) \setminus \Omega_b) \times (B_\alpha(y_0) \setminus \Omega_b)$ the restriction $\nabla u|_{[x,y]}$ is a well-defined $L^1([x, y])$ function. Moreover, there exists a constant $c = c(\theta, \alpha) > 0$ such that, for most pairs $(x, y) \in (B_\alpha(x_0) \setminus \Omega_b) \times (B_\alpha(y_0) \setminus \Omega_b)$,

$$
\int_{[x,y]} \mathrm{dist}(\nabla u, \mathrm{SO}(2)U_0) \, \mathrm{d}\mathcal{H}^1 \leqslant c\mu,
\tag{2.12}
$$

where $[x, y]$ denotes the line segment connecting x and y.

(iii) There exists a constant $c = c(\theta, \alpha) > 0$ such that following estimate is true:

$$
|u(x) - u(y)| \leqslant |U_0(x - y)| + c\mu.
\tag{2.13}
$$

We begin by discussing properties (i) and (ii). To this end we first observe that, by virtue of (2.9),

$$|B_\alpha(x_0) \setminus \Omega_b| \geqslant c\alpha^2, \qquad |B_\alpha(y_0) \setminus \Omega_b| \geqslant c\alpha^2$$

for all sufficiently small η (chosen sufficiently small in dependence of θ in order to guarantee that a sufficiently large volume of 'good points' is left). As in [14] we now consider the function $f(x) := \operatorname{dist}(\nabla u(x), \operatorname{SO}(2)U_0 \cup \operatorname{SO}(2)U_1)\chi_M$. By averaging we show that for almost all $(x, y) \in B_\alpha(x_0) \times B_\alpha(y_0)$,

$$\int_{[x,y]} f \, \mathrm{d}\mathcal{H}^1 < \infty, \tag{2.14}$$

i.e. $f|_{[x,y]} \in L^1([x, y])$. Considering $\nu \in S^1$, the line $t \mapsto x + t\nu$, the vector $\nu_0 := (y_0 - x_0)/|y_0 - x_0|$ and noting that only those lines with $|\nu - \nu_0| \leqslant 3\alpha$ intersect $B_{\alpha r}(y_0) \setminus \Omega_b$, yields

$$\int_{(B_\alpha(x_0)\setminus\Omega_b)\times(B_\alpha(y_0)\setminus\Omega_b)} \int_{[x,y]} f \, \mathrm{d}\mathcal{H}^1$$
$$\leqslant c\alpha \int_{|\nu-\nu_0|\leqslant 3\alpha} \int_{B_\alpha(x_0)\setminus\Omega_b} \int_{\mathbb{R}} f(x + t\nu) \, \mathrm{d}t \, \mathrm{d}x \, \mathrm{d}\nu$$
$$\leqslant C\alpha^2 \int_M f \, \mathrm{d}x$$
$$\leqslant C\alpha^3\mu. \tag{2.15}$$

This shows (2.14). Keeping this in mind, we now prove (i). As in [14] the result follows from a projection argument. In fact we claim that for any $\nu \in S^1$ the set

$$A_\nu := \{x \in B_1 \setminus \Omega_b \colon t \mapsto x + t\nu \text{ intersects } \partial\Omega_b\}$$

satisfies

$$|A_\nu| \leqslant 2\alpha\mathcal{H}^1(\partial\Omega_b) \leqslant c\alpha\eta.$$

Indeed, writing $x = x_0 + s\nu + r\nu^\perp$ for each $x \in A_\nu$, we have that $x_0 + r\nu^\perp$ is contained in the orthogonal projection of $\partial\Omega_b$ onto the line through x_0 parallel to $\nu^\perp$. This yields the claim of (i). Choosing $c = c(\theta, \alpha) > C\alpha^3/\theta$, where C denotes the constant from (2.15), then also yields (ii). Here we exploited that by (i), $f = \operatorname{dist}(\nabla u, \operatorname{SO}(2)U_0)$ along most of the line segments $[x, y]$ and that by our choice of $c = c(\theta, \alpha)$, (2.15) implies that (2.12) holds on a set of measure of size at least $(1-\theta)|B_\alpha(x_0) \times B_\alpha(y_0)|$.

Finally, we present the argument for (iii). By (ii) we have

$$|u(x) - u(y)| \leqslant \int_{[x,y]} |\nabla_\tau u| \, \mathrm{d}\mathcal{H}^1$$
$$\leqslant |U_0(x - y)| + c \int_{[x,y]} \operatorname{dist}(\nabla u, \operatorname{SO}(2)U_0) \, \mathrm{d}\mathcal{H}^1$$
$$\leqslant |U_0(x - y)| + c\mu,$$

where $\nabla_\tau u$ denotes the tangential derivative.

STEP 3 (the lower bound). As in [14], the lower bound is the most delicate part of the proof, since our (piecewise affine) deformation is not necessarily invertible. In addition to this key difficulty, which was overcome by Conti and Schweizer [14] by showing that the deformation is invertible on 'a sufficiently large set', we have to deal with the fact that our deformation is *not a priori regular*. Since we are working with a piecewise affine interpolation of our discrete data, we cannot immediately invoke the degree theory arguments of Conti and Schweizer (which *a priori* only apply to C^1 functions). Instead we use an integrated formula for the degree.

Again we argue in five steps.

(i) *Approximate injectivity.* Let

$$\alpha'' = 3\alpha/2 \quad \text{and} \quad M'' := \operatorname{int} \operatorname{conv}(B_{\alpha''}(x_0) \cup B_{\alpha''}(y_0)).$$

Then there exists $\alpha' \in (7\alpha/4, 2\alpha)$ and an affine deformation $A \colon M \to \mathbb{R}^2$ with gradient in $\mathrm{SO}(2)U_0$ such that for all $z \in A(M'') \setminus u(\Omega_\mathrm{b})$ there exists a unique preimage $x \in M' \cap u^{-1}(z)$. Here $M' := \operatorname{int} \operatorname{conv}(B_{\alpha'}(x_0) \cup B_{\alpha'}(y_0))$.

(ii) Let A be the mapping from (i). Then for the set

$$\Omega_{bi} := \{x \in M' \colon u(x) \in u(\Omega_\mathrm{b}) \cap A(M'')\}$$

we have $|\Omega_{bi}| \leqslant c\eta$.

(iii) We claim that, for most choices of $(x, y) \in (B_{\alpha''}(x_0) \setminus \Omega_\mathrm{b}) \times (B_{\alpha''}(y_0) \setminus \Omega_\mathrm{b})$,

   (a) $[u(x), u(y)] \cap u(\partial \Omega_b) = \emptyset$,

   (b) $[u(x), u(y)] \subset u(M' \setminus \Omega_b)$,

   (c) there exists a piecewise affine curve $\gamma_{xy}(t) \colon [0, 1] \to [u(x), u(y)]$ such that $u \circ \gamma_{xy}$ is a monotonic parametrization of the segment $[u(x), u(y)]$.

(iv) Let γ_{xy} be a piecewise affine curve such that $u \circ \gamma_{xy}$ is a monotonic parametrization of the segment $[u(x), u(y)]$. Then for most pairs $(x, y) \in (B_{\alpha''}(x_0) \setminus \Omega_\mathrm{b}) \times (B_{\alpha''}(y_0) \setminus \Omega_\mathrm{b})$ we have that $\operatorname{dist}(\nabla u, \mathrm{SO}(2)U_0)|_{\gamma_{xy}}$ is an $L^1(\gamma_{xy})$ function. Furthermore, there exists a constant $c = c(\theta, \alpha) > 0$ such that, for most pairs (x, y),

$$\int_{\gamma_{xy}} \operatorname{dist}(\nabla u, \mathrm{SO}(2)U_0) \, \mathrm{d}\mathcal{H}^1 \leqslant c\mu.$$

(v) There exists a constant $c = c(\theta, \alpha) > 0$ such that, for most pairs $(x, y) \in (B_{\alpha''}(x_0) \setminus \Omega_\mathrm{b}) \times (B_{\alpha''}(y_0) \setminus \Omega_\mathrm{b})$,

$$|u(x) - u(y)| \geqslant |U_0(x - y)| - c\mu.$$

The crucial point in the argument is the derivation of (i). As soon as this step is established, the remaining argument follows along the lines of [14].

In order to deduce (i), we argue in various steps. Firstly, following [14] and using (2.5), we observe that

$$\int_M \operatorname{dist}^2(\nabla u, \mathrm{SO}(2)U_0) \, \mathrm{d}x \leqslant C \sum_{(i,j) \in nM} \frac{1}{n^2} \phi_u^{ij} \leqslant C\eta.$$

Hence, the Friesecke–James–Müller rigidity theorem [19] implies that there exists $Q \in SO(2)$ such that

$$\int_M |\nabla u - QU_0|^2 \, \mathrm{d}x \leqslant C\eta.$$

Combined with Poincaré's inequality and setting $A = QU_0 x + b$, this leads to

$$\int_M |\nabla u - \nabla A|^2 + |u - A|^2 \, \mathrm{d}x \leqslant C\eta.$$

Thus, there exists a radius $\alpha' \in (7\alpha/4, 2\alpha)$ such that for $M' := \mathrm{int}\,\mathrm{conv}(B_{\alpha'}(x_0) \cup B_{\alpha'}(y_0))$ we have

$$\int_{\partial M'} |\nabla u - \nabla A|^2 + |u - A|^2 \, \mathrm{d}x \leqslant C\eta.$$

By the embedding of $W^{1,2}(\partial M') \to L^\infty(\partial M')$, we hence infer that

$$\|u - A\|_{L^\infty(\partial M')} \leqslant c\eta^{1/2}.$$

As in [14], this allows us to conclude that for $\alpha'' := 3\alpha/2$, $M'' := \mathrm{int}\,\mathrm{conv}(B_{\alpha''}(x_0) \cup B_{\alpha''}(y_0))$ and a sufficiently small choice of $\eta > 0$, the degree of

$$v_t(x) := tu(x) + (1-t)A(x)$$

is well defined in $A(M'')$ (as $v_t(\partial M') \cap A(M'') = \emptyset$). By homotopy invariance,

$$\deg(u, M', z) = 1 \quad \text{for all } z \in A(M''). \tag{2.16}$$

We note that M'' is open and, as A is affine, this is also true for $A(M'')$. Moreover, $\overline{B_\alpha(x_0) \cup B_\alpha(y_0)}$ is contained in M''. Hence, by the change of variables formula in terms of the degree and the multiplicity function, we have

$$\left.\begin{aligned}
\int_{\mathbb{R}^2} v(z)d(u, M', z) \, \mathrm{d}z &= \int_{M'} v \circ u(x) \det(\nabla u(x)) \, \mathrm{d}x, \\
\int_{\mathbb{R}^2} v(z)N(u, M', z) \, \mathrm{d}z &= \int_{M'} v \circ u(x) |\det(\nabla u(x))| \, \mathrm{d}x
\end{aligned}\right\} \tag{2.17}$$

for all $v \in L^\infty(\mathbb{R}^2)$. Thus, recalling that (by the non-interpenetration condition $u \in \mathcal{A}_n$) $\det(\nabla u) > 0$ almost everywhere in M and choosing functions $v \in L^\infty(\mathbb{R}^2)$ with $\mathrm{supp}(v) \subset A(M'') \setminus u(\Omega_b)$, we obtain

$$\int_{\mathbb{R}^2} v(z) \, \mathrm{d}z = \int_{\mathbb{R}^2} v(z)d(u, M', z) \, \mathrm{d}z = \int_{M'} v \circ u(x) \det(\nabla u(x)) \, \mathrm{d}x$$
$$= \int_{\mathbb{R}^2} v(z)N(u, M', z) \, \mathrm{d}z. \tag{2.18}$$

Therefore,

$$N(u, M', z) = 1 \quad \text{for almost all } z \in A(M'') \setminus u(\Omega_b).$$

This is the desired uniqueness of the preimage of z under u for *almost all* $z \in A(M'') \setminus u(\Omega_b)$. We now argue that this uniqueness statement can be extended to *all* $z \in A(M'') \setminus u(\Omega_b)$. Indeed, this is a consequence of the definition of Ω_b (which is a closed set), the fact that our function u is piecewise affine with a locally invertible

gradient, and the implicit function theorem. We argue by contradiction. Assume that there existed $z \in A(M'') \setminus u(\Omega_\mathrm{b})$ such that it had two preimages $y_1, y_2 \in M'$. By definition, $y_1, y_2 \notin \Omega_\mathrm{b}$. We argue that this already implies the existence of a set of positive measure in $A(M'') \setminus u(\Omega_\mathrm{b})$ on which the injectivity of u is violated, which cannot be the case by our almost everywhere invertibility result from above. To this end, we distinguish three different cases.

(a) We first assume that there exist grid triangles (which without loss of generality we take as '+' triangles) $\Delta_{ij}^{n;+}, \Delta_{kl}^{n;+} \subset M'$ such that $y_1 \in \mathrm{int}(\Delta_{ij}^{n;+})$, $y_2 \in \mathrm{int}(\Delta_{kl}^{n;+})$. By the definition of Ω_b as the *closure* of the 'bad set' and by the piecewise affine definition of u, this yields that also $\Delta_{ij}^{n;+}, \Delta_{kl}^{n;+} \subset M' \setminus \Omega_\mathrm{b}$. Since ∇u is an affine function on each of the triangles, and as $\det(\nabla u) \neq 0$ on these, the implicit function theorem immediately yields that there exist whole neighbourhoods U_1, U_2 of y_1, y_2 such that $u(U_1) = u(U_2)$. In particular, using the openness of $A(M'')$, we would obtain a set $V \subset A(M'') \setminus u(\Omega_\mathrm{b})$ of non-zero measure such that for all $z \in V$ the preimage under u is not unique. This yields a contradiction.

