A Compactness and Structure Result for a Discrete Multi-well Problem with $SO(n)$ Symmetry in Arbitrary Dimension

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Abstract

In this note we combine the “spin-argument” from Kitavtsev et al. (Proc R Soc Edinb Sect A Mater 147(5):1041–1089, 2017) and the n -dimensional incompatible, one-well rigidity result from Lauteri and Luckhaus (An energy estimate for dislocation configurations and the emergence of Cosserat-type structures in metal plasticity, 2016), in order to infer a new proof for the compactness of discrete multi-well energies associated with the modelling of surface energies in certain phase transitions. Mathematically, a main novelty here is the reduction of the problem to an incompatible one-well problem. The presented argument is very robust and applies to a number of different physically interesting models, including for instance phase transformations in shape-memory materials but also anti-ferromagnetic transformations or related transitions with an “internal” microstructure on smaller scales.

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1. Introduction

It is the purpose of this note to provide a short, essentially self-contained compactness argument and structure result for a multi-well discrete-to-continuum problem with $SO(n)$ symmetry arising in the variational modelling of certain phase transitions in arbitrary dimension by combining the ingredients from [12] and [13, 14].

Although similar results were already proved in the context of martensitic phase transitions occurring in the modelling of shape-memory materials in [12] and [2], the present article contains two main novelties: on the one hand, the mathematical argument leading to the structure result is of interest, since in the present note we neither invoke the rigidity results of [7] nor of [5]. Instead, we reduce the problem to the setting of an (incompatible) one-well problem. On the other hand, our arguments extend to a large class of Hamiltonians with possibly quite nonlocal interactions. These cover a number of relevant physical phase transformations, including, for instance, the anti-ferromagnetic transitions. The generality of the systems which are covered here goes far beyond the ones from [12] or [2].

From a mathematical point of view, the result is based on the following idea: instead of relying on [7] or on [5], we combine the “spin argument” from [12] with the n -dimensional strong-supercritical and weak-critical, incompatible, one-well rigidity results from [14] and their consequences from [13]. To this end, we reduce the compatible multi-well problem to an auxiliary, incompatible one-well setting, which allows us to invoke [13]. We believe that this strategy—and in particular the reduction to the auxiliary one-well problem—is interesting in its own right and can be applied to a quite wide range of physically relevant models.

1.1. Outline of the Article

In order to introduce the new ideas in an as simple as possible a set-up, the first part of the article (Sections 2–4) deals with a special Hamiltonian and only considers the physical setting of a martensitic transition in shape-memory alloys. For a nearest neighbour Hamiltonian, which is easy to formulate and which is presented in Section 2, we explain the interplay between the spin argument (c.f. Section 3) and the incompatible, one-well rigidity results from [14] (c.f. Section 4). As the main result in this context, we derive the structure result formulated in Theorem 1.

In Section 5, we then generalize these ideas to a much larger class of physical systems and a much larger family of underlying Hamiltonians. Here we allow for arbitrary finite range interactions. Also in this setting we deduce a compactness and structure result (see Theorem 4). This, in particular, shows the robustness of the underlying mathematical argument.

2. The Set-Up and the Main Result for Martensitic Phase Transformations Modelled by Nearest Neighbour Interactions

2.1. Set-Up

In order to formulate our main result in the context of nearest neighbour interaction models for martensitic phase transformations, we first outline the precise set-up of our n -dimensional, discrete multi-well problem. Here we impose several conditions on the wells, the underlying triangulation and the associated energy, which we explain in the sequel. In order to keep the set-up as simple as possible,

we first discuss a model scenario and postpone the analysis of more general systems (including more nonlocal interactions and periodic internal microstructures which may be present in other physical systems) to Section 5.

We begin by introducing the relevant ingredients in formalizing the precise setting.

2.1.1. Wells Let $U_1, \dots, U_k \in \mathbb{R}^{n \times n}$ be pairwise different, symmetric, positive definite matrices. Let $K = \bigcup_{j=1}^k SO(n)U_j$ denote the union of the (energy) wells $SO(n)U_j$. Assume that the wells are pairwise rank-one connected, that is assume that there exist two rotations $Q_{ij}^\pm$ and vectors $a_{ij}^\pm \in \mathbb{R}^n \setminus \{0\}$, $b_{ij}^\pm \in S^{n-1}$ such that

$$U_i - Q_{ij}^\pm U_j = a_{ij}^\pm \otimes b_{ij}^\pm. \quad (1)$$

Suppose moreover that the wells are separated:

$$\min_{i \neq j} \text{dist}(SO(n)U_i, SO(n)U_j) \geq d > 0. \quad (2)$$

2.1.2. Triangulation Let $\Omega \subset \mathbb{R}^n$ be a bounded open Lipschitz domain. For $m \in \mathbb{N}$ suppose that

$$\mathcal{T}_m = \{T_\alpha : \alpha \in I_m\}$$

is a family of *non-degenerate triangulations* of Ω , that is assume that for each $m \in \mathbb{N}$ we have that

- (i) $I_m = \{1, \dots, N_m\} \subset \mathbb{N}$ is a finite index set such that for some constants $0 < c_1 \leq c_2 < \infty$ which do not depend on m we have $c_1 m^n \leq N_m \leq c_2 m^n$,
- (ii) $\Omega = \bigcup_{\alpha \in I_m} T_\alpha$,
- (iii) the sets T_α are non-degenerate, up to null-sets disjoint tetrahedra.

Here *non-degenerate* means that there are constants $\tilde{c}_{1,T}, \tilde{c}_{2,T} > 0$, which are independent of m , such that for each $\alpha \in I_m$,

$$\tilde{c}_{1,T} m^{-1} \leq r_{i,\alpha} \leq \text{diam}(T_\alpha) \leq \tilde{c}_{2,T} m^{-1},$$

where $r_{i,\alpha}$, $\text{diam}(T_\alpha)$ denote the in-radius and the diameter of the tetrahedron $T_\alpha \in \mathcal{T}_m$.

As a consequence of the non-degeneracy of the triangulation, we obtain that there are constants $c_{1,T}, c_{2,T} > 0$ (which are independent of m) such that, for all $T_\alpha \in \mathcal{T}_m$,

$$c_{1,T} m^{-n} \leq |T_\alpha| \leq c_{2,T} m^{-n}, \quad (3)$$

where $|T_\alpha|$ denotes the Lebesgue measure of T_α . Further assume that the triangulation $\mathcal{T}_m$ is incompatible with the rank-one connections in K , that is there exists $\delta_0 > 0$ (which is independent of m) such that for any $T_\alpha \in \mathcal{T}_m$ and for any normal $b \in S^{n-1}$ associated to an $(n-1)$ -dimensional interface of T_α we have that

$$|b \cdot b_{ij}^\pm| \leq 1 - \delta_0. \quad (4)$$

Here $b_{ij}^\pm \in S^{n-1}$ denotes any normal vector from (1). In particular, by compactness of the involved sets this implies that there exists a constant $\bar{d} > 0$ (depending on $\delta_0 > 0$ and d) such that for all choices of $i_1, i_2 \in \{1, \dots, k\}$ with $i_1 \neq i_2$

$$\min_{Q \in SO(n)} \min_{\substack{b \in S^{n-1} \text{ satisfying (4) \\ for all } i, j \in \{1, \dots, k\}}} \min_{\substack{\tau_1, \dots, \tau_{n-1} \in S^{n-1}, \\ \tau_l \cdot b = 0, \\ \tau_{i_1} \cdot \tau_{i_2} = 0, \\ l_1 \neq l_2}} \max_{\tau_l \in \{\tau_1, \dots, \tau_{n-1}\}} |(U_{i_1} - QU_{i_2})\tau_l| \geq \bar{d} > 0. \quad (5)$$

Indeed, by compactness this minimum is attained; it does not vanish, as this would yield a rank-one connection between $SO(n)U_{i_1}$ and $SO(n)U_{i_2}$, which is different from the ones listed in (1) in Section 2.1.1.

Remark 2.1. We note that by the assumption (4) the constant $\bar{d}$ from (5) has a strictly positive lower bound which is *independent* of m .

2.1.3. Deformation and Energy Let $\mathcal{A}_m$ denote the set of piecewise affine deformations $u \in W^{1,\infty}(\Omega, \mathbb{R}^n)$ adapted to the grid $\mathcal{T}_m$, that is for each $\alpha \in I_m$ we have $\nabla u|_{T_\alpha} = \text{const.}$

For $u \in \mathcal{A}_m$ we then consider the energy

$$E_m(u) = \int_{\Omega} h(\nabla u) dx, \quad (6)$$

where the energy density $h : \mathbb{R}_+^{n \times n} \rightarrow [0, \infty)$ satisfies the comparability condition

$$c_1 \text{dist}^2(M, K) \leq h(M) \text{ for all } M \in \mathbb{R}_+^{n \times n} \quad (7)$$

for some constant $c_1 > 0$. Here the notation $\mathbb{R}_+^{n \times n}$ denotes the positive, definite $n \times n$ matrices. In addition we restrict our attention to sequences of deformations $\{u_m\}_{m \in \mathbb{N}} \subset \mathcal{A}_m$ which are of *surface energy scaling*, that is we assume that there exists a constant $C > 1$ (which does not depend on $m \in \mathbb{N}$) such that

$$E_m(u_m) \leq Cm^{-1}. \quad (8)$$

2.1.4. Remarks on the Assumptions from Sections 2.1.1–2.1.3 Let us comment on the assumptions from Sections 2.1.1–2.1.3:

- Section 2.1.1 asserts that we are considering a non-degenerate multi-well problem, which arises, for instance, in the modelling and analysis of the stress-free deformations of shape-memory materials. We remark that in this context, we could also have added wells with only one or no rank-one connection to the other wells. As our main motivation however stems from microstructures allowing for the *presence* of interfaces, we do not pursue this in the sequel. We also remark that the condition on the symmetry of the matrices U_j is not needed from a mathematical point of view; the restriction is only motivated by the physical application to shape-memory alloys which we have in mind. In Section 5 we will drop this condition.