(b) We now suppose that $y_1 \in \Delta_{ij}^{n;+} \cap M'$, $y_2 \in \Delta_{kl}^{n;+} \cap M'$ are such that at least one of the points y_1 or y_2 lies on $\partial\Delta_{ij}^{n;+}$ or $\partial\Delta_{kl}^{n;+}$, but neither of them is a vertex of the underlying grid. In this case we cannot directly argue via the implicit function theorem as our function is only Lipschitz regular. However, assuming that, for instance, the point y_1 lies at the interface between two grid triangles $\Delta_{rs}^{n;\pm}$ and $\Delta_{ij}^{n;\pm}$ (the superscript $\pm$ that is used here indicates that we do not make an assumption in which of the two grid triangles this may be the case), we can invoke the implicit function theorem in each of the triangles (using the invertibility of the gradient on each of the triangles) to obtain two neighbourhoods

$$\tilde{U}_1 \subset \Delta_{rs}^{n;\pm} \cap M', \qquad \tilde{U}_2 \subset \Delta_{ij}^{n;\pm} \cap M'$$

(for which we use the openness of M') whose closures intersect along a line containing y_1. In order to avoid a contradiction to the almost everywhere invertibility already at this point, u has to be one to one on $U_1 := \tilde{U}_1 \cup \tilde{U}_2$. In particular, u maps U_1 onto a full neighbourhood of $z := u(y_1)$. But arguing similarly for y_2 and using the openness of $A(M'')$ we again obtain a set $V \subset A(M'') \setminus u(\Omega_\mathrm{b})$ of non-zero measure such that u does not have a unique preimage.

(c) Finally, we have to cover the case in which at least one of the points y_1 or y_2 is a vertex of (at least) one of the triangles $\Delta_{ij}^{n;+}$ or $\Delta_{kl}^{n;+}$. However, similarly to above we can again construct full neighbourhoods of y_1 and y_2 on which injectivity is violated, which yields a contradiction.

Hence, we indeed conclude that for all $z \in A(M'') \setminus u(\Omega_\mathrm{b})$ there is a unique preimage $x \in M'$.

We now proceed with the remaining points (ii)–(v). Thanks to (i), this follows along the lines of the argument of Conti and Schweizer [14].

Recalling the definition of Ω_{bi} from (ii), we estimate

$$|\Omega_{bi}| \leqslant |M' \cap \Omega_{\mathrm{b}}| + \int_{M' \setminus \Omega_{\mathrm{b}}} \chi_{\Omega_{bi}} \, \mathrm{d}x$$

$$\leqslant |\Omega_b| + 2 \int_{u(\Omega_{\mathrm{b}}) \cap A(M'')} \#(u^{-1}(z) \cap \Omega' \setminus \Omega_b) \, \mathrm{d}z$$

$$\leqslant C\eta + 2 \int_{u(\Omega_{\mathrm{b}}) \cap A(M'')} \#(u^{-1}(z) \cap \Omega' \setminus \Omega_b) \, \mathrm{d}z.$$

Here we used the closeness of ∇u to $\mathrm{SO}(2)U_0$ away from Ω_{b}. Due to (2.17), for almost every $z \in \Omega_{\mathrm{b}} \cap A(M'')$,

$$\#(u^{-1}(z) \cap M' \setminus \Omega_{\mathrm{b}}) \leqslant 1 + \#(u^{-1}(z) \cap M' \cap \Omega_{\mathrm{b}}).$$

Moreover, the coarea formula, (2.11) and the estimate for the determinant in terms of ϕ_u^{ij} give

$$\int_{u(\Omega_{\mathrm{b}})} \#(u^{-1}(z) \cap \Omega_b) \, \mathrm{d}x = \int_{\Omega_{\mathrm{b}}} |\det(\nabla u)| \, \mathrm{d}x \leqslant C\eta.$$

This yields the claim.

By (ii), for most choices of $(x, y) \in M' \times M'$ we have that $u(x), u(y) \notin u(\Omega_{\mathrm{b}})$. By a similar projection argument to that of step 2, we hence obtain that $[u(x), u(y)] \cap u(\partial\Omega_b) = \emptyset$ for most pairs (x, y). Indeed, to this end, for $z \in \{x_0, y_0\}$ we consider the sets

$$\tilde{B}_{\alpha'}(z) := \left\{ x \in B_{\alpha'}(z) \setminus (\Omega_{\mathrm{b}} \cup \Omega_{bi}) \colon |u(x) - A(x)| \leqslant \frac{\alpha}{4} \right\}.$$

Then, by the size estimates for Ω_{b} and Ω_{bi} (i.e. by (2.9) and claim (ii) in step 3), this still covers nearly the original volume of $B_{\alpha'}(z)$, $i \in \{1, 2\}$, $z \in \{x_0, y_0\}$, if η (as a function of θ) is chosen sufficiently small. Reasoning by a projection argument once more, we consider the lines $t \mapsto \xi + t\nu$ for ν such that $|\nu - (\nabla A)\nu_0| \leqslant 3\alpha$. Considering the set

$$\tilde{A}_\nu := \{\xi \in u(\tilde{B}_{\alpha'}(x_0)) \colon x + t\nu \text{ intersects } u(\partial\Omega_b)\},$$

and using estimate (2.10), we obtain claim (iii)(a). Part (b) now immediately follows from part (a): to this end, we note that for all $x \in \tilde{B}_\alpha(z)$, $z \in \{x_0, y_0\}$, by definition $u(x) \in u(B_{\alpha'}(x_0) \setminus (\Omega_{\mathrm{b}} \cup \Omega_{bi}))$. This then allows us to invoke part (a). Moreover, the claim of (c) follows directly from (b) and the invertibility of u for all $z \in A(M'') \setminus u(\Omega_{\mathrm{b}})$.

The argument for (iv) follows along the lines of [14] and is very similar to step 2(i). We have to, however, establish that for most pairs (x, y) the restrictions of ∇u onto the line segments γ_{xy} are well defined as $L^1(\gamma_{xy})$ functions. Indeed, the well-definedness of the restriction follows from the claim that for most pairs (x, y) the piecewise affine curve γ_{xy} does not contain line segments of $G^n(\Omega)$. To this end, we observe that $u(G^n) := \bigcup_{[z_1, z_2] \in G^n(\Omega)} [u(z_1), u(z_2)]$ forms a zero set in $u(\tilde{B}_{\alpha'}(x_0)) \times u(\tilde{B}_{\alpha'}(y_0))$. Furthermore, γ_{xy} can only contain a line segment in G^n if there exists a line segment $[u(x_1), u(x_2)] \subset [u(x), u(y)]$ with $[u(x_1), u(x_2)] \subset u(G^n)$. But $u(G^n)$ is a zero set, and thus for almost all pairs (x, y) this does not happen.

Last but not least, we observe that, by the monotonicity of u along the curve γ_{xy} and the fact that for most curves γ_{xy} the restriction $\nabla u|_{\gamma_{xy}}$ is a well-defined $L^1(\gamma_{xy})$ function, we have

$$|u(x) - u(y)| = \int_{\gamma_{xy}} |\nabla_\tau u| \, d\mathcal{H}^1 \geqslant \mathcal{H}^1(U_0\gamma_{xy}) - \int_{\gamma_{xy}} \operatorname{dist}(\nabla u, \mathrm{SO}(2)U_0) \, d\mathcal{H}^1$$

$$\geqslant |U_0(x-y)| - c\mu.$$

As before, the requirement that this holds for most pairs $(x, y) \in B_\alpha(x_0) \times B_\alpha(y_0)$ leads to a θ dependence of the constant $c = c(\alpha, \theta) > 0$. This concludes the proof of proposition 2.4. $\qquad \square$

3. Surface energies

In this section we investigate the emergence and form of surface energies. After introducing the limiting surface energies in § 3.1 we deduce some fundamental properties of these in § 3.2 and finally prove the desired Γ-limit in § 3.3.

3.1. Setting

In the context of deformations on Ω that are in the surface energy scaling regime (1.17), we define

$$H_n^1(u_n) := nH_n(u_n).$$

Due to its scaling, we interpret it as a surface energy. Before formulating our main result on the limiting structure of $H_n^1(u_n)$ as $n \to \infty$, we introduce the central objects of this section. We start by defining the *limiting profiles*.

DEFINITION 3.1 (limiting profiles). Let $V \in \{U_0, QU_1\}$ and $V_1, V_2 \in \mathrm{SO}(2)U_0 \cup \mathrm{SO}(2)U_1$ be two rank-one connected matrices. Let $F_\lambda := \lambda U_0 + (1-\lambda)QU_1$ be as in (1.6). Then we define the *limiting profiles* as

$$v_{F_\lambda, V}(x) := \begin{cases} F_\lambda x & \text{for } x \cdot (1,1) \leqslant 0, \\ Vx & \text{for } x \cdot (1,1) > 0, \end{cases}$$

$$v_{V, F_\lambda}(x) := \begin{cases} F_\lambda x & \text{for } x \cdot (1,1) \geqslant 0, \\ Vx & \text{for } x \cdot (1,1) < 0, \end{cases}$$

$$v_{V_1, V_2}^{\pm}(x) := \begin{cases} V_1 x & \text{for } x \cdot (\pm 1, 1) \leqslant 0, \\ V_2 x & \text{for } x \cdot (\pm 1, 1) > 0. \end{cases}$$

With this to hand, we introduce the following boundary and internal layer energies.

DEFINITION 3.2 (boundary and internal layer energies). Let $V \in \{U_0, QU_1\}$ and $V_1, V_2 \in K$ be two rank-one connected matrices. Let F_λ be as in (1.6). Then we define the *left boundary layer energy* $B_+(F_\lambda, V)$, the *internal layer energies*

$C_\pm(V_1, V_2)$, and the *right boundary layer energy* $B_-(F_\lambda, V)$ as

$$
\begin{aligned}
B_+(F_\lambda, V) &:= \inf\Bigg\{ \liminf_{n\to\infty} \sum_{(i,j)\in n\Omega} \frac{1}{n} h_{v_n}^{i,j} : v_n \in \mathcal{A}_{n\Omega},\ v_n \to v_{F_\lambda, V} \text{ in } L^1(\Omega), \\
&\qquad\qquad\qquad v_n(i/n, j/n) = F_\lambda(i/n, j/n) \text{ for } i+j \leqslant -4n \Bigg\}, \\
B_-(V, F_\lambda) &:= \inf\Bigg\{ \liminf_{n\to\infty} \sum_{(i,j)\in n\Omega} \frac{1}{n} h_{v_n}^{i,j} : v_n \in \mathcal{A}_{n\Omega},\ v_n \to v_{V, F_\lambda} \text{ in } L^1(\Omega), \\
&\qquad\qquad\qquad v_n(i/n, j/n) = F_\lambda(i/n, j/n) \text{ for } i+j \geqslant 4n \Bigg\}, \\
C_\pm(V_1, V_2) &:= \inf\Bigg\{ \liminf_{n\to\infty} \sum_{(i,j)\in n\Omega_{4,1}^\pm} \frac{1}{n} h_{v_n}^{i,j} : v_n \in \mathcal{A}_{n\Omega_{4,1}^\pm}, \\
&\qquad\qquad\qquad v_n \to v_{V_1, V_2}^\pm \text{ in } L^1(\Omega_{4,1}^\pm) \Bigg\},
\end{aligned}
\tag{3.1}
$$

where the domains Ω, $\Omega_{l,d}^\pm$ and the sets $\mathcal{A}_{n\Omega_{4,1}^\pm}$ are as in definition 1.1.

We show that in the sense of Γ-limits we can identify the energy H_n^1 with an energy that is concentrated on the jump surfaces of a limiting configuration u_0. We recall that the limiting deformations that arise from passing to the limit $n \to \infty$ of discrete deformations in the surface energy scaling regime (1.17) are *rigid* (see remark 2.6). More precisely, they satisfy the structure result of proposition 2.3 and are hence locally simple laminates. Using this, we give the following definitions.

DEFINITION 3.3 (limiting energy). Let u_0 be a piecewise affine function with gradient $\nabla u_0 \in \mathrm{SO}(2)U_0 \cup \mathrm{SO}(2)U_1$. Suppose that it satisfies the boundary conditions (1.10) and that it has finitely many jump interfaces that pass through the points $(x_l, 0)$, with $l \in \{0, \dots, L-1\}$ for $L \in \mathbb{N}$. Let the boundary and internal layers be as in definition 3.2. Then we set

$$
\begin{aligned}
\bar{E}_{\mathrm{surf}}(u_0) &:= B_+(F_\lambda, \nabla u_0(x_0-, 0)) + \sum_{i=1}^{L-1} C_\pm(\nabla u_0(x_i-, 0), \nabla u_0(x_{i+1}-, 0)) \\
&\quad + B_-(\nabla u_0(x_{(L-1)}-, 0), F_\lambda) \\
&=: \int_{J_{\nabla u_0}} \bar{C}(\nabla u_0(x-, 0), \nabla u_0(x+, 0))\, \mathrm{d}\mathcal{H}^1,
\end{aligned}
\tag{3.2}
$$

where $J_{\nabla u_0}$ denotes the *jump set* of ∇u_0,

$$
u_0(x-) := \lim_{\substack{y=(y_1, y_2)\to x=(x_1, x_2), \\ y_1 \leqslant x_1}} u_0(y),
$$

and, depending on the position and orientation of the jump plane and the values of ∇u_0 at $x \in J_{\nabla u_0}$, the density $\bar{C}(\cdot, \cdot)$ satisfies $\sqrt{2}\bar{C}(\cdot) \in \{B_+(\cdot, \cdot), B_-(\cdot, \cdot), C_\pm(\cdot, \cdot)\}$.

With these notions to hand, we can finally formulate our main result regarding surface energies.

THEOREM 3.4 (surface energies). *With respect to the $L^1(\Omega)$ topology we have that*

$$H_n^1 \overset{\Gamma}{\to} E_{\mathrm{surf}},$$

where

$$E_{\mathrm{surf}}(u) := \begin{cases} \bar{E}_{\mathrm{surf}}(u) & \textit{if } \nabla u(x) = F_\lambda \textit{ for } x_1 + x_2 \leqslant -4, \ |x_2| \leqslant 1, \\ & \nabla u(x) = F_\lambda \textit{ for } x_1 + x_2 \geqslant 4, \ |x_2| \leqslant 1, \\ & \textit{with } \nabla u \in \{U_0, QU_1\} \textit{ and } \nabla u \in \mathrm{BV}_{\mathrm{loc}}(\mathbb{R} \times [-1,1]); \\ \infty & \textit{otherwise.} \end{cases}$$

Here $\bar{E}_{\mathrm{surf}}(u)$ is as in definition 3.3.

Similarly to in [9, 15, 20], the proof of theorem 3.4 is based on a combination of the rigidity result of proposition 2.4 together with a special cutting procedure. Heading for this, we begin by recalling some properties of the energy in §3.2 and then carry out the proof of the Γ-limit in §3.3.

3.2. Properties of the energy and auxiliary results

Before addressing the proof of theorem 3.4, we discuss central properties of the energy and derive auxiliary results. We begin by considering the energy densities from (3.1). For notational convenience we limit ourselves to the case of interior layer energies; the situation for boundary energies is analogous. We start by introducing restricted versions of the internal layer energies from definition 3.2.

DEFINITION 3.5. Let $m_1, m_2 \in \mathbb{R} \setminus \{0\}$ and let $V_1, V_2 \in K$ be two rank-one connected matrices. Then we set

$$C_\pm(V_1, V_2, m_1, m_2) := \inf \left\{ \liminf_{n \to \infty} \sum_{(i,j) \in n\Omega_{m_1,m_2}^\pm} \frac{1}{n} h_{v_n}^{i,j} \colon v_n \in \mathcal{A}_{n\Omega_{m_1,m_2}^\pm}, \right.$$
$$\left. v_n \to v_{V_1,V_2}^\pm \text{ in } L^1(\Omega_{m_1,m_2}^\pm) \right\}. \quad (3.3)$$

Analogous definitions hold for the boundary layer energies. We claim that the energies $C_\pm(V_1, V_2, m_1, m_2)$ do not depend on the dimension m_1 and are linear in the m_2 dimension.

LEMMA 3.6. *Let $m_1, m_2 \in \mathbb{R} \setminus \{0\}$ and let either $V_1 = U_0$, $V_2 = QU_1$ or $V_1 = QU_1$, $V_2 = U_0$, with the matrix Q from (1.5). Let $C_\pm(V_1, V_2, m_1, m_2)$ be as in definition 3.2. Then there exist constants $C_\pm$ depending only on the normals $(\pm 1, 1)$ such that*

$$C_\pm(V_1, V_2, m_1, m_2) = C_\pm(V_1, V_2, 1, 1)m_2 = C_\pm m_2. \quad (3.4)$$

Proof. The proof follows from averaging and scaling as in [15, lemma 3.2] (due to our discrete set-up, however, we make small errors for each fixed $n \in \mathbb{N}$, which vanish in the limit $n \to \infty$). We only present the argument for $C_-(V_1, V_2, m_1, m_2)$ (the one for $C_+(V_1, V_2, m_1, m_2)$ is analogous) and only argue that $C_-(V_1, V_2, m_1, m_2)$ is independent of m_1, the other dependencies being more direct. We begin by noticing

that, by definition, $C_-(V_1, V_2, m_1, m_2)$ is an increasing function in m_1. We claim that, moreover,

$$C_-(V_1, V_2, \alpha m_1, \alpha m_2) = \alpha C_-(V_1, V_2, m_1, m_2).$$

Indeed, assuming that n is sufficiently large and setting $\bar{n} := [\alpha n]$, we have

$$\sum_{(i,j) \in n\Omega_{\alpha m_1, \alpha m_2}^-} \frac{1}{n} h_{v_n}^{ij} = \alpha \sum_{(i,j) \in n\Omega_{m_1\alpha, m_2\alpha}^-} \frac{1}{\alpha n} h_{v_n}^{ij}$$

$$= \alpha \sum_{(i,j) \in \bar{n}\Omega_{m_1, m_2}^-} \frac{1}{\bar{n}} h_{u_{\bar{n}}}^{ij} + O\left(\frac{1}{\bar{n}}\right),$$

where $u_{\bar{n}}(i,j) := (1/\alpha)v_{\bar{n}}(\alpha i, \alpha j)$. Fixing α and taking the $\liminf$ as $n \to \infty$ yields the claim.

Next, we show that

$$C_-\left(V_1, V_2, m_1, \frac{m_2}{m}\right) \leqslant \frac{1}{m} C_-(V_1, V_2, m_1, m_2).$$

This follows from averaging and translating. More precisely, we have

$$\sum_{k=0}^{m-1} \left(\sum_{(i,j) \in n\Omega_{m_1, m_2/m}^-} \frac{1}{n} h_{v_n^k}^{ij} \right) = \sum_{(i,j) \in n\Omega_{m_1, m_2}^-} \frac{1}{n} h_{v_n^{ij}} + O\left(\frac{m}{n}\right),$$

where

$$(v_n^k)^{ij} := v_n(i/n + km/n, j/n + km/n).$$

Therefore, there exists $k_0 \in \{0, \ldots, m-1\}$ such that

$$\sum_{(i,j) \in n\Omega_{m_1, m_2/m}^-} \frac{1}{n} h_{v_n^k}^{ij} = \frac{1}{m} \sum_{(i,j) \in n\Omega_{m_1, m_2}^-} \frac{1}{n} h_{v_n^{ij}} + O\left(\frac{m}{n}\right).$$

Again the claim follows by taking the $\liminf$ as $n \to \infty$. Hence, for all $m \in \mathbb{R} \setminus \{0\}$, we deduce that

$$\frac{1}{m} C_-(V_1, V_2, m_1, m_2) = C_-\left(V_1, V_2, \frac{m_1}{m}, \frac{m_2}{m}\right) \leqslant C_-\left(V_1, V_2, m_1, \frac{m_2}{m}\right)$$

$$\leqslant \frac{1}{m} C_-(V_1, V_2, m_1, m_2). \quad (3.5)$$

Here the first inequality follows from monotonicity in m_1 and the second one from averaging. Thus, equality holds in all estimates in (3.5). In particular, for all $m \in \mathbb{R} \setminus \{0\}$,

$$C_-\left(V_1, V_2, \frac{m_1}{m}, m_2\right) = C_-(V_1, V_2, m_1, m_2),$$

which yields the independence of $C_-(V_1, V_2, m_1, m_2)$ of m_1. $\qquad \square$

As a consequence, the limiting energies only depend on the corresponding normal direction to the interface by means of the constants $C_\pm$, but *do not* depend on the extension m_1 of the domain in the direction $(\pm 1, 1)$. Similar to proposition 2.3, this already partially confirms the expectation that the continuum energy will be a 'line energy'. Hence, after a normalization step, it is always possible to assume that the given layer energy is defined in a unit parallelogram. Relying on proposition 2.4 from the previous section, we also obtain the following *vertical cutting mechanism*.

PROPOSITION 3.7 (vertical cutting). *Let $d, l > 0$ and let $u_n \in \mathcal{A}_{n\Omega_{2d,2l}^-}$ be piecewise affine on the grid Ω_n. Suppose that*

$$\sum_{(i,j) \in n\Omega_{2d,2l}^-} \frac{1}{n^2}(\phi_{u_n}^{ij} + |\nabla_n \phi_{u_n}^{i,j}|) \leqslant \eta < \infty, \tag{3.6}$$

where $\phi \in C^{0,1}((\mathbb{R}^2)^4, \mathbb{R})$ and

$$\phi_{u_n}^{ij} := \phi(\partial_1 u_n^{ij}, \partial_2 u_n^{ij}, \partial_1 u_n^{i-1,j}, \partial_2 u_n^{i-1,j})$$

denotes a one-well energy function with well given by one of the sets $\mathrm{SO}(2)U_i$, $i = 1, 2$, and with quadratic growth, i.e.

$$c_1 \operatorname{dist}^2(\nabla u_n^{ij}, \mathrm{SO}(2)U_i) \leqslant \phi_{u_n}^{ij} \leqslant c_2 \operatorname{dist}^2(\nabla u_n^{ij}, \mathrm{SO}(2)U_i). \tag{3.7}$$

Then there exist a constant $C > 0$ and a modified deformation $\tilde{u}_n \in \mathcal{A}_{n\Omega_{2d,l/2}^-}$ such that along a subsequence

(a) $H_n(\tilde{u}_n^{i,j}) \leqslant C H_n(u_n^{i,j})$ *for $(i,j) \in n\Omega_{2d,l/2}^-$,*

(b) *for $x \in \Omega_{2d,l/2}^-$ it holds that*

$$\nabla \tilde{u}_n(x) = U_0 \qquad \text{for } x \cdot \begin{pmatrix} -1 \\ 1 \end{pmatrix} \geqslant \tfrac{3}{8}nd$$

and

$$\tilde{u}_n(x) = u_n(x) \quad \text{for } x \cdot \begin{pmatrix} -1 \\ 1 \end{pmatrix} \leqslant \tfrac{1}{4}nd.$$

REMARK 3.8. The previous 'cutting result' will play a major role in our Γ-convergence proof (in the construction of the recovery sequence). We emphasize that for our proof it is necessary to pass from the larger domain $\Omega_{2d,2l}$ to the smaller set $\Omega_{2d,l/2}$ in the formulation of proposition 3.7. However, this does not pose difficulties in the proof of the Γ-convergence result, as we can exploit the scaling behaviour of the boundary and layer energies, which was formulated in lemma 3.6.

Proof. The proof of the cutting lemma follows along the lines of [15, proposition 5.2] and [13]. During the procedure in which we modify u_n to $\tilde{u}_n$, however, we have to ensure admissibility. This corresponds to two requirements: firstly, we have to preserve impenetrability; secondly we also have to make sure that the final function $\tilde{u}_n$ is still defined on the original lattice $(\Omega_n, \Delta_{i,j}^{n,\pm})$.

STEP 1 (energy estimates). There exist many values of $c_0 \in [\frac{1}{4}n, \frac{3}{8}n] \cap \mathbb{Z}$ such that, for all $\delta \in (0,1)$,

$$\frac{1}{\delta} \sum_{\substack{(i,j) \in n\Omega^-_{2d,2l}, \\ c_0 - [\delta n] \leqslant i-j \leqslant c_0}} \frac{1}{n^2}(\phi^{i,j}_{u_n} + |\nabla_n \phi^{i,j}_{u_n}|) \leqslant c\eta.$$

This follows by a covering argument as in [15].

STEP 2 (construction of the reference grid G^n_{R}). The construction of the grid G^n_{R} is similar to in [15] but with respect to the direction $(1,-1)$. It refines dyadically with vertical distances that we denote by h_k. However, instead of refining up to *infinite* order, we limit ourselves to *finite* scales such that h_k is larger than or equal to $1/n$. We denote the finest scale by $h^n_{k_0}$ and assume that $h^n_{k_0} \in [1/n, 100/n]$.

More precisely, we define $l_1 := 2\sqrt{2}[l]$ and $h_1 := [2d]$. Furthermore, we then set $l_k := 2^{-k}l_1$ and $h_k := 2^{-k}h_1$ as long as $h_k \geqslant h^n_{k_0}$ and stop the refining procedure after that. Then we divide the line segment in $\Omega^-_{2d,2l}$ with coordinates $i_k - j_k := c_0 - [h_k n]$ into intervals of equal size that are arranged symmetrically with respect to the line $j = 0$. The boundaries of the intervals constitute the vertices of the grid G^n_{R}. The grid is formed by connecting the vertices along neighbouring lines. We remark that the degeneracy of the triangles depends on the ratio l/d.

STEP 3 (energy scaling). In this step we prove the optimal scaling of the energy in the respective triangles. This follows from the discrete analogue of the arguments in [15]. We apply step 1 with $\delta = h_k$:

$$\sum_{\substack{(i,j) \in n\Omega^-_{2d,2l}, \\ c_0 - [h_k n] \leqslant i-j \leqslant c_0}} \frac{1}{n^2}(\phi^{i,j}_{u_n} + |\nabla_n \phi^{i,j}_{u_n}|) \leqslant c\eta h_k. \tag{3.8}$$

Therefore, there exists a parameter $c_k \in [c_0 - [h_k n], c_0] \cap \mathbb{Z}$ such that

$$\sum_{\substack{(i,j) \in n\Omega^-_{2d,2l}, \\ i-j=c_k}} \frac{1}{n}(\phi^{i,j}_{u_n} + |\nabla_n \phi^{i,j}_{u_n}|) \leqslant c\eta.$$

From the previous two estimates we infer that the following hold.

(a) We have

$$\sum_{\substack{(i,j) \in n\Omega^-_{2d,2l}, \\ i-j=c_k}} \frac{1}{n}|\nabla_n \phi^{i,j}_{u_n}| \leqslant c\eta.$$

Spelling this out and considering the diagonal derivatives, we in particular obtain

$$\sum_{\substack{(i,j) \in n\Omega^-_{2d,2l}, \\ i-j=c_k}} |\phi^{i+1,j}_{u_n} - \phi^{i,j}_{u_n}| \leqslant c\eta.$$

(b) There exists $j_k \in [-n, n] \cap \mathbb{Z}$ such that for the point $(i_k, j_k) \in n\Omega_{2d,2l}^-$ with $i_k - j_k = c_k$ it holds that

$$\phi_{u_n}^{i_k, j_k} \leqslant c\eta.$$

Thus, combining these two points by writing out a telescope sum, we observe that, on $i - j = c_k$,

$$|\phi_{u_n}^{i,j} - \phi_{u_n}^{i_k, j_k}| \leqslant \sum_{\substack{(i,j) \in n\Omega_{2d,2l}^-, \\ i-j=c_k}} |\phi_{u_n}^{i+1,j} - \phi_{u_n}^{i,j}| \leqslant c\eta.$$

Due to the bound on $\phi_{u_n}^{i_k, j_k}$ from (b), this implies an L^∞ estimate along the whole strip $i - j = c_k$, $|j| \leqslant n$:

$$|\phi_{u_n}^{i,j}| \leqslant c\eta. \tag{3.9}$$

Defining $S_c := \{(i,j) \mid c_0 - [h_k n] \leqslant i - j \leqslant c_0, \ [d] \leqslant i + j \leqslant [d] + [h_k n]\}$ for any $d \in \{-n, \ldots, n - [h_k n]\}$ and invoking Poincaré's inequality in combination with (3.8) and (3.9) then yields

$$\sum_{(i,j) \in S_c} \frac{1}{n^2} \phi_{u_n}^{i,j} \leqslant 2 \left(h_k^2 \max_{\substack{(i,j) \in n\Omega_{2d,2l}^-, \\ i-j=c_k, |j| \leqslant n}} |\phi_{u_n}^{i,j}| + h_k \sum_{(i,j) \in S_c} \frac{1}{n^2} |\nabla_n \phi_{u_n}^{i,j}| \right) \leqslant c\eta h_k^2. \tag{3.10}$$

STEP 4 (construction of $\tilde{u}_n$).