- The conditions in Section 2.1.2 render our problem a discrete problem, since in Section 2.1.3 we only consider piecewise affine deformations adapted to the triangulation. The set of admissible grids is quite large; in particular we do not require the underlying triangulations to be periodic and only ask for a mild non-degeneracy in (3). Requiring the condition (4) is however crucial for our purposes since it implicitly provides a “surface energy” regularizing contribution in the energy (6) (this “finite element regularization” was observed for perhaps the first time in the work of Lorent [16], c.f. also the references therein).
- The energy densities h which we consider are also only subject to mild restrictions. The requirement in (7) ensures that in tetrahedra with low energy the deformation gradient is close to the energy wells from Section 2.1.1. Finally, the condition (8) ensures that we only consider deformations with the simplest possible microstructures, that is we only consider deformations of which we expect that they are very close to being exact solutions to the differential inclusion $\nabla u \in K$. The smallness condition in (8) is such that it for instance excludes microstructures which display branching phenomena.

2.2. The Main Result

We assume that the conditions from Section 2.1 hold. Motivated by discrete-to-continuum limits as in [2, 11, 12], we then seek to deduce the following convergence and structure result:

Theorem 1. *Let $n \geq 2$ and assume that $U_1, \dots, U_k, K, E_m$ are as in Section 2.1. Let $\{u_m\}_{m \in \mathbb{N}} \subset \mathcal{A}_m$ be a sequence satisfying (8). Then, there exist (up to null-sets) disjoint Caccioppoli partitionings*

$$\Omega = \bigcup_{j=1}^k \Omega_j, \quad \Omega_j = \bigcup_{i=1}^{\infty} \Omega_{j,i},$$

with underlying characteristic functions $\chi_j, \chi_{j,i} : \Omega \rightarrow \{0, 1\}$, which in particular satisfy

$$\sum_{j=1}^k \chi_j = 1, \quad \sum_{i=1}^{\infty} \chi_{j,i} = \chi_j, \quad \sum_{j=1}^k \sum_{i=1}^{\infty} |D\chi_{j,i}|(\Omega) < \infty,$$

a deformation $u \in W^{1,\infty}(\Omega)$ with $\nabla u \in BV(\Omega, K)$ and rotations $R_{j,i}$ such that

$$\nabla u_m \rightarrow \nabla u \text{ in } L^2(\Omega), \quad \nabla u = \sum_{j=1}^k \sum_{i=1}^{\infty} R_{j,i} U_j \chi_{j,i}.$$

Here and in the sequel we use the convention that we denote the full (distributional) derivative of a (BV) function χ by $D\chi$ and use $\nabla\chi$ for its absolutely continuous part. The total variation measure of a BV function is denoted by $|D\chi|(\cdot)$.

As in [2], Lemma 4.2, in addition to the structure result of Theorem 1 one can show that the jump interfaces of ∇u are locally flat and can only intersect in “corners” (that is lower dimensional objects).

The main idea of the proof of Theorem 1 is to combine the “spin-argument” from Lemma 2.1 in [12] (which we briefly recall in Section 3), which was simultaneously also derived in [2], with the one-well, incompatible supercritical rigidity estimate from [13] (c.f. also [14]). Here the reduction of the multi-well problem to an (incompatible) auxiliary one-well problem is of particular interest and constitutes the main novelty of the proof. We repeat that while in the context of the modelling and analysis of shape memory alloys the compactness result itself is not new, the generality in which it holds (c.f. the physical models covered in Section 5) and the argument for this result are new and of interest in themselves.

3. The “Spin-Argument”

For self-containedness and completeness, we briefly recall the “spin-argument” from [12] and [2]. As a slight extension with respect to the argument from [12] we directly prove it in arbitrary dimension.

Lemma 3.1. *Let $n \geq 2$. Let $\mathcal{T}_m$ be as in Section 2.1.2 and assume that $T_{i_1}, T_{i_2} \in \mathcal{T}_m$ are adjacent grid tetrahedra, that is assume that T_{i_1} and T_{i_2} have a common $(n-1)$ -dimensional interface with interface normal $b \in S^{n-1}$. Let*

$$c_0 := \min\{\bar{d}, d\}, \quad (9)$$

where $d, \bar{d} > 0$ are the constants from (2) and (5). Suppose further that for $u \in \mathcal{A}_m$,

$$|\nabla u|_{T_{i_1}} - U_{i_1}| \leq \frac{c_0}{100}, \quad (10)$$

but

$$|\nabla u|_{T_{i_2}} - QU_{i_1}| > \frac{c_0}{100} \quad (11)$$

for all $Q \in SO(n)$. Then,

$$\text{dist}(\nabla u|_{T_{i_2}}, K) > \frac{c_0}{100}. \quad (12)$$

Proof. We show that for any $j \in \{1, \dots, k\} \setminus \{i_1\}$ and for any $Q \in SO(n)$ we have

$$|\nabla u|_{T_{i_2}} - QU_j| > \frac{c_0}{100}, \quad (13)$$

where $c_0 > 0$ (c.f. Remark 2.1) is the constant from (9). By our assumption (11) the claim of Lemma 3.1 follows, once (13) is shown.

To this end we note that as T_{i_1}, T_{i_2} are neighbouring grid tetrahedra, they share a common $(n-1)$ -dimensional interface with normal $b \in S^{n-1}$. In particular,

$$(\nabla u|_{T_{i_1}} - \nabla u|_{T_{i_2}})\tau = 0 \quad (14)$$

for all $\tau \in S^{n-1}$ with $\tau \cdot b = 0$. By virtue of (10) and (14) we infer that

$$\max_{\tau \in S^{n-1}, \tau \cdot b = 0} |(U_{i_1} - \nabla u|_{T_{i_2}})\tau| \leq \frac{c_0}{100}. \quad (15)$$

Building on these observations and by definition of c_0 and $\bar{d}$ (c.f. (5)), the triangle inequality leads to

$$\begin{aligned} |\nabla u|_{T_{i_2}} - \bar{Q}U_{j_0}| &\geq |(U_{i_1} - \bar{Q}U_{j_0})\tau_0| - \max_{\tau \in S^{n-1}, \tau \cdot b = 0} |(\nabla u|_{T_{i_1}} - U_{i_1})\tau| \\ &\quad - \max_{\tau \in S^{n-1}, \tau \cdot b = 0} |(\nabla u|_{T_{i_1}} - \nabla u|_{T_{i_2}})\tau| \\ &\geq c_0 - \frac{c_0}{100} - 0 > \frac{c_0}{100}. \end{aligned}$$

Here the vector $\tau_0 \in S^{n-1}$, $\tau_0 \cdot b = 0$ is chosen such that the inequality (5) holds. This yields (13), which thus concludes the argument for the lemma.

Lemma 3.2. *Let $n \geq 2$, and assume that the conditions from Section 2.1 hold. Then,*

$$\# \left\{ \alpha \in I_m : \text{dist}^2(\nabla u_m|_{T_\alpha}, K) \geq \frac{c_0^2}{100^2} \right\} \leq \frac{C 100^2}{c_0^2 c_1 c_{1,T}} m^{n-1}. \quad (16)$$

Proof. The claim follows from the energy estimate (8) and a counting argument. Indeed, let $N := \#\{\alpha \in I_m : \text{dist}^2(\nabla u_m|_{T_\alpha}, K) \geq \frac{c_0^2}{100^2}\}$. Then, by (8), (7) and (3),

$$N c_1 100^{-2} c_0^2 c_{1,T} m^{-n} \leq N \text{dist}^2(\nabla u_m|_{T_\alpha}, K) \inf_{\alpha} |T_\alpha| \leq E_m(u) \leq C m^{-1}.$$

Solving for N yields the claim.

Proposition 1. *Let $n \geq 2$ and suppose that the conditions from Section 2.1 are valid. Assume that $\{u_m\}_{m \in \mathbb{N}}$ is a sequence of deformations satisfying (8). Further, for $j \in \{1, \dots, k\}$, let*

$$\begin{aligned} \Omega_{j,m} &:= \{T_\alpha \in \mathcal{T}_m : \text{dist}(\nabla u_m|_{T_\alpha}, SO(n)U_j) \leq \frac{c_0}{100}\}, \\ \Omega_{b,m} &:= \{T_\alpha \in \mathcal{T}_m : \text{dist}(\nabla u_m|_{T_\alpha}, K) > \frac{c_0}{100}\}. \end{aligned}$$

Then there exist Caccioppoli sets $\Omega_1, \dots, \Omega_k \subset \Omega$ such that

$$\chi_{\Omega_{j,m}} \rightarrow \chi_{\Omega_j}, \quad \chi_{\Omega_{b,m}} \rightarrow 0 \text{ in } L^1(\Omega), \quad \Omega = \bigcup_{j=1}^k \Omega_j.$$

Here $\chi_{\Omega_{j,m}}, \chi_{\Omega_{b,m}}, \chi_{\Omega_j} : \Omega \rightarrow \{0, 1\}$ denote the characteristic functions associated with the corresponding sets.

Proof. The proof follows from the Lemmas 3.1 and 3.2. Indeed, for $j \in \{1, \dots, k\}$,

$$\begin{aligned} \text{Per}(\Omega_{j,m}) &\leq \#\{T_\alpha \in \mathcal{T}_m : \text{dist}(\nabla u|_{T_\alpha}, SO(n)U_j) > \frac{c_0}{100}\} \max_{T_\alpha \in \mathcal{T}_m} |\partial T_\alpha| \\ &\leq \#\{T_\alpha \in \mathcal{T}_m : \text{dist}(\nabla u|_{T_\alpha}, K) > \frac{c_0}{100}\} \max_{T_\alpha \in \mathcal{T}_m} |\partial T_\alpha| \\ &\leq \frac{C100^2}{c_0^2 c_1 c_{1,T}} m^{n-1} 3\tilde{c}_{2,T} m^{1-n} \leq \frac{3C100^2 \tilde{c}_{2,T}}{c_0^2 c_1 c_{1,T}}. \end{aligned}$$

Here in the first estimate we used that at boundary tetrahedra Lemma 3.1 asserts that the local energy is larger than $\frac{c_0}{100}$. In the second inequality we just extended the relevant set, and in the last inequality we invoked the bound from Lemma 3.2. Hence, in particular, $|D\chi_{\Omega_{j,m}}|(\Omega) \leq \frac{3C100^2 \tilde{c}_{2,T}}{c_0^2 c_1 c_{1,T}}$, which yields that along a subsequence

$\chi_{\Omega_{j,m}} \rightarrow \chi_{\Omega_j}$ in $L^1(\Omega)$ and $\chi_{\Omega_j} \in BV(\Omega)$. As $\text{Per}(\Omega_{b,m}) \leq \sum_{j=1}^k \text{Per}(\Omega_{j,m})$ we thus also obtain a similar uniform perimeter bound for $\Omega_{b,m}$ and therefore $\chi_{\Omega_{b,m}} \rightarrow \chi_{\Omega_b}$ along a further subsequence. Since $\Omega = \Omega_{b,m} \cup \bigcup_{j=1}^k \Omega_{j,m}$, the sets $\Omega_{b,m}, \Omega_{1,m}, \dots, \Omega_{k,m}$ hence form a Caccioppoli partitioning of Ω with a uniform (in m) perimeter bound. As a consequence, $\Omega_b, \Omega_1, \dots, \Omega_k$ also form a Caccioppoli partitioning of Ω (c.f. Theorem 4.19 in [3]).

Finally, we note that $|\Omega_b| = 0$, as by Lemma 3.2 we have that

$$\begin{aligned} |\Omega_b| &\leq \#\{T_\alpha \in \mathcal{T}_m : \text{dist}(\nabla u|_{T_\alpha}, K) > \frac{c_0}{100}\} \max_{T_\alpha \in \mathcal{T}_m} |\partial T_\alpha| \\ &\leq \frac{C100^2}{c_0^2 c_1 c_{1,T}} m^{n-1} c_{1,T} m^{-n} \\ &= C100^2 (c_0^2 c_1)^{-1} m^{-1} \rightarrow 0 \text{ as } m \rightarrow \infty. \end{aligned}$$

This concludes the argument.

4. Proof of Theorem 1

4.1. A Compactness Result for Incompatible Fields Close to Rotations

With the result of Lemma 1 to hand, we approach the proof of our main result. In this context, we will frequently identify vector fields $v \in L^2(\Omega, \mathbb{R}^n)$ with co-vectorfields $\omega = v^\flat = \sum_{j=1}^n v_j dx_j \in L^2(\Omega, \Lambda^1)$. If $A \in L^2(\Omega, \mathbb{R}^{n \times n})$ we correspondingly identify it with $\omega \in L^2(\Omega, \Lambda^1)^n$. Furthermore, with slight abuse of notation for $v \in C_0^\infty(\Omega, \mathbb{R}^n)$ we do not distinguish between $\text{Curl}(v) = (*dv)^\sharp$, where $*$ denotes the Hodge star operator and $\sharp$ the sharp operator (c.f. [15]), and the two-form $dv^\flat = d\omega$, where

$$dv^\flat = \sum_{j < k} \left(\frac{\partial v^j}{\partial x_k} - \frac{\partial v^k}{\partial x_j} \right) dx^j \wedge dx^k.$$

If v is less regular, we interpret $\frac{\partial v^j}{\partial x_k} - \frac{\partial v^k}{\partial x_j}$ distributionally. If $\frac{\partial v^j}{\partial x_k} - \frac{\partial v^k}{\partial x_j}$ is a Radon measure, we write $|\text{Curl}(v)|(\cdot)$ to denote its total variation. We denote the set of bounded Radon measures on Ω with values in Λ^k by $\mathcal{M}_b(\Omega, \Lambda^k)$. Analogously, we use the notation $\mathcal{M}_b(\Omega, \Lambda^k)^n$ for vectors of bounded Radon measures.

With this preparation in hand, we recall a consequence of the estimates in [13], which will be of central relevance to us.

Proposition 2. (Proposition 3 in [13]) *Let $\Omega \subset \mathbb{R}^n$, $n \geq 2$, be a bounded, open, simply connected set and consider a sequence of matrix fields $A_j \in L^2(\Omega, \mathbb{R}^{n \times n})$ such that*

$$\lim_{j \rightarrow \infty} \|\text{dist}(A_j, SO(n))\|_{L^2(\Omega)} = 0, \quad \sup_{j \in \mathbb{N}} |\text{Curl}(A_j)|(\Omega) \leq C,$$

where the operator Curl is understood as explained above.

Then, up to subsequences, $\{A_j\}_{j \in \mathbb{N}}$ converges strongly in $L^2(\Omega)$ to a matrix field $A \in BV(\Omega, SO(n))$ and

$$|DA|(\Omega) \leq C |\text{Curl}(A)|(\Omega).$$

For the convenience of the reader, we include here a (rough) sketch of the proof of Proposition 2. To this end, we first recall important observations from [14]. Here the starting point is the identity

$$T \, d\omega + dT\omega = \omega, \tag{17}$$

where T is the *averaged linear homotopy operator* (cf. [14]), which holds for every differential form $\omega \in L^1(B, \Lambda^r)$ on the unit ball $B = B(0, 1) \subset \mathbb{R}^n$, whose exterior derivative is a bounded Radon measure $d\omega \in \mathcal{M}_b(B, \Lambda^{r+1})$. It can be shown that T is a “weakly singular” operator (that is it maps L^∞ continuously into itself), c.f. (4) in [14] and the discussion following it. Combining the properties of T with the weak geometric rigidity estimate from [6, Corollary 4.1] entails the following *weak critical (that is for the exponent $1^* := \frac{n}{n-1}$) geometric rigidity estimate for incompatible fields* (cf. [14, Theorem 3]):

Theorem 2. *Let $B := B(0, 1) \subset \mathbb{R}^n$ with $n \geq 2$. There exists a constant $C = C(n) > 0$, which depends only on the dimension n such that for every matrix field $A \in L^{1^*, \infty}(B, \mathbb{R}^{n \times n})$ whose distributional Curl is a bounded Radon measure, that is $A \in \mathcal{M}_b(B, \Lambda^2)^n$, there exists an associated rotation $R \in SO(n)$ such that*

$$\|A - R\|_{L^{\frac{n}{n-1}, \infty}(B, \mathbb{R}^{n \times n})} \leq C \left(\|\text{dist}(A, SO(n))\|_{L^{\frac{n}{n-1}, \infty}(B, \mathbb{R}^{n \times n})} + |\text{Curl}(A)|(B) \right). \tag{18}$$

Moreover, it can be checked that ∇T is the sum of a weakly singular operator and a Calderón-Zygmund operator. Using this observation, it is possible to prove the following quantitative geometric rigidity result (cf. [14, Theorem 4]):

Theorem 3. *Let $B := B(0, 1) \subset \mathbb{R}^n$ and $p > 1^*(n)$. There exists a constant $C = C(n, p) > 0$, which depends only on the dimension n and the exponent p , such that for every matrix field $A \in L^p(B, \mathbb{R}^{n \times n})$ such that $dA^b \in \mathcal{M}_b(B, \Lambda^2)^n$, there exists an associated rotation $R \in SO(n)$ such that*

$$\|A - R\|_{L^p(B, \mathbb{R}^{n \times n})}^p \leq C \left\{ \|\text{dist}(A, SO(n))\|_{L^p(B, \mathbb{R}^{n \times n})}^p + |\text{Curl}(A)|^{\frac{n}{n-1}}(B) \right\}. \quad (19)$$

Clearly, the constants in (18) and (19) are scaling invariant. With Theorem 2 and Theorem 3 at hand one can approach the proof of Proposition 2 (cf. also [14, Proposition 1]). This is based on two steps, which we only sketch here.