(a) *Construction of the perturbed grid G_{P}^n.* This follows in the same way as in [15]. As in the construction of the reference grid, however, we only refine up to $h_k \sim n^{-1}$, and recall that this finest scale is denoted by $h_{k_0}^n$.

We recall the precise construction from [15]. Here the perturbed grid G_{P}^n is obtained from the grid G_{R}^n by perturbations along rigid directions. We seek to apply proposition 2.4 so that all the resulting new grid edges are rigid (see remark 2.6). In order to remain within $\Omega_{2d,2l}^-$, in this procedure we restrict our construction to the subgrid that is fully contained in $\Omega_{2d,l}^-$. We begin by defining $\alpha = \frac{1}{10} c(d, l)$, where $c(d, l) > 0$ should be thought of as a small constant dealing with the degeneracy of the grid. Then we enumerate the grid vertices of G_{R}^n and denote them by v_m. We apply proposition 2.4 in a ball $B_m := B_{\alpha h_k}(v_m)$, where v_m is a vertex on the layer $i_k - j_k = c_0 - [n h_k]$. Then for two neighbouring balls $B_m, B_{m'}$ there are many rigid points $(w_m, w_{m'})$ according to proposition 2.4. Following [15], we now describe our choice of the new grid vertices by iteratively defining *possible choices at step m*.

- *Possible choices at step 0.* These are all $w_m \in B_m$.

- *Possible choices at step m.* These are all points $w_m \in B_m$ such that w_m forms a rigid pair with many points of all neighbouring balls.

- *Possible choices at step $m + 1$.* These are all possible choices from step m without those points $w \in B_{m'}$ with $m' > m$ such that $v_{m'}$ is a neighbour of the v_m but (w, w_m) is not rigid.

As in [15], we claim that this algorithm works (i.e. the set of possible choices in step m always forms a set of positive measure) and yields a new set of vertices that defines our new grid G_{P}^n. We give a proof for this in appendix D (see lemma D.1).

As in [15], interpolation on the resulting triangles leads to a new piecewise affine grid function v on the new grid G_{P}^n. Furthermore, as in [14], proposition 2.4 and the bound (3.10) further yield estimates of type

$$\left. \begin{aligned} |\nabla v(T_m) - Q_m U_0| &\leqslant C \frac{1}{h_k} \|\operatorname{dist}(\nabla u, K)\|_{L^2(T_m)}, \\ |\nabla v(T_m) - Q_m U_0| &\leqslant C \sqrt{\eta} \end{aligned} \right\} \tag{3.11}$$

for some rotation Q_m associated with each triangle T_m of the grid G_{P}^n (which is spanned by neighbouring vertices). Here we used (3.10) and (3.7) to obtain the second estimate in (3.11) from the first one. The notation $\nabla v(T_m)$ refers to the gradient of v in the interior of the triangle T_m (we recall that v is a piecewise affine function on the perturbed grid G_{P}^n). Furthermore, the facts that two neighbouring triangles T_m, T_m' of G_{P}^n share a common edge and that on both triangles ∇v has a controlled distance to the wells in K (see (3.11)) imply that

$$\left. \begin{aligned} |\nabla v(T_m) - \nabla v(T_m')| &\leqslant C \frac{1}{h_k} \|\operatorname{dist}(\nabla u, K)\|_{L^2(T_m)}, \\ |Q_m' U_0 - Q_m U_0| &\leqslant C \frac{1}{h_k} \|\operatorname{dist}(\nabla u, K)\|_{L^2(T_m)}. \end{aligned} \right\} \tag{3.12}$$

We now modify v into a function $\tilde{v}_n$ on the original discrete grid Ω_n. To this end, we define $\tilde{v}_n$ as the interpolation of v with respect to the grid Ω_n (for most of the triangles, the interpolated gradient $\nabla \tilde{v}_n$ will equal the original gradient ∇v as the triangles in G_{P}^n are in general much larger than those in Ω_n, due to the choice $h_{k_0}^n \sim n^{-1}$ and as v is affine on these). This yields a function that is defined on

$$\Omega_{2d,l/2} \cap \operatorname{conv}\{(i/n, j/n) \colon i - j \leqslant c_0 - [n h_{k_0}^n]\}.$$

In the interpolation process we obtain new error terms at the interfaces of two triangles in G_{P}^n, since the grid G_{P}^n does not match the original grid Ω_n. However, for these new interpolations we note that $\nabla \tilde{v}(\Delta_{ij}^{n,\pm}) \in \operatorname{conv}_{l \in \{1,\ldots,m\}}(\nabla v(T_l))$, where the index l denotes all the involved neighbouring triangles in G_{P}^n (in particular, the maximal number of involved triangles m is independent of n). But due to (3.12) this error is controlled. For example, in the case in which $\nabla \tilde{v}_n(\Delta_{ij}^{n,+}) = \lambda \nabla v(T_m) + (1-\lambda) \nabla v(T_m')$ we have

$$\int_{\Delta_{ij}^{n,+}} |\nabla \tilde{v}_n(\Delta_{ij}^{n,+}) - \lambda Q_m U_0 - (1-\lambda) Q_m' U_0|^2 \, \mathrm{d}x$$

$$\leqslant 4 \left(\int_{T_m} |\nabla v(T_m) - \lambda Q_m U_0|^2 \, \mathrm{d}x + \int_{T_m'} |\nabla v(T_m') - Q_m' U_0|^2 \, \mathrm{d}x \right)$$

$$\leqslant C \|\operatorname{dist}(\nabla u, K)\|_{L^2(T_m)}^2 + C \|\operatorname{dist}(\nabla u, K)\|_{L^2(T_m')}^2,$$

where we have used (3.11). Summing over all triangles hence yields that

$$H_n(\tilde{v}_n) \leqslant C H_n(u_n).$$

Moreover, due to the second estimate in (3.11), we note that v and similarly $\tilde{v}_n$ satisfy the non-interpenetration condition.

(b) *Estimates on the original grid Ω_n close to the line $i - j = c_0$.* We estimate the contributions of ∇u on the original grid Ω_n in the domain given by $\Omega' := \{(i,j): |j| \leqslant n, \ c_0 - [10h_{k_0}^n n] \leqslant i - j \leqslant c_0\}$. In contrast to the argument in the previous steps, we do not construct a perturbed grid but seek to obtain estimates on the closeness of ∇u_n^{ij} to $\mathrm{SO}(2)U_0$ on each individual grid triangle $\Delta_{ij}^{n,\pm}$. For this we use the one-well rigidity theorem of [19] together with (3.8). In particular, on the scale $h_k \sim n^{-1}$ these immediately yield pointwise bounds and we infer that

$$|\phi_{u_n}^{i,j}| \leqslant c\eta \quad \text{on each triangle } \Delta_{ij}^{n,\pm} \subset \Omega'. \tag{3.13}$$

Therefore, there exist rotations Q_{ij} with

$$\left.\begin{aligned}
|\nabla u_n(\Delta_{ij}^{n,\pm}) - Q_{ij}U_0| &\leqslant C\sqrt{\eta} \quad \text{for all triangles } \Delta_{ij}^{n,\pm} \subset \Omega', \\
|Q_{kl}U_0 - Q_{ij}U_0| &\leqslant C\sqrt{\eta} \quad \text{for neighbouring triangles } \Delta_{ij}^{n,\pm}, \Delta_{kl}^{n,\pm} \subset \Omega', \\
\sum_{(i,j)\in n\Omega'} \frac{1}{n^2} h_{u_n}^{ij} &\leqslant C \int_{\Omega'} \mathrm{dist}(\nabla u, K)^2 \, \mathrm{d}x,
\end{aligned}\right\} \tag{3.14}$$

where the last line follows from the one-well rigidity result, the observation that $\mathrm{dist}(\nabla u, \mathrm{SO}(2)U_0) \leqslant \mathrm{dist}(\nabla u, K)$ on $\Delta_{ij}^{n,\pm} \subset \Omega'$, and the two-growth behaviour of $h_{u_n}^{ij}$ close to the energy wells.

(c) *Construction of the interpolation function.* Using the estimate from steps (a) and (b), we now construct an interpolation function $w_n: \Omega_{2d,l/2}^- \to \mathbb{R}^2$ between u_n and $\tilde{v}_n$,

$$w_n(x) := \gamma(nx)u_n(x) + (1 - \gamma)(nx)\tilde{v}_n(x),$$

where γ is a smooth function with $\gamma(z) = 1$ for $z_1 - z_2 \in [c_0/n - [2h_{k_0}^n n]/n, c_0/n]$, $\gamma(z) = 0$ for $z_1 - z_2 \leqslant c_0/n - [9h_{k_0}^n n]/n$. Here, for completeness, u_n and $\tilde{v}_n$ are set to equal zero in the domains in which they have not yet been defined. We claim that the resulting function w_n satisfies the following energy bound:

$$H_n(w_n) \leqslant CH_n(u_n). \tag{3.15}$$

Indeed, for $i - j \geqslant c_0 - [2h_{k_0}^n n]$ and for $i - j \leqslant c_0 - [9h_{k_0}^n n]$ this follows from the respective bounds for $\tilde{v}_n$ and u_n that were stated in steps (a) and (b). It thus remains to argue that this is also true in the interpolation region

$$c_0 - [9h_{k_0}^n n] \leqslant i + j \leqslant c_0 - [2h_{k_0}^n n].$$

To this end, we note that as $h_{k_0}^n \sim n^{-1}$, $\nabla\tilde{v}(\Delta_{ij}^{n,\pm}) \in \mathrm{conv}(\nabla u(\Delta_{kl}^{n,\pm}))$, where $\Delta_{kl}^{n,\pm}$ are neighbouring triangles of $\Delta_{ij}^{n,\pm}$ (or triangles within a certain uniformly bounded distance from $\Delta_{ij}^{n,\pm}$). As a consequence, by the triangle inequality and the estimates (3.11), (3.12), (3.14), we infer that

$$|\nabla u_n(\Delta_{ij}^{n,\pm}) - \nabla\tilde{v}_n(\Delta_{ij}^{\pm})| \leqslant C\frac{1}{h_k} \sum_{(kl)\in\mathcal{N}(i,j)} \|\mathrm{dist}(\nabla u_n, K)\|_{L^2(\Delta_{kl}^\pm)}. \tag{3.16}$$

Assuming growth of order 2 for the energy density h_n at infinity, setting

$$\Omega'' := \{(x_1, x_2): x_1 - x_2 \in [c_0/n - [9h_{k_0}^n n]/n, c_0/n], \ |x_2| \leqslant 1\}$$

and using (3.16), we hence obtain

$$
\begin{aligned}
H_n(w_n) &= H_n(u_n + \gamma(\tilde{v}_n - u_n)) \\
&\leqslant C H_n(u_n) + \sum_{(i,j) \in n\Omega''} \frac{1}{n^2} |\nabla u_n^{ij} - \nabla \tilde{v}_n^{ij}|^2 \\
&\quad + C \sum_{\substack{(i,j) \in n\Omega_{2d,l/2}^-, \\ c_0 - [9h_{k_0}^n n] < i-j < c_0 - [2h_{k_0}^n n]}} \frac{1}{n^2} |\nabla \gamma|^2 |u_n^{ij} - \tilde{v}_n^{ij}|^2 \\
&\leqslant C H_n(u_n) + \sum_{(i,j) \in n\Omega''} \frac{1}{n^2} |\nabla u_n^{ij} - \nabla \tilde{v}_n^{ij}|^2 \\
&\quad + \sum_{\substack{(i,j) \in n\Omega_{2d,l/2}^-, \\ c_0 - [h_k n] < i+j < c_0}} \frac{1}{n^2} n^2 |u_n^{ij} - \tilde{v}_n^{ij}|^2 \\
&\leqslant C H_n(u_n) + C \sum_{\substack{(i,j) \in n\Omega_{2d,l/2}^-, \\ c_0 - [h_k n] < i-j < c_0}} \frac{1}{n^2} |\nabla u_n^{ij} - \nabla \tilde{v}_n^{ij}|^2 \\
&\leqslant C H_n(u_n),
\end{aligned}
$$

where we used (3.16) in passing from the third to the fourth line and Poincaré's inequality to estimate the term involving $|u_n - \tilde{v}_n|$. Moreover, due to the L^∞ estimates in (3.11), (3.12) and (3.14), the admissibility of w_n is preserved. Hence, setting $\tilde{u}_n = w_n$ provides the desired modification of u_n. $\qquad\square$

An analogous cutting result holds for the limiting profiles v_{V_1,V_2}^+.

3.3. Proof of the Γ-convergence result

In this section we finally prove the Γ-convergence result of theorem 1.11. Here the Γ-$\liminf$ inequality essentially follows directly from the definition of the limiting energy and the independence result of lemma 3.6. The construction of the Γ-$\limsup$ inequality, however, is more involved (as in [13–15]). Here we have to invoke the cutting result of proposition 3.7.

Proof of the Γ-$\liminf$ inequality. Using the definition (3.1), the Γ-$\liminf$ inequality follows directly. Without loss of generality we may assume that

$$
\liminf_{n \to \infty} H_n^1(u_n) \leqslant C < \infty.
$$

In this setting, the compactness result of proposition 2.3 holds. Thus, along a subsequence, we obtain a limiting deformation u_0 that is a simple laminate. In particular, its gradient attains values in $K = \mathrm{SO}(2)U_0 \cup \mathrm{SO}(2)U_1$ and only has finitely many, say $L \in \mathbb{N}$, jump interfaces. Furthermore, we claim that it suffices to assume that the jump interfaces of ∇u_0 *do not* intersect on $\partial\Omega$. Indeed, this follows from the observation that if there were intersections of jump interfaces on the boundary, then we could carry out the procedure that is described below in domains that slightly stay away from the boundary. More precisely, for any given $\varepsilon > 0$ we would only

cover a $(1 - \varepsilon)$ fraction of the jump set (i.e. only the interior parts of the jump set, which are at distance $\varepsilon/2$ away from the boundary) by the sets Ω_n^k that are described below. By virtue of the arbitrariness of ε, this yields our claim.