On the one hand, Theorem 3 gives compactness with respect to the strong L^2 topology, that is, up to a subsequence, $A_j \rightarrow A \in L^2(\Omega, \mathbb{R}^{n \times n})$ strongly in $L^2(B, \mathbb{R}^{n \times n})$. The argument for this itself relies in two steps (c.f. [13], proof of Proposition 3).

- First, weak L^2 convergence is used to pass to the limit in (19) yielding that for every $x \in \mathbb{R}^n$, $\rho > 0$ there exists $R_{\rho, x} \in SO(n)$ such that

$$\|A - R_{\rho, x}\|_{L^2(B_{\rho, x}, \mathbb{R}^{n \times n})}^2 \leq CT(B_{\rho, x})^{\frac{n}{n-1}},$$

where T is the weak- $*$ -limit of $|\text{Curl}(A_j)|(\cdot \cap B_\rho(x))$.

- In a second step, a covering argument, in which the scaling invariance of the original inequality (19) is crucial, shows that

$$\dim_{\mathcal{H}}(\{x \in \Omega : A \notin SO(n)\}) \leq n - 1.$$

On the other hand, as the second main step, the BV structure of the limit field A can be deduced using Theorem 2. Indeed, one can always approximate the field A with a piecewise constant one of the form

$$A_\rho := \sum_i R_i^{(\rho)} \chi_{Q_{i, \rho}},$$

where the cubes $Q_{i, \rho} = Q(x_i, \rho)$ of side length $\rho > 0$ (whose interiors are mutually disjoint) define a tessellation of $\mathbb{R}^n$, the sum is extended over those cubes which intersect the domain Ω and the rotations $R_i^{(\rho)}$ are given by Theorem 2 applied to the balls $B(x_i, \frac{3}{2}\rho)$. The total variation of A_ρ is then estimated in terms of dA , using the fact that the weak- L^p norm is comparable to the strong- L^p norm for constant functions. For the precise details of this argument, we refer to the proof of Proposition 3 in [13].

4.2. Proof of Theorem 1

Relying on Proposition 2, we now present the proof of Theorem 1.

Proof of Theorem 1. *Step 1: Truncation.* Using a truncation argument (c.f. for instance [10]) we may, without loss of generality, assume that $u_m \in W^{1,\infty}(\Omega)$. Indeed, if this were not the case, it would always be possible to replace the sequence u_m by a sequence v_m with the property that for a constant $\bar{c} > 0$ which only depends on Ω, n :

$$\|\nabla v_m\|_{L^\infty(\Omega)} \leq \bar{c}100d, \quad \|\nabla u_m - \nabla v_m\|_{L^2(\Omega)}^2 \leq \bar{c} \int_{\{|\nabla u_m| \geq 100d\}} |\nabla u_m|^2 dx \leq \bar{c} \frac{C}{m}.$$

Here we used the energy bound (8) to infer the last estimate. In particular, v_m satisfies the energy bounds of the same type as u_m . Therefore, in the sequel, we always assume that we already have that $u_m \in W^{1,\infty}(\Omega)$.

Step 2: Reduction to the one-well problem. Invoking the energy estimate (8) and the bound (7), we obtain

$$\int_{\Omega} \text{dist}^2 \left(\sum_{j=1}^k \chi_{j,m} \nabla u_m U_j^{-1}, SO(n) \right) dx \leq C c_1^{-1} m^{-1}, \quad (20)$$

where for $j \in \{1, \dots, k\}$ the functions $\chi_{j,m} := \chi_{\Omega_{j,m}}$ are the characteristic functions from Proposition 1. Using the boundedness of ∇u_m and the convergence $\chi_{j,m} \rightarrow \chi_j := \chi_{\Omega_j}$, which was derived in Proposition 1, implies that the vector fields

$$A_{j,m}(x) := \chi_j|_{U_j^{-1}x} \nabla u_m|_{U_j^{-1}x} U_j^{-1} \quad (21)$$

satisfy

$$\int_{\tilde{\Omega}_j} \text{dist}^2(A_{j,m}, SO(n)) dx \leq 2C c_1^{-1} m^{-1}, \quad (22)$$

$$|\text{Curl}(A_{j,m})| \leq C |D\chi_j|_{U_j^{-1}} \text{ as measures, that is,}$$

$$|\text{Curl}(A_{j,m})|(\Omega') \leq C |D\chi_j|(U_j^{-1}\Omega') \text{ for all } \Omega' \subset \tilde{\Omega}_j. \quad (23)$$

Here we set $\tilde{\Omega}_j = U_j\Omega_j$, and have used that

$$\text{Curl}(\nabla u_m|_{U_j^{-1}x} U_j^{-1}) = \text{Curl}(\nabla u_m(U_j^{-1}\cdot)) = 0.$$

Indeed, (22) directly follows from (20), while (23) follows from the computation of the distributional curl of $A_{j,m}$, a mollification argument (on the level of u_m) and the fact that $\nabla u_m \in L^\infty(\Omega)$, which is a consequence of the Lipschitz truncation from Step 1. We elaborate on the derivation of (23): For $\varepsilon > 0, \delta > 0$, we first define the regularized field $A_{j,m}^{\varepsilon,\delta}(x) := \chi_j^\delta|_{U_j^{-1}x} \nabla u_m^\varepsilon|_{U_j^{-1}x} U_j^{-1}$, where

- u_m^ε is a regularization of u_m such that $\nabla u_m^\varepsilon \rightarrow \nabla u_m$ in $L^1(\Omega)$ as $\varepsilon \rightarrow 0$ and such that for each $\varepsilon > 0$ it holds $\|\nabla u_m^\varepsilon\|_{L^\infty(\Omega)} \leq C \|\nabla u_m\|_{L^\infty(\Omega)}$,

– χ_j^δ is a regularization of χ_j such that $\chi_j^\delta \rightarrow \chi_j$ in $L^1(\Omega)$ and $|\nabla \chi_j^\delta|(\Omega) \rightarrow |\nabla \chi_j|(\Omega)$, c.f. Theorem 2 in Section 5.2.2 in [8].

Then, as $\nabla u_m|_{U_j^{-1}x} U_j^{-1}$ is a gradient,

$$\begin{aligned} \left| \int_{\Omega} A_{j,m} \operatorname{Curl}(\varphi) dx \right| &= \left| \lim_{\delta \rightarrow 0} \lim_{\varepsilon \rightarrow 0} \int_{\Omega} A_{j,m}^{\varepsilon, \delta} \operatorname{Curl}(\varphi) dx \right| \\ &\leq \lim_{\delta \rightarrow 0} \lim_{\varepsilon \rightarrow 0} \int_{\Omega} |\varphi| |\nabla \chi_j^\delta|_{U_j^{-1}} |U_j^{-1}| |\nabla u_m^\varepsilon|_{U_j^{-1}} |U_j^{-1}| dx \\ &\leq \lim_{\delta \rightarrow 0} \lim_{\varepsilon \rightarrow 0} \|\varphi\|_{C^0(\Omega)} \|\nabla \chi_j^\delta\|_{L^1(\Omega)} \|U_j^{-1}\| \\ &\quad \times \|\nabla u_m^\varepsilon\|_{L^\infty(\Omega)} |U_j^{-1}| \\ &\leq \|\varphi\|_{C^0(\Omega)} |D\chi_j|_{U_j^{-1}}(\Omega) |U_j^{-1}| \|\nabla u_m\|_{L^\infty(\Omega)} |U_j^{-1}|. \end{aligned}$$

Here we integrated by parts, used that $\nabla u_m|_{U_j^{-1}x} U_j^{-1}$ is a gradient and then applied the bounds for the regularizations. Taking the supremum in φ with $\|\varphi\|_{C^0(\Omega)} = 1$ and recalling the L^∞ bound from step 1 then implies the desired result.

Step 3: Application of the one-well rigidity result and conclusion. Combining the estimates (22) and (23) with Proposition 2, we infer that $A_{j,m} \rightarrow A_j$ in $L^2(\Omega)$ with $A_j \in SO(n)$ and

$$|DA_j|(\Omega) \leq C |\operatorname{Curl}(A_j)|(\Omega) \leq C |D\chi_j|(\Omega). \quad (24)$$

Here we used (23) and the lower semicontinuity of the perimeter in order to deduce the last estimate in (24). In particular, since by the energy estimate (8) there exists u with $\nabla u_m \rightharpoonup \nabla u$ in $L^2(\Omega)$, the strong L^2 convergence of $A_{j,m}$ yields that $\nabla u_m \rightarrow \nabla u$ in $L^2(\Omega)$. We can therefore pass to the $(L^2(\tilde{\Omega}))$ -limit in the identity (21) and infer that

$$A_j(x) = \chi_j|_{U_j^{-1}x} \nabla u|_{U_j^{-1}x} U_j^{-1}.$$

We note that due to (24) the associated jump sets satisfy $J_{A_j} \subset J_{\chi_j \circ U_j^{-1}}$. In particular this entails that $A_j \in SBV(\Omega, SO(n))$. Moreover, it implies that on $\tilde{\Omega}_j \setminus \partial^* \tilde{\Omega}_j$ we have $\nabla A_j = 0$ and thus $A_j = R_{j,i}$ for some $R_{j,i} \in SO(n)$, which is constant on each of the at most countably many BV indecomposable components of $\tilde{\Omega}_j$ (c.f. Proposition 2.13 in [7] or 4.2.25 in [9]). As a consequence, there exist characteristic functions $\tilde{\chi}_{j,i}$, $\chi_{j,i}$ and $R_{j,i} \in SO(n)$ with

$$A_j(x) = \sum_{i=1}^{\infty} \tilde{\chi}_{j,i}(x) R_{j,i} =: \sum_{i=1}^{\infty} \chi_{j,i}(U_j^{-1}x) R_{j,i}.$$

Using that this is valid for all $j \in \{1, \dots, k\}$ and rewriting it in terms of ∇u therefore results in

$$\nabla u(x) = \sum_{j=1}^k \sum_{i=1}^{\infty} \chi_{j,i}(x) R_{j,i} U_j,$$

where $\sum_{j=1}^k \sum_{i=1}^{\infty} |D\chi_{j,i}|(\Omega) \leq C \sum_{j=1}^k |D\chi_j|(\Omega) < \infty$. This concludes the argument.

5. Generalizations

In this section, we show that the arguments which were presented in Sections 2–4 generalize to a much larger class of physical systems. These include the martensitic phase transformations from Sections 2–4 as special cases. In order to achieve this degree of generality, we consider Hamiltonians which allow for a *periodic* ground state structure, corresponding to settings in which there is an “internal” microstructure in the different phases. In particular, the associated Hamiltonians can be much more “nonlocal” and cover a significantly larger class of physically interesting phase transformations (c.f. Examples 1 and 2 on anti-ferromagnetic transformations and on more general transformations with internal twinning structure).

5.1. Setting

We seek to generalize the structure result of Theorem 1 to a larger class of Hamiltonians. Let us be more precise about this. First, adopting a microscopic point of view, we consider deformations $X_i : \mathbb{Z}^n \rightarrow \mathbb{R}^n$. Given a set $\hat{\Omega} \subset \mathbb{Z}^n$, we study Hamiltonians $H : \mathbb{Z}^n \rightarrow \mathbb{R}$ with a translation and rotation invariant energy density $h : \mathbb{R}^{n \times q} \rightarrow \mathbb{R}_+$ such that

$$H(X_j) = \sum_{j \in \mathbb{Z}^n : \tau_j(\Lambda) \subset \hat{\Omega}} h(X_{j+i})_{i \in \Lambda}. \quad (25)$$

Here $\Lambda \subset \hat{\Omega}$ with $\max\{\#\Lambda, \text{diam}(\Lambda)\} = q < \infty$ and $\tau_j(\Lambda) := \{i \in \mathbb{Z}^n : i - j \in \Lambda\}$. The notation $h(X_{j+i})_{i \in \Lambda}$ is used to abbreviate a dependence of h on all the values X_{j+r} , $r \in \Lambda$. Invoking the translation invariance and denoting the canonical basis of $\mathbb{R}^n$ by $e_1, \dots, e_n$, we observe that the Hamiltonian (25) can be rewritten as a function of the discrete gradient

$$\nabla_d X_i := (X_{i+e_1} - X_i, \dots, X_{i+e_n} - X_i)^t, \quad i \in \mathbb{Z}^n$$

only (which we evaluate on a finite range of lattice points). More precisely, by virtue of the translation invariance of the problem, the Hamiltonian takes the form

$$H(X_j) = \sum_{j \in \mathbb{Z}^n : \tau_j(\Lambda) \subset \hat{\Omega}} \tilde{h}(\nabla_d X_{j+i})_{i \in \Lambda},$$

where $\tilde{h} : \mathbb{R}^{n \times n \times q} \rightarrow \mathbb{R}_+$ is obtained from the energy density h . Also, using a piecewise affine interpolation on an underlying triangulation of $\mathbb{Z}^n$, we can always identify the discrete deformation $X_j : \mathbb{Z}^n \rightarrow \mathbb{R}^n$ with its piecewise affine interpolation $X : \mathbb{R}^n \rightarrow \mathbb{R}^n$ (on a fixed triangulation of the lattice). On the underlying dual lattice triangles we in particular have $\nabla_d X_i = \nabla X(i)$. In the sequel, we will often switch between the discrete and continuous viewpoints without further comment.

In deriving our main structure result, we will further suppose that the following conditions hold:

(H1) The ground states (or rather their gradients) are periodic. More precisely, there exist deformations $Z_{l,j} : \mathbb{Z}^n \rightarrow \mathbb{R}^n$, $l \in \{1, \dots, k\}$, such that the following conditions hold:

(a) The gradients $\nabla_d Z_{l,j}$ are periodic functions with a rectangular period cell $Q_l \subset \mathbb{Z}^n$ of finite diameter $\text{diam}(Q_l) \leq L_l < \infty$. We set $L_0 := \max_{l \in \{1, \dots, k\}} \{\text{diam}(Q_l)\}$ and $Q_0 := [0, L_0]^n$;

(b) We have

$$\begin{aligned} \sum_{j \in \mathbb{Z}^n} h(X_{j+i})_{i \in \Lambda} &= 0 \\ \Leftrightarrow X_j &= RZ_{l,j} + b \text{ for some } l \in \{1, \dots, k\}, R \in SO(n), b \in \mathbb{R}^n \\ &\text{and all } j \in \mathbb{Z}^n; \end{aligned}$$

(c) For each $l \in \{1, \dots, k\}$ the averaged gradients

$$U_l := |Q_l|^{-1} \int_{Q_l} \nabla_d Z_l(x) dx$$

are invertible. In particular, the gradients of the ground states can be split into a mean deformation (which averages out the microscopic oscillations) and an oscillatory part with average zero:

$$\nabla_d Z_l = U_l + (\nabla_d Z_l - U_l);$$

(d) The ground states are incompatible in the sense that

$$\text{dist}(SO(n)\nabla_d Z_{l_1,i}, SO(n)\nabla_d Z_{l_2,i})|_{i \in Q_0} \geq d > 0, \quad (26)$$

where for two mappings $Y_1(i), Y_2(i)$, a set $B \subset \mathbb{Z}^n$ and a point $j_0 \in \mathbb{Z}^n$ we set $\text{dist}(Y_1(i), Y_2(i))|_{i \in B+j_0} := \max_{i \in B+j_0} \text{dist}(Y_1(i), Y_2(i))$.

(H2) There exists $p \in (1, \infty)$ and a box $\tilde{\Lambda}$ which strictly contains Λ and $2Q_0 := [0, 2L_0]^n$, that is $\Lambda \subset \tilde{\Lambda}$ and $2Q_0 \subset \tilde{\Lambda}$, such that if for all $R \in SO(n)$, for some $j_0 \in \mathbb{Z}^n$ with $\tau_{j_0}(\tilde{\Lambda}) \subset \tilde{\mathcal{Q}}$ and $\kappa \in \mathbb{R}_+$ it holds that

$$\max_{l \in \{1, \dots, k\}} \text{dist}(R\nabla_d Z_{l,i}, \nabla_d X_i)|_{i \in \tilde{\Lambda}+j_0} \geq \kappa,$$

then it follows that

$$\sum_{j \in \mathbb{Z}^n: \tau_j(A) \subset \tilde{A} + j_0} h(X_{j+i})_{i \in A} \geq c\kappa^p.$$

$$\text{Here } \text{dist}(R\nabla_d Z_{l,i}, \nabla_d X_i)|_{i \in \tilde{A} + j_0} := \max_{i \in \tilde{A} + j_0} \text{dist}(R\nabla_d Z_{l,i}, \nabla_d X_i).$$

Let us comment on these assumptions: The Hamiltonian (25) is allowed to depend on a quite large range of values; it is significantly more “nonlocal” than the Hamiltonian which was considered in our model set-up in Section 2.1. Moreover, we emphasize that the Hamiltonians presented here are not only tailored to cover martensitic phase transitions, but also allow for other classes of classical phase transformations, including for example anti-ferromagnetic ones (c.f. Examples 1, 2). The conditions (H1)–(H2) ensure that they nevertheless mathematically display similar structural properties as the Hamiltonian from Section 2.1.3:

- The first condition (H1) determines the energy wells of the Hamiltonian and implies that it can for instance be used to describe martensitic phase transformations. However, by assuming that (the gradients of) the ground states are periodic instead of being constant, we also cover a number of other interesting phase transformations, in particular it can be used to describe *phase-antiphase* boundaries. A typical system, which for instance is included, is an anti-ferromagnetic Ising type model.