With this discussion in mind (in particular, assuming that the interfaces are separated from each other and do not intersect on $\partial\Omega$), we now cover the jump set of ∇u_0 by subdomains Ω_k^n, of which each only contains a single jump interface or one of the boundary layers given by the points (x_1, x_2) with $x_1 + x_2 \leqslant -4$ and $x_1 + x_2 \geqslant 4$ and $|x_2| \leqslant 2$. We consider associated subenergies $H_n^{1,k}(\cdot)$ determined by the sets Ω_k^n and the interfaces and boundaries of the limiting configuration u_0:

$$H_n^1(u_n) = H_n^{1,0}(u_n \chi_{\Omega_k^n}) + \sum_{k=1}^{L-1} H_n^{1,k}(u_n \chi_{\Omega_k^n}) + H_n^{1,L}(u_n \chi_{\Omega_L^n}).$$

By the compactness result of proposition 2.3, there exist points $x_k^n \in \Omega$ with $x_k^n \to x_k \in \Omega$ such that, up to subsequences,

$$u_n(\cdot - x_k^n)\chi_{\Omega_k^n} \to v_{V_k, V_{k+1}}^{\pm} \quad \text{in } L^1(\Omega_k^n), \tag{3.17}$$

where the functions $v_{V_k, V_{k+1}}^{\pm}$ are defined in definition 3.1. We furthermore observe that for all $k \in \{0, \dots, L\}$ and for each $\varepsilon > 0$ there exists $N_{\varepsilon,k} \in \mathbb{N}$ such that, for all $n \geqslant N_{\varepsilon,k}$,

$$H_k^1(u_n \chi_{\Omega_k^n}) \geqslant \liminf_{n \to \infty} H_k^1(u_n \chi_{\Omega_k^n}) - \varepsilon.$$

Then, however, with $\varepsilon > 0$ arbitrary but fixed and $N_\varepsilon := \max_{k \in \{0,\dots,L\}} N_{\varepsilon,k}$, we immediately infer that, for $n \geqslant N_\varepsilon$ (where we invoke the independence result of lemma 3.6 and (3.17)),

$$H_n^1(u_n) = H_n^{1,0}(u_n \chi_{\Omega_k^n}) + \sum_{k=1}^{L-1} H_n^{1,k}(u_n \chi_{\Omega_k^n}) + H_n^{1,L}(u_n \chi_{\Omega_L^n})$$

$$\geqslant H_n^{1,0}(u_n \chi_{\Omega_k^n}) - \varepsilon + \sum_{k=1}^{L-1} \left(\liminf_{n \to \infty} H_n^{1,k}(u_n \chi_{\Omega_k^n}) - \varepsilon \right) + H_n^{1,L}(u_n \chi_{\Omega_L^n}) - \varepsilon$$

$$\geqslant \sum_{k=1}^{L-1} \inf \left\{ \liminf_{n \to \infty} H_n^{1,k}(v_n \chi_{\Omega_k^n}), \; v_n \to v_{V_k, V_{k+1}}^{\pm} \text{ in } L^1(\Omega_k^n) \right\}$$

$$+ \inf \left\{ \liminf_{n \to \infty} H_n^{1,0}(v_n \chi_{\Omega_0^n}), \; v_n \to v_{F_\lambda, V_1} \text{ in } L^1(\Omega_0^n), \right.$$

$$\left. v_n(i/n, j/n) = F_\lambda(i/n, j/n) \text{ for } i + j \leqslant -4n \right\}$$

$$+ \inf \left\{ \liminf_{n \to \infty} H_n^{1,L}(v_n \chi_{\Omega_0^n}), \; v_n \to v_{V_L, F_\lambda} \text{ in } L^1(\Omega_0^n), \right.$$

$$\left. v_n(i/n, j/n) = F_\lambda(i/n, j/n) \text{ for } i + j \geqslant 4n \right\} - (L+1)\varepsilon$$

$$\geqslant E_{\text{surf}}(u_0) - \varepsilon.$$

In the second last inequality, we carried out a translation of u_n in order to match the boundary conditions for the right boundary layer. Since this estimate holds for any $\varepsilon > 0$, this concludes the proof of the Γ-lim inf inequality. $\qquad\square$

We now proceed to the proof of the Γ-lim sup inequality. As in [13–15], this is the harder part of the argument. In the presence of multiple interfaces we have to cut and paste the different internal and boundary layers, which are provided by the minimization problem that defines the densities of $E_{\mathrm{surf}}(\cdot)$. This has to be achieved in a way that leads to an overall admissible sequence. In particular, we have to preserve the non-interpenetration condition. To ensure these issues, we rely on the cutting procedure from proposition 3.7.

Proof of the Γ-lim sup inequality. For the purpose of this proof, we introduce

$$H_n^{1,\pm}(v, m_1, m_2) := \sum_{(i,j) \in n\Omega_{m_1,m_2}^{\pm}} \frac{1}{n} h_v^{ij} \tag{3.18}$$

to denote the energies that were used as a building block in definition 3.2 and lemma 3.6.

STEP 1 (reduction to proposition 3.7). Given u_0, which is piecewise affine and whose gradient in Ω attains values in $K = \mathrm{SO}(2)U_0 \cup \mathrm{SO}(2)U_1$, we have to construct a sequence of u_n that is admissible, converges to u_0 in $L^1(\Omega)$ and satisfies

$$\limsup_{n \to \infty} H_n^1(u_n) \leqslant E_{\mathrm{surf}}(u_0).$$

As $E_{\mathrm{surf}}(u_0)$ is defined by a sum of boundary and internal layer energies, and as each of these is determined by a minimization process (see (3.1) and (3.2)), for each jump interface of ∇u_0 we find subsequences n_j and $u_{n_j}^k : \Omega_{d,4}^- \to \mathbb{R}^2$ such that (with the notation from (3.18)), for instance,

$$\lim_{j \to \infty} H_{n_j}^{1,-}(u_{n_j}^k, d, 4) = C_-(V_k, V_{k+1}, d, 4) = 4C_-.$$

In what follows, we concentrate on this single jump interface; the results for the other internal and boundary layers follow analogously. We seek to modify these functions $u_{n_j}^k$ into new functions $\tilde{u}_{n_j}^k$ such that they are defined in (part of) our original domain Ω and have affine boundary data. Then, if we can extend the functions $\tilde{u}_{n_j}^k$ to a full sequence in $n \in \mathbb{N}$ (not just the subsequence $\{n_j\}_{j \in \mathbb{N}} \subset \mathbb{N}$; this is done in step 3), then the affine boundary data would allow us to glue the individual pieces together. This would hence yield a global recovery sequence defined on Ω.

Returning to our interface with orientation $(-1,1)$ between the gradients V_k, V_{k+1}, we claim that there is a sequence $\tilde{u}_n^k$ (derived from the function $u_{n_j}^k$) such that in $\Omega_{d,1}^-$ we have the following:

(a) $\tilde{u}_n^k \to u_0$ in $L^1(\Omega_{d,1}^-)$;

(b) $\tilde{u}_n^k$ is affine away from the interface; more precisely, there are orientation preserving isometries I_n, I_n',

$$u_n^k(x,y) = \begin{cases} I_n \circ u_0 & \text{for } x - y \geqslant 4/5d, \\ I_n' \circ u_0 & \text{for } x - y \leqslant -4/5d, \end{cases}$$

and $I_n, I_n' \to Q, Q' \in \mathrm{SO}(2)$;

(c) $H_n^1(\tilde{u}_n^k) = H_n^{1,-}(\tilde{u}_n^k, d, 1) \to C_-(V_k, V_{k+1}, 1, 1) = C_-$.

The claims (a)–(c) are deduced by an application of proposition 3.7. In order to do so, we first observe the independence of $C_-(V_k, V_{k+1}, m_1, m_2)$ on the extension of the domain $\Omega^-_{m_1,m_2}$ in the direction orthogonal to the interface (see lemma 3.6). Next, by the definition of $E_{\text{surf}}(u_0)$ and by lemma 3.6, we directly infer that for each $\eta > 0$ there exists a number $N_\eta \in \mathbb{N}$ such that

$$\sum_{\substack{(i,j)\in n\Omega^-_{d,1}, \\ [n/2]\leqslant|i-j|\leqslant[n]}} \frac{1}{n} h^{ij}_{u^k_n} \leqslant C\eta \quad \text{for all } n \geqslant N_\eta. \tag{3.19}$$

Let us then choose d, l in the assumptions of proposition 3.7 so that

$$n\Omega^-_{2d,l/2} = \{(i,j) \in n\Omega^-_{d,1}, \ [n/2] \leqslant i - j \leqslant [n]\}$$

or

$$n\Omega^-_{2d,l/2} = \{(i,j) \in n\Omega^-_{d,1}, \ -[n] \leqslant i - j \leqslant -[n/2]\}.$$

Finally, in step 2 we construct the one-well energy satisfying (3.6). Combining these observations allows us to apply proposition 3.7, and hence to replace our minimal sequence $u^k_{n_j}$ by the corresponding modification $\tilde{u}^k_{n_j}$. The resulting sequence $\tilde{u}^k_{n_j}$ satisfies an analogous energy bound and consequently yields statements (a)–(c) from above. In particular, its boundary data are affine and lie in the respective energy wells. These affine boundary data then permit us (after a suitable translation) to glue together the individual functions $\tilde{u}^k_{n_j}$, $k \in \{1, \dots, L\}$, that were obtained for the individual interfaces. Hence, it remains to construct the one-well energy satisfying (3.6). This is the content of the next step.

STEP 2 (reduction to a one-well energy). Seeking to apply the two-well rigidity result of proposition 2.4, we construct a one-well energy density that satisfies the necessary bounds.

We begin by considering the following one-well energy density

$$\phi^{ij}_u := \gamma(|U^{i,j}|) \min\{\bar{h}^{i,j}_{u,U_0}, \bar{c}/10\} + (1 - \gamma)(|U^{i,j}|)k(|U^{ij}|). \tag{3.20}$$

Here $\bar{h}^{ij}_{u,U_0}$ denotes the one-well function from remark 1.6, $\bar{c}$ is the constant from (1.4),

$$U^{i,j} := (\partial_1 u^{i,j}, \partial_1 u^{i-1,j}, \partial_2 u^{i,j}, \partial_2 u^{i,j-1}).$$

The function $\gamma \in C^\infty(\mathbb{R}, \mathbb{R})$ is a cut-off function with $\gamma(t) = 1$ for all $|t| \leqslant 10 \max\{10\bar{c}, 100\}$ and $\gamma(t) = 0$ for $|t| \geqslant 20 \max\{10\bar{c}, 100\}$. Moreover, k is chosen such that

$$c_1 \operatorname{dist}(\nabla u^{ij}, \operatorname{SO}(2)U_0)^2 \leqslant k(U^{ij}) \leqslant c_2 \operatorname{dist}(\nabla u^{ij}, \operatorname{SO}(2)U_0)^2 \tag{3.21}$$

for some constants $c_1, c_2 > 0$. Similarly to in remark 1.6, we interpret ϕ_u as the composition of a Lipschitz continuous function ϕ. with the piecewise constant function ∇u.

We claim that, for any $u \in \mathcal{A}_n$,

$$|\nabla_n \phi^{ij}_u| \leqslant Cn h^{ij}_u, \tag{3.22}$$

where h_u^{ij} denotes our original model Hamiltonian from definition 1.8. Indeed, as

$$|\nabla_n \phi_u^{ij}| \leqslant Cn(|\phi_u^{i+1,j} - \phi_u^{i,j}| + |\phi_u^{i,j+1} - \phi_u^{i,j}|),$$

(3.22) directly follows in the region where $\operatorname{dist}(\nabla u^{ij}, \mathrm{SO}(2)U_0)^2 \leqslant \bar{c}/100$ from (3.20). This is due to the fact that in this region, in (3.20) we have

$$\phi_u^{ij} = \gamma(|U^{ij}|)\bar{h}_{u,U_0}^{ij} + (1-\gamma)(|U^{ij}|)k(|U^{ij}|).$$

But then for $(i,j) \in n\Omega$ with $\operatorname{dist}(\nabla u^{ij}, \mathrm{SO}(2)U_0)^2 \leqslant \bar{c}/100$ this first term in the bracket is controlled by our original Hamiltonian h_u^{ij} (as also here the first bracket is active while the second one is bounded below).

In the region where $\operatorname{dist}(\nabla u^{ij}, \mathrm{SO}(2)U_1) \leqslant \operatorname{dist}(\nabla u^{ij}, \mathrm{SO}(2)U_0)$ and $|\nabla u^{ij}| \leqslant \max\{100, 10\bar{c}\}$, the function ϕ_u^{ij} is constant, and hence $0 = |\nabla_n \phi_u^{ij}| \leqslant h_u^{ij}$. Thus, by compactness (and by the Lipschitz regularity of ϕ.), the bound (3.22) follows for all values of ∇u^{ij} with $|\nabla u^{ij}| \leqslant \max\{100, 10\bar{c}\}$. Finally, for $|\nabla u^{ij}| \geqslant \max\{100, 10\bar{c}\}$, the bound follows from the two-growth assumption (3.21), which is satisfied by both h_u^{ij} and ϕ_u^{ij}.

Using (3.22), we thus infer that

$$\sum_{\substack{(i,j) \in n\Omega, \\ -[n/2] \leqslant |i-j| \leqslant [n]}} \frac{1}{n^2} |\nabla_n \phi_u^{ij}| \leqslant C \sum_{\substack{(i,j) \in n\Omega, \\ -[n/2] \leqslant |i-j| \leqslant [n]}} \frac{1}{n} h_u^{ij} \leqslant c\eta.$$

This then permits us to invoke proposition 2.4.

Hence, on the level of our subsequence $u_{n_j}^k$ we have obtained a recovery sequence. In order to pass to a full sequence, we invoke a scaling argument as in [15].

STEP 3 (passage from the subsequence n_j to a full sequence in $n \in \mathbb{N}$). The proof of the extension of the recovery sequence from a subsequence to a full sequence follows along the argument given by Conti and Schweizer [14]. It relies on a combination of a scaling argument and the energy control from (3.19). As before we restrict our attention to a single interface that has a normal pointing in the $(-1, 1)$ direction. For the situation with more interfaces we argue locally around each interface.