The invertibility condition which is stated in (H1)(c) is a mathematical artefact of our proof. We however emphasize that we only require the *averages* U_l to be invertible, in particular the full ground state deformation gradient $\nabla_d Z_{l,i}$ may include strong oscillations. The invertibility condition can be viewed as having density estimates from above and below.

For some simple physical systems the invertibility requirement can be relaxed by modifying the ground states. For instance, for one dimensional systems such as the anti-ferromagnetic spin system from Example 1, this can be achieved by passing from the deformations $Z_{l,j}$ to deformations $\tilde{Z}_{l,j} := Z_{l,j} + Cj$, where $C \in \mathbb{R}_+$ is a large positive constant. Choosing $C > 0$ sufficiently large, then ensures the invertibility of the corresponding averaged gradients U_l . For more complex physical systems with rotation invariance, the invertibility condition however cannot be recovered by such a simple argument in general.

- Property (H2) implies that the Hamiltonian is bounded from below by a power of the distance function to the wells. The requirement $p \in (1, \infty)$ yields a growth condition for the Hamiltonian in the neighbourhoods of the wells. It also replaces Lemma 3.1, which ensures that we necessarily catch interfacial energy, when switching between the wells. By a similar argument, it further allows us to average on microscopic scales and hence to ignore the (possibly large) oscillations on these scales. The restriction to $p \in (1, \infty)$ is a mathematical artefact ensuring the validity of one-well rigidity estimates.

Example 1. (Anti-ferromagnetic spin model) An example of a phase transition to which our set-up applies is a (one-dimensional) anti-ferromagnetic spin Hamiltonian. We begin by discussing a nearest neighbour interaction. In order to show

Fig. 1. The two ground state configurations for the spin system from Example 1 consist of a combination of an “up” and a “down” spin (illustrated over two periods in panel **a**) or a “down” and an “up” spin (illustrated over two periods in **b**). This is a typical example of a system with a phase and an antiphase displaying phase-antiphase transitions. If there is a transition between the two ground states (as for instance illustrated in **c**), this costs energy as for instance a “down” spin is next to another “down” spin

how this fits into our framework, we use a (for this model) slightly cumbersome notation (which is chosen in order to resemble the set-up layed out in the conditions (H1)–(H2)). Let $\Omega = [0, L]$ and set

$$H(X_j) := \sum_{j \in \mathbb{Z} \cap [0, L-1]} [(\nabla_d X_j)(\nabla_d X_{j+1}) + 1], \quad (27)$$

where $X_i : \mathbb{Z} \cap \Omega \rightarrow \{\pm 1\}$ (which in particular entails that $\nabla_d X_i \in \{0, \pm 1\}$). Up to translations, the ground states of this Hamiltonian are given by the following two piecewise affine, periodic deformations $Z_{1,j}$, $Z_{2,j}$, which are determined by the requirements

$$\nabla_d Z_{1,j} = 2, \quad \nabla_d Z_{1,j+1} = -2 \text{ or } \nabla_d Z_{2,j} = -2, \quad \nabla_d Z_{2,j+1} = 2.$$

We remark that a transition between $Z_{1,j}$, $Z_{2,j}$ necessarily costs interfacial energy as it involves two parallel spin vectors, c.f. Fig. 1. In particular, if an energy bound as in (30) below is assumed to hold, the number of transitions between the states $Z_{1,j}$ and $Z_{2,j}$ is uniformly controlled.

While the conditions (H2) on the Hamiltonian can be checked to be satisfied, the invertibility requirement in condition (H1)(c) is violated (as the average of (the gradient of) the sawtooth function is clearly not invertible). As the Hamiltonian however only depends on the finitely many values of the (discrete) gradient (we recall that $X_i \in \{\pm 1\}$), the problem (27) is “equivalent” to a setting in which the saw-tooth ground states are mapped to ground states which are invertible. More precisely, the ground states only involve the gradients ± 2 (general deformations, which are not necessarily ground states, might also have 0 as a third option for its gradient, but cannot attain more values, since the admissible deformations X_i are constraint to attain only the values ± 1). Hence, the anti-ferromagnetic spin model could have been mapped to a model in which the ground states attain the gradient values 1, 2. The additionally possible gradient value 0 could be mapped to any number different from 1, 2. With this modification, the anti-ferromagnetic spin system is admissible in our framework, as now the invertibility constraint is also satisfied. In order to have an explicit setting in mind, we remark that an associated Hamiltonian could for instance be given by

Fig. 2. An example of a ground state, which consists of a twin between two variants A, B . There are different “realizations” of this, some examples are indicated in the three figures. Although these are physically only shifts of a single “parent phase” and hence give rise to phase-antiphase transitions, we treat these mathematically as different phases for simplicity of notation

$$\tilde{H}(\nabla X_j) = \sum_{j \in \mathbb{Z} \cap [0, L-1]} [(\nabla_d X_j) - 1][(\nabla_d X_{j+1}) - 2] + 1$$

for the class of deformations, which only attain the values $\nabla_d X_j \in \{1, \frac{3}{2}, 2\}$.

We note that instead of considering the simple nearest neighbour anti-ferromagnetic spin Hamiltonian, we could also have considered more complicated anti-ferromagnetic Hamiltonians, which involve longer range interactions. For possible microstructures that arise in this more general framework we refer to [1, 4].

Remark 5.1. We observe that in the previous example the two ground states $Z_{1,j}$, $Z_{2,j}$ are physically not really different “phases”. As they only differ by a shift, they could be considered as being the same phase but in a different shifted form. In physical terms they correspond to antiphases, their interfaces are *phase-antiphase boundaries*. Mathematically, this could have been emphasized and formalized by working with two variables, one denoting the phase, one the shift. In order to avoid further technicalities, we have opted not to pursue this here, and have instead subsumed both the variants of the phases and the different phases in the collection $Z_{l,j}$ of the ground states (c.f. (H1)).

Example 2. (Phases with internal microstructure) A higher dimensional example of the setting which is covered by our class of Hamiltonians is given by phase transformations with an “internal microstructure”. A model setting of this consists for instance of ground states which are themselves twinned, see Fig. 2. Here the different “variants” consist of translations of the twinning structure. Moreover, rotations of the structures are also possible, these are however identified as corresponding to the same phase. A macroscopic state could combine several mesoscopic states, involving both different phases and different “microphases”.

As we are interested in the limit from the microscopic to the macroscopic scales, we next introduce a lattice on a fixed domain $\Omega \subset \mathbb{R}^n$ and consider a rescaled version of the Hamiltonian from above. To formulate this more precisely, we use the following notation: For an arbitrary set $B \subset \mathbb{R}^n$ and any number $m \in \mathbb{R}_+$ we define

$$mB := \{x \in \mathbb{R}^n : m^{-1}x \in B\}. \quad (28)$$

With this notation at hand, we set $\hat{\Omega} := m\Omega$ for each $m \in \mathbb{N}$ and work with

$$H_m(X_i) := \sum_{j \in \mathbb{Z}^n: \tau_j(\Lambda) \subset \hat{\Omega}} m^{-n} \tilde{h}(\nabla_d X_{j+i})_{i \in \Lambda}.$$

For a fixed triangulation of the underlying lattice, the piecewise affine interpolation at scale m^{-1} associated with the microscopic mapping $X_i : \mathbb{Z}^n \rightarrow \mathbb{R}^n$ is then given by

$$u_m(m^{-1}i) := m^{-1}X_i. \quad (29)$$

In addition to the conditions on the Hamiltonian, which have been explained in (H1)–(H2) from above, we will always assume a “low energy condition”, which essentially corresponds to surface energy scaling. To this end, we assume that any sequence of deformations $\{(X_m)_i\}_{m \in \mathbb{N}}$, which will be considered in the following, satisfies the bound

$$H_m(X_{m,i}) \leq Cm^{-1} \quad (30)$$

for some $C > 0$, which is independent of m .

5.2. The Main Result

In the sequel, we seek to prove the following analogue of Theorem 1, which also yields a corresponding structure result in the setting of the more general phase transformations discussed in the present section.

Theorem 4. *Let $\Omega \subset \mathbb{R}^n$ with $n \geq 2$ be an open, bounded Lipschitz domain. Let H_m be a Hamiltonian as described in Section 5.1, in particular assume that the conditions (H1)–(H2) hold. Further, suppose that $\{(X_m)_i\}_{m \in \mathbb{N}}$ with*

$$(X_m)_i : \mathbb{Z}^n \rightarrow \mathbb{R}^n \text{ for each } m \in \mathbb{N}$$

is a sequence of deformations satisfying (30) (with a uniform constant $C > 0$). Denote for each $m \in \mathbb{N}$ by $u_m \in W_{loc}^{1,\infty}(\mathbb{R}^n, \mathbb{R}^n)$ the interpolation of $(X_m)_i$, which was defined in (29). Then there exists a function $u \in BV(\Omega, \mathbb{R}^n)$ and a Caccioppoli partitioning

$$\Omega = \bigcup_{l=1}^k \bigcup_{j=1}^{\infty} \Omega_{l,j},$$

with associated characteristic functions $\chi_{l,j}$ such that

$$\begin{aligned} -u_m &\rightharpoonup u \text{ in } W_{loc}^{1,p}(\Omega, \mathbb{R}^n) \text{ (where } p \in (1, \infty) \text{ denotes the exponent from (H2))} \\ &\text{and } \nabla u \in BV_{loc}(\Omega), \end{aligned}$$

– there exist countably many $R_{l,j} \in SO(n)$ with

$$\nabla u(x) = \sum_{j=1}^{\infty} \sum_{l=1}^k \chi_{l,j}(x) R_{l,j} U_l.$$

Here $U_l := |Q_l|^{-1} \int_{Q_l} \nabla Z_l(y) dy$, with Q_l being the box of periodicity in condition (H1)(a). The following properties are satisfied by the characteristic functions $\chi_{l,j}$:

- (i) $\sum_{j=1}^{\infty} \sum_{l=1}^k |D\chi_{l,j}| \leq C < \infty$;
- (ii) $\chi_l(x) = \sum_{j=1}^{\infty} \chi_{l,j}(x)$ for almost every $x \in \Omega$.

We again emphasize that from a physical point of view the different ground states Z_l do not necessarily denote different phases, but can in principle also represent different shifts of a common “parent phase” (c.f. the explanations in Remark 5.1 after Example 1). In this case the corresponding boundaries of the domains Ω_l , $l \in \{1, \dots, k\}$, should be interpreted as phase-antiphase boundaries.

5.3. Proofs

In order to prove Theorem 4, we argue similarly as in Sections 3 and 4.

Indeed, we first observe that (H1)–(H2) suffice to prove an analogue of the spin argument from Proposition 1 from Section 3.

Proposition 3. *Let $n \geq 1$ and suppose that (H1)–(H2) and (30) are valid. Assume that for any $m \in \mathbb{N}$ we have a sequence of deformation $\{(X_m)_i\}_{i \in \mathbb{Z}^n}$ satisfying (30) with a constant $C > 0$ which is independent of m . Furthermore, for $l \in \{1, \dots, k\}$, let*

$$\begin{aligned} \Omega_{l,m} &:= \left\{ j \in m^{-1}\mathbb{Z}^n \cap \Omega : \tau_{mj}(Q_0) \subset \hat{\Omega} \text{ and there is } R \in SO(n) \text{ s.t.} \right. \\ &\quad \left. \text{dist}(\nabla_d X_i, R \nabla_d Z_{l,i})_{i \in Q_0+mj} \leq \frac{d}{100} \right\}, \\ \Omega_{b,m} &:= \left\{ j \in m^{-1}\mathbb{Z}^n \cap \Omega : \tau_{mj}(Q_0) \subset \hat{\Omega} \text{ and for all } l \in \{1, \dots, k\} \text{ and} \right. \\ &\quad \left. \text{for all } R \in SO(n) \text{ we have } \text{dist}(\nabla_d X_i, R \nabla_d Z_{l,i})_{i \in Q_0+mj} > \frac{d}{100} \right\}, \\ \Omega_{bd,m} &:= \left\{ j \in m^{-1}\mathbb{Z}^n \cap \Omega : \tau_{mj}(Q_0) \cap (\mathbb{Z}^n \setminus \hat{\Omega}) \neq \emptyset \right\}. \end{aligned}$$

Then there exist Caccioppoli sets $\Omega_1, \dots, \Omega_k \subset \Omega$ such that

$$\chi_{\Omega_{l,m}} \rightarrow \chi_{\Omega_l}, \chi_{\Omega_{b,m}} \rightarrow 0, \chi_{\Omega_{bd,m}} \rightarrow 0 \text{ in } L^1(\Omega), \quad \Omega = \bigcup_{j=1}^k \Omega_j.$$

Here $\chi_{\Omega_{l,m}}, \chi_{\Omega_{b,m}}, \chi_{\Omega_l}, \chi_{\Omega_{bd,m}} : \Omega \rightarrow \{0, 1\}$ denote the characteristic functions associated with the corresponding sets.

Remark 5.2. The sets $\Omega_{b,m}$ consists of all points of comparatively large local energy density. The set $\Omega_{bd,m}$ corresponds to a boundary layer, which is present due to the finite range interactions in our Hamiltonian and the boundedness of the set $\hat{\Omega}$.

Proof. The argument for Proposition 3 follows from the assumptions (H1), (H2) and the energy bound (30) similarly as in the proof of Proposition 1.

First, we note that the energy bound (30) in combination with (H2) ensures that at most $\tilde{C}m^{d-1}$ lattice points have a local energy larger than a fixed constant. This can be seen by a counting argument as in Lemma 3.2. In particular, this directly implies the vanishing of $\Omega_{b,m}$ in the limit $m \rightarrow \infty$.

Next, we observe that (H1) combined with (H2) controls the length of the interfaces between the different phases $Z_{l,i}$, $l \in \{1, \dots, k\}$, and hence replaces Lemma 3.1. More precisely, (H1) and (H2) yield that for $c_0 = d/100$ the following property is satisfied: If for some $j_0 \in m^{-1}\mathbb{Z}^n \cap \Omega$ and some $i_0 \in \{1, \dots, n\}$ it holds that for some $R \in SO(n)$, for all $\tilde{R} \in SO(n)$ and some $l \in \{1, \dots, k\}$

$$\text{dist}(R\nabla_d Z_{l,i}, \nabla_d X_i)_{i \in Q_0 + mj_0} \leq c_0/100,$$

$$\text{dist}(\tilde{R}\nabla_d Z_{l,i}, \nabla_d X_i)_{i \in Q_0 + mj_0 + e_{i_0}} > c_0/100,$$

then for any $Q \in SO(n)$ and any $r \in \{1, \dots, k\}$

$$\text{dist}(Q\nabla_d Z_{r,i}, \nabla_d X_i)_{i \in \tilde{\Lambda} + mj_0} > c_0/100.$$

Here $\tilde{\Lambda}$ denotes the box from the condition (H2) and e_{i_0} is a canonical unit vector in $\mathbb{Z}^n$. This follows from an application of the triangle inequality in conjunction with the control (26). As, by assumption $\text{dist}(\tilde{R}\nabla_d Z_{l,i}, \nabla_d X_i)_{i \in Q_0 + mj_0 + e_{i_0}} > c_0/100$ for all $\tilde{R} \in SO(n)$, it suffices to show that for all $Q \in SO(n)$ and all $r \in \{1, \dots, k\} \setminus \{l\}$

$$\text{dist}(Q\nabla_d Z_{r,i}, \nabla_d X_i)_{i \in \tilde{\Lambda} + mj_0} > c_0/100.$$

This, however, is a consequence of the following lower bound which uses (26): for all $Q, R \in SO(n)$,

$$\begin{aligned} \text{dist}(Q\nabla_d Z_{r,i}, \nabla_d X_i)_{i \in \tilde{\Lambda} + mj_0} &\geq \text{dist}(Q\nabla_d Z_{r,i}, R\nabla_d Z_{l,i})_{i \in Q_0 + mj_0} \\ &\quad - \text{dist}(R\nabla_d Z_{l,i}, \nabla_d X_i)_{i \in Q_0 + mj_0} \\ &\geq d - \frac{c_0}{100} > \frac{c_0}{100}. \end{aligned}$$

Finally, as an additional point in the present more general set-up, we note that the size of the boundary layer $\Omega_{bd,m}$ is controlled by

$$|\Omega_{bd,m}| \leq Cqm^{-1}, \quad \text{Per}(\Omega_{bd,m}) \leq C.$$

This follows from the finite interaction range which is determined by the choice of $\Lambda \in \mathbb{Z}^n$.

As in the proof of Proposition 1 these three observations imply the uniform perimeter bounds on $\chi_{\Omega_{l,m}}$. These then lead to the remaining claims by general compactness arguments in the space BV (see the proof of Proposition 1 for the details).

With the spin result at hand, we can proceed to the proof of Theorem 4. This follows along the same lines as in Section 4 and mainly relies on a reduction to a one-well problem. As an additional technical aspect with respect to the proof of Theorem 1, we have to deal with the fact that the ground states are now periodic in general and that only the *average* deformation gradients U_l are invertible. Hence, we introduce an additional auxiliary averaging step.

Proof of Theorem 4. Recalling that u_m denotes the piecewise affine interpolation of $(X_m)_i$ (c.f. (29)), we first observe that by a truncation argument, we may again assume that ∇u_m is bounded. In order to avoid boundary effects, we define for each small parameter $\varepsilon > 0$ the set $\Omega_\varepsilon := \{x \in \Omega : \text{dist}(x, \partial\Omega) > \varepsilon\}$ and the associated Caccioppoli sets $\Omega_{l,\varepsilon} := \Omega_\varepsilon \cap \Omega_l$. Here Ω_l with $l \in \{1, \dots, k\}$ are the sets from Proposition 3.