(a) *Scaling.* We claim that for each $n \in \mathbb{N}$ there exists a function $v_n \colon \Omega_{d,1}^- \to \mathbb{R}^2$ such that (with the abbreviation from (3.18))

$$\limsup_{n \to \infty} H_n^{1,-}(v_n, \infty, 1) \leqslant C_-,$$

and there exists $L_n > 0$ such that

$$\nabla v_n(x_1, x_2) = \begin{cases} U_0 & \text{for } x_1 - x_2 \geqslant L_n, \\ QU_1 & \text{for } x_1 - x_2 \leqslant -L_n. \end{cases}$$

The claim follows from scaling. Indeed, by the definition of $C_-(U_0, QU_1, d, 1)$ there exist sequences n_j and u_{n_j} such that

$$H_n^{1,-}(u_{n_j}, d, 4) \to 4C_- \quad \text{and} \quad u_{n_j} \to v_{U_0, QU_1}^- \quad \text{in } L^1(\Omega_{d,4}^-).$$

By proposition 3.7 this implies that there exists a sequence $\tilde{u}_{n_j}$ with affine boundary data such that

$$H_n^{1,-}(\tilde{u}_{n_j}, d, 1) \to C_- \quad \text{and} \quad \tilde{u}_{n_j} \to v_{U_0, QU_1}^- \quad \text{in } L^1(\Omega_{d,1}^-).$$

Let $\varepsilon_j := |H_n^{1,-}(\tilde{u}_{n_j}, d, 1) - C_-|$ denote the error at stage j and assume that n_j is a monotone increasing sequence. Then, for given $n \in \mathbb{N}$, let $n_j \in \mathbb{N}$ be the smallest element in $\{n_j\}_{j \in \mathbb{N}}$ such that $n^2 < n_j$ and write $\alpha := n_j/n > n$. Moreover, define

$$\tilde{v}_n(i,j) := \alpha \tilde{u}_n(i/\alpha, j/\alpha).$$

Thus, the scaling of the energy (see the proof of lemma 3.6) yields

$$H_n^{1,-}(\tilde{v}_n, \alpha d, \alpha) = \alpha H_n^{1,-}(\tilde{u}_{n_j}, d, 1) \leqslant \alpha C_- + \alpha \varepsilon_j + \frac{c}{\alpha n}.$$

By translating, it is possible to find a point $(\bar{i}, \bar{j}) \in \Omega_{\alpha d, \alpha}^-$ with distance d away from the boundary such that for $v_n(i,j) := \tilde{v}_n(i, j + \bar{j})$ we have

$$H_n^{1,-}(v_n, \alpha d, 1) = H_n^{1,-}(\tilde{u}_{n_j}, d, 1) \leqslant C_- + \varepsilon_j + \frac{c}{\alpha^2 n}. \tag{3.23}$$

As by construction ∇v_n^{ij} is in the energy wells if $i - j \geqslant \alpha$ or $i - j \leqslant -\alpha$, this proves the claim with $L_n := \alpha$.

(b) *Energy bounds.* We claim that there exist $h > 0$, $L > 2h$, $\delta > 0$, all independent of n, a function $w_n \colon \Omega_{L,d}^- \to \mathbb{R}^2$ such that

$$\limsup_{n \to \infty} H_n^{1,-}(w_n, L, 1) \leqslant C_-,$$

and:

(i) for half of all points (i,j) with $i - j \in (Ln - hn, Ln)$,

$$\operatorname*{ess\,inf}_{j \in (-n,n) \cap \mathbb{Z}^2} \operatorname{dist}(\nabla w_n^{i,j}, \mathrm{SO}(2)U_1) \geqslant \delta;$$

(ii) there exists a value $j_n \in (-Ln, Ln - 2hn)$ (depending on n) such that for half of the points (i,j) with $i - j \in (j_n, j_n + hn)$ it holds that

$$\operatorname*{ess\,inf}_{j \in (-n,n) \cap \mathbb{Z}^2} \operatorname{dist}(\nabla w_n^{i,j}, \mathrm{SO}(2)U_0) \geqslant \delta.$$

This shows (in a weak form) that the transition from $\mathrm{SO}(2)U_1$ to $\mathrm{SO}(2)U_0$ already takes place in the smaller domain $\Omega_{L,d}^-$. The proof follows from the energy control in (3.23). More precisely, we choose $\delta < \operatorname{dist}(\mathrm{SO}(2)U_0, \mathrm{SO}(2)U_1)/10$ and consider

$$f_{U_0}(c) := \#\{(i,j) \in n\Omega_{\infty,1}^- : i - j = c, \ \operatorname{dist}(\nabla v_n^{i,j}, \mathrm{SO}(2)U_0) \leqslant \delta\},$$
$$f_{U_1}(c) := \#\{(i,j) \in n\Omega_{\infty,1}^- : i - j = c, \ \operatorname{dist}(\nabla v_n^{i,j}, \mathrm{SO}(2)U_1) \leqslant \delta\}.$$

In order to prove the statement, we show that f_{U_0}, f_{U_1} are essentially characteristic functions. For this we observe the following points.

- As $H_n^{1,-}(v_n, \infty, 1) \leqslant c$, we have

$$\#\{c \colon f_{U_0}(c) + f_{U_1}(c) < \tfrac{3}{2}\} \leqslant c_1 n.$$

- As a transition from $\mathrm{SO}(2)U_0$ to $\mathrm{SO}(2)U_1$ costs a finite amount of energy (see the argument in lemma A.3),

$$\#\{c \colon f_{U_0}(c) \neq 0, f_{U_1}(c) \neq 0\} \leqslant c_2 n.$$

- It holds that

$$f_{U_0}(c) = \begin{cases} 2n & \text{for } c \geqslant nL_n, \\ 0 & \text{for } c \leqslant -nL_n. \end{cases}$$

- If $f_{U_0}(c_a) \geqslant \tfrac{3}{2}n$ and $f_{U_1}(c_b) \geqslant \tfrac{3}{2}n$, then for $\bar{v}_n(i,j) := v(i+i_c, j+j_c)$, where $i_c - j_c = (c_a + c_b)/2$,
$$H_n^{1,-}(\bar{v}_n, |c_a - c_b|, 1) \geqslant c.$$

Combining these we obtain that there exists sets M_0, M_1, M_2 of points (i,j) such that $\#M_2 \leqslant (c_1 + c_2)n^2$,

$$\begin{aligned} f_{U_0}(c) \geqslant \tfrac{3}{2}n, \quad & f_{U_1}(c) = 0 \quad && \text{for } (i,j) \in M_0 \text{ with } i+j = c, \\ f_{U_0}(c) = 0, \quad & f_{U_1}(c) \geqslant \tfrac{3}{2}n, \quad && \text{for } (i,j) \in M_1 \text{ with } i+j = c. \end{aligned}$$

In other words, M_0 denotes the set of lines such that $\mathrm{SO}(2)U_0$ is the preferred value of ∇u on these lines. M_2 plays the same role for lines on which ∇u is mostly in $\mathrm{SO}(2)U_1$. Finally, M_3 denotes the 'mixed' lines where both $\mathrm{SO}(2)U_0$ and $\mathrm{SO}(2)U_1$ appear in a large volume fraction.

We observe that the number of interfaces between M_0, M_1 is bounded by a constant c_3 (which is uniform in n). Defining

$$c_a := \inf\{c \in \mathbb{Z} \colon \text{for all } (i,j) \text{ with } i - j \in (c - j, c), \ (i,j) \notin M_1\}$$

and choosing $h \geqslant 2(c_1 + c_2)$ yields (ii) in the interval given by (i,j) with $i - j \in (c_a - h, c_a)$. Choosing a large number L with $L > (c_3 + 2)h$ and dividing the interval of points in which $i - j \in (c_a - L, c_a - h)$ into sections of size h, we note that, by definition, all of them intersect M_1. For sufficiently large L there exists one section that does not intersect M_0, which follows as the number of interfaces between M_1 and M_0 is bounded by c_3. This yields the existence of the desired value c_n from (ii). The function w_n is obtained by an appropriate translation of the function v_n.

(c) *Compactness and conclusion.* Finally, we construct the desired full sequence u_n in $\Omega_{d,1}^-$. This sequence both satisfies the energy bound (3.19) and converges against the desired limiting profile. To this end, we claim that there exists a rotation R, a point $a \in (-L + h/2, L - h/2)$ and a translation vector $b \in \mathbb{R}^2$ such that

$$\|Rw_n(i + i_a, j + j_a) + b - v_{U_0, QU_1}^-(i/n, j/n)\|_{L^1(\Omega_{d,1}^-)} \to 0. \tag{3.24}$$

Indeed, this follows from compactness. Assume that it were not the case. Then, by the boundedness of the energy of w_n we can invoke proposition 2.3 along the 'bad sequence' that satisfies the energy bound (3.19) but does not obey (3.24) and

obtain a limiting deformation w_∞ with $\nabla w_\infty \in K$. For $i - j \leqslant -L$ and $i - j \geqslant L$ it respectively attains the gradient values $R_1 U_0$ and $R_2 U_1$ with $R_1, R_2 \in \mathrm{SO}(2)$. Moreover, by step 2, the interface must have the normal $(-1, 1)$. Hence, the limiting deformation w_∞ involves *at least one* interface between the energy wells and the corresponding interface has the right orientation. Furthermore, it cannot involve more interfaces, as these would cost a non-vanishing additional amount of energy (see the proof of the Γ-lim inf inequality). This yields a contradiction to our assumption that w_n does not converge to the desired limiting profile after translation and rotation. Rotating and translating w_n appropriately yields the definition of u_n and concludes the proof. $\qquad\square$

Acknowledgements

Appendix A. Mapping the microscopic two-well problem to a spin system

In this section we map the two-well problem to a spin system and prove one-sided energy bounds that are crucially used in the compactness result of §2.1. For convenience of notation, throughout the section we assume that the constant $\bar{c}$ from (1.4) is such that $\bar{c} \leqslant \bar{c}^2$. In this section, the discrete nature of our problem is strongly used. In this context, a number of arguments simplify with respect to the analogous continuous models. It is in this part of our argument that the origins of the surface energies in the discrete model appear for the first time. We begin by introducing the corresponding definitions and abbreviations.

DEFINITION A.1 (spin Hamiltonian). Let $\bar{c}$ be as in (1.4) and $u \in \mathcal{A}_n^{F_\lambda}$. Then we set

$$\tilde{\Omega}_0^n := \{(i/n, j/n) \in \Omega \colon h_{u_n}^{i,j} \leqslant \tfrac{1}{10}\bar{c} \text{ and } \mathrm{dist}(\nabla u_n^{i,j}, \mathrm{SO}(2)U_0) \leqslant \tfrac{1}{10}\bar{c}\},$$

and $\tilde{\Omega}_1^n := \Omega_n \setminus \tilde{\Omega}_0^n$. We further define the *discrete spin function* $\sigma_n \colon (n^{-1}\mathbb{Z})^2 \cap \Omega \to \{\pm 1\}$ as

$$\sigma_n^{i,j} := \begin{cases} 1 & \text{if } (i/n, j/n) \in \tilde{\Omega}_0^n, \\ -1 & \text{otherwise,} \end{cases} \tag{A 1}$$

and correspondingly the *spin Hamiltonian* as

$$H_n^s(\sigma_n^{i,j}) := \sum_{(i/n, j/n) \in G^n \cap \Omega} \;\; \sum_{(k,l) \in \{(i+1,j),(i,j+1),(i-1,j),(i,j-1)\}} n^{-2}(\sigma_n^{i,j} - \sigma_n^{k,l})^2.$$

Next, we claim the following one-sided comparability of the two-well and spin Hamiltonians.

PROPOSITION A.2. *Let $u \in \mathcal{A}_n^{F\lambda}$. Then there exists a constant $0 < C = C(a,b) < \infty$ such that*

$$H_n(u_n) \geqslant C H_n^s(\sigma_n^{i,j}). \qquad (A\,2)$$

In order to prove this proposition, we first show the following auxiliary result.

LEMMA A.3. *Let $u \in \mathcal{A}_n^{F\lambda}$ and $(i/n, j/n) \in \tilde{\Omega}_0^n$ but assume that $((i+1)/n, j/n) \notin \tilde{\Omega}_0^n$. Then,*

$$h_u^{i+1,j} > \frac{\bar{c}}{100}.$$

Proof. Indeed, this follows from the two-body interactions that are involved in the definition of h_u^{ij} close to the two wells $\mathrm{SO}(2)U_0 \cup \mathrm{SO}(2)U_1$. In order to see this, we argue by contradiction and assume that the conclusion of the lemma is false. This would entail that (in the notation of remark 1.6)

$$\bar{h}_{u,U_0}^{ij} \leqslant \frac{\bar{c}}{4} \quad \text{and} \quad \bar{h}_{u,U_1}^{i+1,j} \leqslant \frac{\bar{c}}{4}.$$

However, this is not possible as the first assumption implies that

$$(|\partial_1 u^{i,j}|^2 - a^2)^2 \leqslant \frac{\bar{c}}{4},$$

while the second condition ensures that

$$(|\partial_1 u^{i,j}|^2 - b^2)^2 \leqslant \frac{\bar{c}}{4}.$$

As by virtue of the choice of $\bar{c}$ these are not possible simultaneously, we obtain a contradiction. Thus, we obtain the desired result. $\qquad \square$

Using the previous lemma, we can proceed with the proof of proposition A.2.

Proof of proposition A.2. By definition we have that $(\sigma_n^{i,j} - \sigma_n^{k,l})^2 \in \{0, 4\}$ for each $(i/n, j/n) \in \Omega_n$ and any of its neighbours $(k/n, l/n) \in \Omega_n$. Thus, we only have to argue that the number of points on which $h_u^{i,j}$ is uniformly bounded from below, for example, by $\bar{c}/100$, is larger than or equal to the number of points on which $(\sigma_n^{i,j} - \sigma_n^{k,l})^2$ attains the value 4. But this is ensured by lemma A.3. $\qquad \square$

As a direct corollary of proposition A.2 and the energy bound (1.17), we obtain that for each $n \in \mathbb{N}$ the set of edges in G^n that connects two vertices such that $(\sigma_n^{i,j} - \sigma_n^{k,l})^2$ attains the value 4 has a uniformly (in n) bounded one-dimensional Hausdorff measure. It divides Ω into two connected components Ω_0^n and Ω_1^n such that $\sigma_n^{i,j} = 1$ for $(i/n, j/n) \in \Omega_0^n$ and $\sigma_n^{i,j} = -1$ for $(i/n, j/n) \in \Omega_1^n$. Both are Caccioppoli sets, whose perimeter is uniformly bounded in n. Moreover, we can interpolate the lattice function σ_n^{ij} constantly and define a function $\sigma \in \mathrm{BV}(\Omega)$ that is equal to ± 1 for $x \in \Omega_{0,1}^n$, respectively. Hence, by the compactness results for sequences of Caccioppoli sets (see for instance, [2]), along subsequences we obtain the existence of limiting Caccioppoli sets Ω_0 and Ω_1 of the sets Ω_0^n and Ω_1^n. This is summarized in the next proposition.