We note that the assumption (H2) yields that for any deformation $Y_i : \mathbb{Z}^n \rightarrow \mathbb{R}^n$

$$\sum_{j \in \mathbb{Z}^n, \tau_j(\Lambda) \subset \tilde{\Lambda} + j_0} h(Y_{j+i})_{i \in \Lambda} \geq c \min_{p \in \{1, \dots, k\}} \text{dist}^p(R_{j_0} \nabla_d Z_{p,i}, \nabla_d Y_i)_{i \in \tilde{\Lambda} + j_0},$$

where $R_{j_0} \in SO(n)$ is the rotation which satisfies

$$R_{j_0} := \operatorname{argmin}_{R \in SO(n)} \min_{q \in \{1, \dots, k\}} \text{dist}(R \nabla_d Z_{q,i}, \nabla_d Y_i)_{i \in \tilde{\Lambda} + j_0}.$$

For convenience of notation and without loss of generality we assume that

$$\min_{q \in \{1, \dots, k\}} \text{dist}^p(R_{j_0} \nabla_d Z_{q,i}, \nabla_d Y_i)_{i \in \tilde{\Lambda} + j_0} = \text{dist}^p(R_{j_0} \nabla_d Z_{l,i}, \nabla_d Y_i)_{i \in \tilde{\Lambda} + j_0}.$$

Since

$$\text{dist}(R_{j_0} \nabla_d Z_{l,i}, \nabla_d Y_i)_{i \in \tilde{\Lambda} + j_0} \geq \text{dist}(R_{j_0} U_l, \nabla_d \bar{Y}_{j_0})$$

(where we used that $Q_l \subset \tilde{\Lambda}$ for all $l \in \{1, \dots, k\}$), we then also infer that

$$\sum_{j \in \mathbb{Z}^n, \tau_j(\Lambda) \subset \tilde{\Lambda} + j_0} h(Y_{j+i})_{i \in \Lambda} \geq c \text{dist}^p(R_{j_0} U_l, \nabla_d \bar{Y}_{j_0}) \chi_{m, \Omega_{l,\varepsilon}}(j_0). \quad (31)$$

Here $U_l : \mathbb{Z}^n \rightarrow \mathbb{R}^n$ is the average deformation which was defined in the formulation of the theorem and $\nabla_d \bar{Y}_j : \mathbb{Z}^n \rightarrow \mathbb{R}^n$ denotes a similarly averaged field:

$$\nabla_d \bar{Y}_j = |Q_l|^{-1} \int_{Q_l + j} \nabla_d Y(x) dx$$

(we remark that the size of the averaging domain depends on the value of $l \in \{1, \dots, k\}$).

We apply this observation to $Y_i = (X_m)_i$, invoke the energy bound (30), sum over all values $i \in \mathbb{Z}^n \cap \hat{\Omega}_{l,\varepsilon}$ and use the boundedness of $\nabla_d X$ together with the bounds for $|\Omega_{bd,m}|$, $|\Omega_{b,m}|$. If, for convenience, we denote the (rescaled) piecewise

affine interpolation of $\bar{X}_i$ by $\bar{u}_m$ (here the interpolation is considered in the sense of (29) and $\bar{X}_i$ is a suitable antiderivative of $\nabla \bar{X}_i$), this leads to

$$\int_{\Omega_{l,\varepsilon}} \text{dist}^p(\nabla \bar{u}_m, SO(n)U_l) dx \leq CL_0^n m^{-1}, \quad (32)$$

where L_0 denotes the constant from condition (H1)(a).

With (32) at hand, we can now argue as in the proof of Theorem 1. As in the argument for Theorem 1, we first note that by setting $x = U_l^{-1}y$ (where we use the invertibility condition from the requirement (H1)(c)), the function $\nabla \bar{u}_m(x)U_l^{-1}$ can be rewritten as

$$\nabla \bar{u}_m(U_l^{-1}y)U_l^{-1} = \nabla \varphi_m(y),$$

with $\varphi_m(y) = \bar{u}_m(U_l^{-1}y)$ being piecewise affine. Hence, by the change of coordinates formula and by recalling (32), we deduce for each $l \in \{1, \dots, k\}$ that

$$\int_{\tilde{\Omega}} \text{dist}^p(\chi_{\tilde{\Omega}_{l,\varepsilon}} \nabla \varphi_m, SO(n)) dx = \int_{\tilde{\Omega}_{l,\varepsilon}} \text{dist}^p(\nabla \varphi_m, SO(n)) dx \leq CL_0^n m^{-1},$$

where $\tilde{\Omega} := U_l(\Omega)$ and $\tilde{\Omega}_{l,\varepsilon} := U_l(\Omega_{l,\varepsilon})$.

Setting

$$A_{l,m,\varepsilon}(y) := \chi_{\tilde{\Omega}_{l,\varepsilon}}(y) \nabla \varphi_m(y),$$

we note that for some constant $C > 0$ which is independent of m ,

$$|\text{Curl}(A_{l,m,\varepsilon})| \leq C |D\chi_{\tilde{\Omega}_{l,\varepsilon}}|_{U_l^{-1}} \text{ as measures.} \quad (33)$$

As a consequence, Proposition 2 is applicable and yields $A_{l,m,\varepsilon} \rightarrow A_{l,\varepsilon}$ in $L^p(\tilde{\Omega})$ for $m \rightarrow \infty$ with $A_{l,\varepsilon} \in SO(n)$ and

$$|DA_{l,\varepsilon}|(\Omega') \leq |\text{Curl}(A_{l,\varepsilon})|(\Omega') \leq C |D\chi_{\tilde{\Omega}'_{l,\varepsilon}}|(U_l^{-1}\Omega) \quad (34)$$

for all $\Omega' \subset \tilde{\Omega}$.

This entails that there exist countably many characteristic functions $\tilde{\chi}_{l,i}$ and matrices $R_{l,i} \in SO(n)$ with

$$\begin{aligned} A_{l,m,\varepsilon}(y) &\rightarrow A_{l,\varepsilon}(y) = \sum_{i=1}^{\infty} \tilde{\chi}_{l,i}(y) R_{l,i} \text{ in } L^p(\tilde{\Omega}_{l,\varepsilon}) \\ \text{and } \sum_{i=1}^{\infty} |D\tilde{\chi}_{l,i}| &\leq C |D\chi_{\tilde{\Omega}_{l,\varepsilon}}|. \end{aligned} \quad (35)$$

In particular, by definition of $A_{l,m,\varepsilon}$,

$$\nabla \varphi_m(y) \rightarrow \sum_{i=1}^{\infty} \tilde{\chi}_{l,i}(y) R_{l,i} \text{ in } L^p(\tilde{\Omega}_{l,\varepsilon}).$$

Changing coordinates again then leads to

$$\nabla \bar{u}_m - \sum_{i=1}^{\infty} \tilde{\chi}_{l,i}(U_l x) R_{l,i} U_l \rightarrow 0 \text{ in } L^p(\Omega_{l,\varepsilon}). \quad (36)$$

We combine (36) with the weak convergence of ∇u_m . On the one hand, the boundedness of the energy (30) yields

$$\nabla u_m \rightharpoonup \nabla u \text{ in } L^p(\Omega_{l,\varepsilon}). \quad (37)$$

On the other hand, the periodicity of ∇Z_l implies that the weak limits of ∇u_m and $\nabla \bar{u}_m$ agree. Indeed, since in the phase l the function $\nabla \bar{u}_m$ is defined by averaging ∇u_m over the (shifted) period cell Q_l , we have $\nabla \bar{u}_m = \nabla u_m * \chi_{Q_{l,m}}$, where $\chi_{Q_{l,m}}$ is the characteristic function of $m^{-1}Q_l \subset \Omega$. Thus, for all $\psi \in C_c^\infty(\Omega)$,

$$\begin{aligned} & \lim_{m \rightarrow \infty} \int_{\mathbb{R}^n} \nabla \bar{u}_m(x) \psi(x) dx \\ &= \lim_{m \rightarrow \infty} \int_{\mathbb{R}^n} \nabla u_m(x) (\psi * \chi_{Q_{l,m}})(x) dx = \int_{\mathbb{R}^n} \nabla u(x) \psi(x) dx. \end{aligned}$$

Here we used that $\nabla u_m \rightharpoonup \nabla u$ and $\psi * \chi_{Q_{l,m}} \rightarrow \psi$ in $L^2(\Omega)$. Hence, by (36) and defining $\chi_{l,i}(x) := \tilde{\chi}_{l,i} U_l$,

$$\nabla u(x) = \sum_{i=1}^{\infty} \tilde{\chi}_{l,i}(x) R_{l,i} U_l \text{ for } x \in \Omega_{l,\varepsilon}. \quad (38)$$

Using that an identity of this type holds for any $\varepsilon > 0$ then shows (by considering a countable family of $\varepsilon \rightarrow 0$) that an identity of the form (38) holds for any subdomain of Ω_l . Moreover, considering suitable diagonal sequences implies that the corresponding limits have to agree on the intersection of the various sets $\Omega_{l,\varepsilon}$, in particular (up to boundary effects) neither the characteristic functions $\tilde{\chi}_{l,i}$ nor the rotations $R_{l,i}$ depend on $\varepsilon > 0$. Since ∇u is defined in any compact set of Ω , this provides the desired representation result. The control of the BV norms of the characteristic functions $\tilde{\chi}_{l,i}$ follows from this and from the estimate in (35).

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Conflict of interest

The authors declare that they have no conflict of interest.

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