PROPOSITION A.4. *Let $\{u_n\}_{n \in \mathbb{N}}$ be a sequence of lattice deformations with $u_n \in \mathcal{A}_n^{F\lambda}$ satisfying the energy bound (1.17). Let Ω_0^n be as above. Then there exists a*

subsequence $\{n_j\}_{j\in\mathbb{N}}$ *and (up to zero sets) disjoint Caccioppoli sets* Ω_0, Ω_1 *such that*

$$\Omega_0^{n_j} \to \Omega_0 \quad and \quad \Omega_1^{n_j} \to \Omega_1 \quad in\ measure,$$

that is,

$$|\Omega_0^{n_j}\Delta\Omega_0| \to 0 \quad and \quad |\Omega_1^{n_j}\Delta\Omega_1| \to 0.$$

Moreover, $\Omega = \Omega_0 \cap \Omega_1$.

Finally, in the next proposition we relate the limiting sets Ω_0 and Ω_1 to corresponding limiting sets of 'low energy deformations' (see 1.17) of the two-well problem.

PROPOSITION A.5. *Let* $\{u_n\}_{n\in\mathbb{N}} \subset \mathcal{A}_n^{F_\lambda}$ *be piecewise affine functions on the grid* Ω_n *satisfying (1.17). Then*

$$\left.\begin{array}{ll} \operatorname{dist}(\nabla u_n, \mathrm{SO}(2)U_0) \to 0 & in\ L^2(\Omega_0), \\ \operatorname{dist}(\nabla u_n, \mathrm{SO}(2)U_1) \to 0 & in\ L^2(\Omega_1). \end{array}\right\} \tag{A 3}$$

More precisely, for $l \in \{0,1\}$,

$$\int_{\Omega_l} \operatorname{dist}^2(\nabla u_n, \mathrm{SO}(2)U_l)\,\mathrm{d}x \leqslant 100(c+1)H_n(u_n) + (100c)^2|\Omega_l\Delta\Omega_l^n|.$$

Proof. We only provide the proof for $l = 0$; for $l = 1$ the argument is analogous. We have

$$\int_{\Omega_0} \operatorname{dist}^2(\nabla u_n, \mathrm{SO}(2)U_0)\,\mathrm{d}x = \int_{\Omega_0^n} \operatorname{dist}^2(\nabla u_n, \mathrm{SO}(2)U_0)\,\mathrm{d}x$$
$$+ \int_{\Omega_0\setminus\Omega_0^n} \operatorname{dist}^2(\nabla u_n, \mathrm{SO}(2)U_0)\,\mathrm{d}x$$
$$\leqslant H_n(u_n) + \int_{\Omega_0\setminus\Omega_0^n} \operatorname{dist}^2(\nabla u_n, \mathrm{SO}(2)U_0)\,\mathrm{d}x. \tag{A 4}$$

We continue by estimating the second term:

$$\int_{\Omega_0\setminus\Omega_0^n} \operatorname{dist}^2(\nabla u_n, \mathrm{SO}(2)U_0)\,\mathrm{d}x$$
$$\leqslant \int_{\Omega_0\setminus\Omega_0^n} \chi_{\{|\nabla u_n|\leqslant 100\bar{c}\}} \operatorname{dist}^2(\nabla u_n, \mathrm{SO}(2)U_0)\,\mathrm{d}x$$
$$+ \int_{\Omega_0\setminus\Omega_0^n} \chi_{\{|\nabla u_n|\geqslant 100\bar{c}\}} \operatorname{dist}^2(\nabla u_n, \mathrm{SO}(2)U_0)\,\mathrm{d}x$$
$$\leqslant (100\bar{c})^2|\Omega_0\Delta\Omega_0^n|$$
$$+ 100\bar{c}\int_{\Omega_0\setminus\Omega_0^n} \operatorname{dist}^2(\nabla u_n, \mathrm{SO}(2)U_0 \cup \mathrm{SO}(2)U_1)\,\mathrm{d}x$$
$$\leqslant (100\bar{c})^2|\Omega_0\Delta\Omega_0^n| + 100\bar{c}H_n(u_n).$$

Inserting this back into (A 4) yields the desired bound. $\square$

REMARK A.6. We observe that the convergence $|\Omega_0 \Delta \Omega_0^n| \to 0$ (which follows as a consequence of the discussion of the spin system given in appendix A) can be arbitrarily slow. Indeed, as an example, one could consider a finite number of stripes, in which $\nabla u_n \in \mathrm{SO}(2)U_1$, with size n^α for any arbitrary $\alpha \in (0, 1)$.

Appendix B. Second derivative control

In this section we derive an important property of the Hamiltonian H_n. Although this is not directly used in the argument that leads to the Γ-limit of theorem 1.11, this property in part explains the comparability of the continuous model from [15] and our discrete model. In fact the Hamiltonian from definition 1.8 not only controls the deviation of the gradients of u from the energy wells, but also the discrete *second* derivatives of u.

In what follows we use C to denote a universal constant that only depends only on a and b and may change from line to line.

LEMMA B.1 (second derivative control). *Let $u \in \mathcal{A}_n^{F_\lambda}$. Then there exists a constant $C = C(a, b) > 0$ such that*

$$n^2 |u^{i+1,j} + u^{i-1,j} - 2u^{i,j}| \leqslant Cn\sqrt{h_u^{i,j}},$$
$$n^2 |u^{i,j+1} + u^{i,j-1} - 2u^{i,j}| \leqslant Cn\sqrt{h_u^{i,j}},$$
$$n^2 |u^{i+1,j+1} - u^{i,j+1} - u^{i+1,j} + u^{i,j}| \leqslant Cn\big(\sqrt{h_u^{i,j}} + \sqrt{h_u^{i+1,j}} + \sqrt{h_u^{i-1,j}}\big).$$

More concisely, we will also abbreviate this as $|\nabla_n^2 u| \leqslant Cn\sqrt{h_u^{i\pm1,j\pm1}}$, where ∇_n^2 denotes the tensor of second finite differences of u.

Proof. We recall that the density of the Hamiltonian can be rewritten in terms of the lengths and angles of the deformation (see (1.13)). In what follows, for notational convenience we will use the abbreviations $v^{i,j} := \nabla_1 u^{i,j}$, $w^{i,j} := \nabla_2 u^{i,j}$.

STEP 1 (horizontal difference quotients). We begin by estimating the horizontal second-order difference quotient. Here we distinguish two cases, the first concerning the smallness of h.

(a) *The case in which $h_u^{i,j} \leqslant c$.* In the first case we assume that $h_u^{i,j} \leqslant c$, where $c = c(a, b) > 0$ is a constant that is much smaller than the distance between the wells (and much smaller than 1). In particular, we may assume that one of the brackets in the definition of h_u^{ij} is much smaller than 1 while the other is of the order $C(a, b)$, which is a universal constant that only depends on a, b. Without loss of generality, we assume that the first bracket in the definition of h_u^{ij}, i.e. (1.13), is the small one. Thus, we obtain that, for some constant $C = C(a, b)$,

$$(|v^{i,j}| - |v^{i-1,j}|)^2 \leqslant 4((|v^{i,j}| - a)^2 + (|v^{i-1,j}| - a)^2) \leqslant Ch_u^{i,j}.$$

Moreover, we infer that

$$|(v^{i,j}, w^{i,j})| + |(v^{i-1,j}, w^{i,j})| \leqslant Ch_u^{i,j}.$$

However, by linear algebra and the non-interpenetration condition, this implies that

$$n^4 |u^{ij} + u^{i-1,j} - 2u^{i,j}|^2 = n^2 |v^{ij} - v^{i-1,j}|^2 \leqslant Cn^2 h_u^{i,j},$$

which yields the desired estimate.

(b) *The case in which $h_u^{ij} \geqslant c$.* In the case in which $h_u^{ij} \geqslant c > 0$ for some fixed constant $c = c(a, b)$, we directly use the triangle inequality:

$$n^4 |u^{ij} + u^{i-1,j} - 2u^{i,j}|^2 \leqslant 4n^2 (|v^{i,j}|^2 + |v^{i-1,j}|^2) \leqslant Cn^2 h_u^{i,j} + n^2 C(a, b) \leqslant Cn^2 h_u^{i,j}.$$

Here the last estimate follows from the lower bound assumption on h. Combining the results of (a) and (b) thus yields the full control on the horizontal second difference quotient. A similar estimate holds true for the vertical second difference quotient.

STEP 2 (mixed second-order differences). Again we consider two cases, which depend on the local energy density of two neighbouring points.

(a) *Small local energy density.* We assume that for a sufficiently small constant $c = c(a, b) > 0$ we have $h^{i,j} + h^{i+1,j} \leqslant c(a, b)$. In this case we may assume that $\nabla u^{i,j}$ and $\nabla u^{i+1,j}$ are sufficiently close to a common energy well, i.e. we may, for instance, assume that the first bracket in the definition of h_u is controlled in terms of h_u for both points (i, j) and $(i + 1, j)$ (this follows directly from the definition of $\tilde{h}_u$ but can also be inferred from lemma 1.7). Then

$$(|w^{i,j}| - a)^2 \leqslant h_u^{i,j} \quad \text{and} \quad (|w^{i+1,j}| - a)^2 \leqslant h_u^{i+1,j},$$

which implies that

$$(|w^{ij}| - |w^{i+1,j}|)^2 \leqslant h_u^{i,j} + h_u^{i+1,j}. \tag{B 1}$$

Moreover,

$$\left.\begin{aligned} (|v^{i,j}| - b)^2 &\leqslant h_u^{i,j} + h_u^{i+1,j}, \\ |(w^{i,j}, v^{i,j})| &\leqslant h_u^{i,j}, \\ |(w^{i+1,j}, v^{i,j})| &\leqslant h_u^{i,j} + h_u^{i+1,j}. \end{aligned}\right\} \tag{B 2}$$

Arguing as above, by linear algebra and the non-interpenetration condition (which can also be interpreted as a condition on the orientation of the image triangles), the combination of (B 1) and (B 2) implies that

$$n^4 |u^{i+1,j+1} - u^{i,j+1} - u^{i+1,j} + u^{i,j}|^2 \leqslant n^2 |w^{ij} - w^{i+1,j}|^2$$
$$\leqslant n^2 (h_u^{i,j} + h_u^{i+1,j}),$$

which is the desired result.

(b) *Large local energy density.* We assume that $h^{i,j} + h(\nabla u^{i+1,j}) \geqslant c(a, b) > 0$. As in step 1(a), we directly conclude by using the triangle inequality:

$$n^4 |u^{i+1,j+1} - u^{i+1,j} - u^{i,j+1} + u^{ij}|^2$$
$$\leqslant 4n^4 (|u^{i+1,j+1} - u^{i+1,j}|^2 + |u^{i,j+1} - u^{ij}|^2)$$
$$\leqslant n^2 (4(|w^{ij}| - a)^2 + 8(a^2 + b^2) + 4(|w^{i+1,j}| - a)^2)$$
$$\leqslant 4n^2 (h_u^{i,j} + h_u^{i+1,j}) + n^2 C(a, b)$$
$$\leqslant C(a, b) n^2 (h_u^{i,j} + h_u^{i+1,j}).$$

This concludes the proof. □

Appendix C. Sketch of proof of the discrete coarea formula

In this section we give a (very rough) sketch of the proof of the discrete coarea formula. More precisely, we show that for any grid function $f^{ij}\colon \Omega_n \to \mathbb{R}$ the following holds:

$$\int_0^\infty \mathrm{Per}_M(\{(i,j)\colon f^{ij} \geqslant t\})\,\mathrm{d}t \leqslant C \sum_{(i,j)\in nM} \frac{1}{n^2}|\nabla_n f^{ij}|. \tag{C1}$$

Similarly to the continuous case (see [17]), this is a consequence of an integration by parts argument in combination with the bathtub principle. We consider the super-level sets $E_t := \{(i,j)\colon f^{ij} \geqslant t\}$ associated with the function f^{ij}. Let $\sigma^{ij} = (\sigma_1^{ij}, \sigma_2^{ij})\colon \Omega_n \to \mathbb{R}^2$ be any test function with $|\sigma^{ij}| \leqslant 1$. Then we have

$$\sum_{(i,j)\in nM} \frac{1}{n^2}[n(f^{i+1,j} - f^{i,j})\sigma_1^{i,j} + n(f^{i,j+1} - f^{i,j})\sigma_2^{i,j}]$$

$$= \int_0^\infty \sum_{(i,j)\in\partial(nE_t)} \frac{1}{n}(\sigma^{i,j}, \nu^{i,j})\,\mathrm{d}t. \tag{C2}$$

Here $\nu(x)\colon \partial(nE_t) \to \mathbb{R}^2$ denotes 'the outer unit normal field' to $\partial(nE_t)$. As $\partial(nE_t)$ is only piecewise affine, we define it as the classical outer unit normal field at all points at which the boundary is C^1. Due to the choice of our interpolation, the only possibility of violating the C^1 condition for the boundary is by forming corners of $45°$, $90°$, $180°$, $225°$, $270°$. These corners are given as the intersection of two C^1 curves that are tangential to two grid edges. Hence, at these corner points (i,j) we define $\nu^{ij} = \lim_{x_1\to(i,j)} \nu(x_1) + \lim_{x_2\to(i,j)} \nu(x_2)$, where x_1, x_2 are points approaching the corner along the two intersecting grid edges.

We note that the left-hand side of (C2) is clearly bounded from above by

$$\sum_{(i,j)\in nM} \frac{1}{n^2}[n|f^{i+1,j} - f^{i,j}| + n|f^{i,j+1} - f^{i,j}|].$$

Hence,

$$\int_0^\infty \sum_{(i,j)\in\partial(nE_t)} \frac{1}{n}(\sigma^{i,j}, \nu^{i,j})\,\mathrm{d}t \leqslant \sum_{(i,j)\in nM} \frac{1}{n^2}[n|f^{i+1,j} - f^{i,j}| + n|f^{i,j+1} - f^{i,j}|].$$

Choosing σ^{ij} such that $(\sigma^{i,j}, \nu^{i,j}) = 1$ on $\partial(nE_t)$ proves (C1).

Appendix D. Proof of the well-definedness of the algorithm for the perturbed grid construction

In this section we present a proof of the well-definedness of the algorithm that yields the new grid in step 4(a) of the proof of proposition 3.7.

$$\overset{I_1}{\longmapsto} \quad \longrightarrow \quad \overset{I_2}{\longmapsto} \quad \longrightarrow \quad \overset{I_3}{\longmapsto} \quad \longrightarrow \quad \overset{I_4}{\longmapsto} \quad \longrightarrow \quad \cdots$$
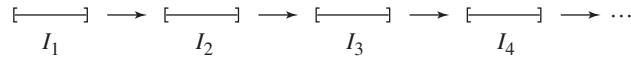
Figure 3. The one-dimensional chain of intervals described in step 1. Without loss of generality we may assume that the intervals are given as $I_n = [n-1, n]$ with $n \in \mathbb{N}$. The arrow between the intervals indicates the neighbouring relation. In a *chain of intervals* each of the intervals only has one neighbour.

LEMMA D.1. *The algorithm in step 4(a) of the proof of proposition 3.7 is well-defined, i.e. it is possible to choose the parameter $\theta > 0$ such that there exists a number $c_\theta > 0$ with the property that the volume fraction of possible choices in each step is non-empty and bounded from below:*

$$|\{\text{possible choices in step } m\}| \geqslant c_\theta |B_m|. \tag{D 1}$$

The main difficulty here is to ensure that in the selection of the *possible choices in step $m+1$* not too many points are deleted. In particular, we have to ensure that although for each pair B_m, B_{m+1} there always is a volume fraction of $(1-\theta)|B_m \times B_{m+1}|$ rigid pairs, these pairs do not involve too many points that had to be deleted during one of the previous m steps. If this were the case, it could in principle occur that the algorithm terminates without having constructed a new grid.

Proof. We divide the proof into two steps and first show the analogous result in the setting of one-dimensional intervals of equal length that form a one-dimensional chain (see figure 3). In the second step we then show that our algorithm essentially reduces to the previous setting.

STEP 1. We argue in the context of one-dimensional intervals of equal size, which form a one-dimensional chain (see figure 3). More precisely, we imagine that we have a partition of the real half-line into intervals $I_n := [n, n+1]$ for $n \in \mathbb{N} \cup \{0\}$. The end-points are the vertices of our one-dimensional grid. We assume that we have an analogue of proposition 2.4, asserting that for each neighbouring pair I_n, I_{n+1} of intervals, the volume of rigid pairs (x, y) of points in $I_n \times I_{n+1}$ has volume at least $(1-\theta)|I_n \times I_{n+1}|$. We apply the algorithm described in step 4(a) of the proof of proposition 3.7 to this one-dimensional 'chain of intervals' (where B_m is replaced by I_m). We claim that this algorithm is well-defined in the sense of (D 1), and hence does not terminate before having constructed a new perturbed grid.

To this end, we prove that at any stage of the algorithm the points that are rigid in I_m and are *possible choices in step $m+1$* never become the empty set. On the contrary, we show that they satisfy the bound (D 1). We claim that this is true, since θ (which is fixed throughout the algorithm and in particular does not depend on the step m) can be chosen sufficiently small. Indeed, for each pair I_m, I_{m+1} the volume of rigid pairs $(x, y) \in I_m \times I_{m+1}$ is $(1-\theta)|I_m \times I_{m+1}|$. However, this might be diminished by the points that have been removed in the previous steps of the algorithm (as it could be the case that all of these deleted points were rigid points for the next step; see figure 4). Hence, the effective volume of rigid pairs could be smaller than $(1-\theta)|I_m \times I_{m+1}|$. In this context the worst case scenario is given by the following setting: all points of I_{m+1} form rigid pairs with the 'bad set' I_m^{bad}
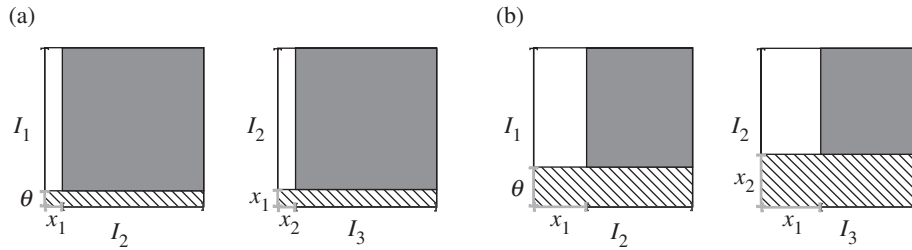
(a)

(b)

Figure 4. The worst case scenario described in step 1 in the proof of lemma D.1. Although the overall volume fraction of rigid points between two intervals I_m, I_{m+1} is always given by $(1-\theta)|I_m \times I_{m+1}|$, it is in principle possible that the *effectively* useful volume fraction in step m of rigid pairs in the algorithm is smaller than that. This is due to the possibility that a lot of rigid points are given by pairs (x, y) with $x \in I_m$, $y \in I_{m+1}$ such that $x \in I_m^{\text{bad}}$, i.e. that many points x lie in the set that had to be deleted from being a possible choice in a previous step of the algorithm. Here this is illustrated for (a) $\theta = 0.1$ and (b) $\theta = 0.25$. Here the rigid points are given by the union of the dashed and the dark grey rectangles. The white rectangle is the set of non-rigid points between the intervals. In the first step the intervals I_0 and I_1 have a volume fraction of $(1-\theta)|I_0 \times I_1|$ rigid pairs. Hence, after deleting the non-rigid pairs a volume fraction of at least θ points of I_1 is rigid. However, a volume fraction of up to θ of I_1 consists of bad points, which had to be deleted. In the next step, which is depicted as the first schematic illustration in (a), the intervals I_1, I_2 still have a volume fraction of $(1-\theta)|I_1 \times I_2|$ rigid points. These are schematically depicted as the union of the dashed and the dark grey rectangles. However, it is possible that a large amount of rigid pairs involve points in I_1^{bad}. These are indicated as the points in the dashed rectangle. (The light grey interval on the vertical axis corresponds to the bad points I_1^{bad} of I_1. Thus, in order to construct the new perturbed grid, only the grey pairs are of use. However, this implies that in I_2 the light grey interval of length x_1^θ is deleted by the algorithm, yielding a bad set I_2^{bad} of length $x_1^\theta := \theta/(1-\theta)$.) In the next step, which is depicted in the second illustration in (a), this could happen again: a large fraction of rigid points is given by pairs in which the first component lies in I_2^{bad}. Thus, again, only the dark grey square can be used as rigid points in order to construct the new grid. Thus, $|I_2^{\text{bad}}| =: x_2^\theta = \theta/(1 - x_1^\theta)$. As (a) indicates, for $\theta = 0.1$ the sequence $x_m^{0.1}$ converges quite fast to the value $\bar{x}^{0.1} \sim 0.112702$. The figure (b) on the right depicts the same scenario for the $\theta = 0.25$. This is the largest value of θ for which convergence still holds with $\bar{x}^{0.25} = 0.5$. For larger values of θ the algorithm terminates before having created a new grid.

of I_m, i.e. with those points that were removed from being possible choices in the previous steps of the algorithm, and the volume of the points in I_{m+1} that form rigid pairs with points in $I_m \setminus I_m^{\text{bad}}$ is minimized (see figure 4). In the first step of the algorithm the 'bad set' I_m^{bad} can be of measure at most θ. However, in principle this could increase in the next steps. We have to show that the 'bad set' remains small (depending on θ). Indeed, following the description of the previous worst case scenario, we estimate the 'bad set' I_m^{bad}. Computing the volume of the bad set in step m (see figure 4), we infer that the bad set I_m^{bad} is bounded by the solution of the recursion relation

$$x_m^\theta = \frac{\theta}{1 - x_{m-1}^\theta}, \quad x_0^\theta = \theta.$$

However, if $\theta \leqslant \frac{1}{4}$, this recursion relation converges to the limit $\bar{x}^{\theta} := \frac{1}{2}(1 - \sqrt{1 - 4\theta})$, due to monotonicity. Hence, the bad set remains bounded. This yields our claim (D 1).

STEP 2. We claim that the previous step implies that the grid construction algorithm in the proof of proposition 3.7 works for our two-dimensional set-up. First we note that the fact that the balls become smaller does not matter, as the result only depends on the respective volume fractions involved. Secondly, we note that also in the two-dimensional case, we have to rule out the worst case scenario of an accumulating 'bad set' and that the recursion relation from above would still give the desired bound if there was only a single neighbour to each vertex. Finally, we notice that the presence of *finitely* many neighbouring vertices (instead of having a single vertex only) does not change the convergence of the algorithm (if θ is decreased according to the number of possible neighbouring vertices). This is a consequence of the fact that in comparison to the setting in step 1, additional points are deleted in the presence of several neighbours only finitely many times. □

References

1   R. Alicandro and M. Cicalese. A general integral representation result for continuum limits of discrete energies with superlinear growth. *SIAM J. Math. Analysis* **36** (2004), 1–37.
2   L. Ambrosio, N. Fusco and D. Pallara. *Functions of bounded variation and free discontinuity problems*, vol. 254 (Oxford: Clarendon Press, 2000).
3   I. Baele, G. Van Tendeloo and S. Amelinckx. Microtwinning in Ni–Mn resulting from the $\beta \to \theta$ martensitic transformation. *Acta Metall.* **35** (1987), 401–412.
4   J. Ball and R. James. Fine phase mixtures as minimizers of energy. *Arch. Ration. Mech. Analysis* **100** (1987), 13–52.
5   J. M. Ball and C. Mora-Corral. A variational model allowing both smooth and sharp phase boundaries in solids. *Commun. Pure Appl. Analysis* **8** (2009), 55–81.
6   K. Bhattacharya. *Microstructure of martensite*, Oxford Series on Materials Modelling (Oxford University Press, 2003).
7   X. Blanc, C. L. Bris and P.-L. Lions. From molecular models to continuum mechanics. *Arch. Ration. Mech. Analysis* **64** (2002), 341–381.
8   A. Braides. *From discrete systems to continuum problems.* Lecture Notes given at the University of Wuerzburg, 2012. (Available at http://www.mat.uniroma2.it/~braides/1112/LectureNotesWuerzburg.pdf.)
9   A. Braides and M. Cicalese. Surface energies in nonconvex discrete systems. *Math. Models Meth. Appl. Sci.* **17** (2007), 985–1037.
10   A. Braides and M. S. Gelli. Asymptotic analysis of microscopic impenetrability constraints for atomistic systems. *J. Mech. Phys. Solids* **96** (2016), 235–251.
11   J. Braun and B. Schmidt. On the passage from atomistic systems to nonlinear elasticity theory for general multi-body potentials with p-growth. *Networks Heterogen. Media* **8** (2013), 879–912.
12   S. Conti. Branched microstructures: scaling and asymptotic self-similarity. *Commun. Pure Appl. Math.* **53** (2000), 1448–1474.
13   S. Conti and B. Schweizer. Gamma convergence for phase transitions in impenetrable elastic materials. In *Multi-scale problems and asymptotic analysis*, GAKUTO International Series: Mathematical Sciences and Applications, vol. 24, pp. 105–118 (Tokyo: Gakkotosho, 2006).
14   S. Conti and B. Schweizer. Rigidity and gamma convergence for solid–solid phase transitions with SO(2) invariance. *Commun. Pure Appl. Math.* **59** (2006), 830–868.
15   S. Conti and B. Schweizer. A sharp-interface limit for a two-well problem in geometrically linear elasticity. *Arch. Ration. Mech. Analysis* **179** (2006), 413–452.
16   G. Dolzmann and S. Müller. Microstructures with finite surface energy: the two-well problem. *Arch. Ration. Mech. Analysis* **132** (1995), 101–141.

17   L. C. Evans and R. F. Gariepy. *Measure theory and fine properties of functions* (Boca Raton, FL: CRC Press, 2015).

18   G. Friesecke and F. Theil. Validity and failure of the Cauchy–Born hypothesis in a two-dimensional mass-spring lattice. *J. Nonlin. Sci.* **12** (2002), 445–478.

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

20   G. Kitavtsev, S. Luckhaus and A. Rüland. Surface energies arising in microscopic modeling of martensitic transformations. *Math. Models Meth. Appl. Sci.* **25** (2015), 647–683.

21   R. V. Kohn and S. Müller. Branching of twins near an austenite-twinned-martensite interface. *Phil. Mag.* A **66** (1992), 697–715.

22   A. C. Kort and F. Otto. A quantitative rigidity result for the cubic to tetragonal phase transition in the geometrically linear theory with interfacial energy. *Proc. R. Soc. Edinb.* A **142** (2012), 273–327.

23   A. Lorent. The two-well problem with surface energy. *Proc. R. Soc. Edinb.* A **136** (2006), 795–805.

24   A. Lorent. The regularisation of the N-well problem by finite elements and by singular perturbation are scaling equivalent in two dimensions. *ESAIM: Control Optim. Calc. Variations* **15** (2009), 322–366.

25   S. Luckhaus and L. Mugnai. On a mesoscopic many body Hamiltonian describing elastic shears and dislocations. *Continuum Mech. Thermodyn.* **22** (2010), 251–290.

26   S. Müller. Variational models for microstructure and phase transitions. In *Calculus of variations and geometric evolution problems* (ed. S. Hildebrandt and M. Struwe), Lecture Notes in Mathematics, vol. 1713, pp. 85–210 (Springer, 1999).

27   P. Rosakis. Continuum surface energy from a lattice model. *Networks Heterogen. Media* **9** (2014), 1556–1801.