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Calculus of Variations

Local minimizers and planar interfaces in a phase-transition model with interfacial energy

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Abstract Interfacial energy is often incorporated into variational solid-solid phase transition models via a perturbation of the elastic energy functional involving second gradients of the deformation. We study consequences of such higher-gradient terms for local minimizers and for interfaces. First it is shown that at slightly sub-critical temperatures, a phase which globally minimizes the elastic energy density at super-critical temperatures is an L^1-local minimizer of the functional including interfacial energy, whereas it is typically only a $W^{1,\infty}$-local minimizer of the purely elastic functional. The second part deals with the existence and uniqueness of smooth interfaces between different wells of the multi-well elastic energy density. Attention is focussed on so-called planar interfaces, for which the deformation depends on a single direction $x \cdot N$ and the deformation gradient then satisfies a rank-one ansatz of the form $Dy(x) = A + u(x \cdot N) \otimes N$, where A and $B = A + a \otimes N$ are the gradients connected by the interface.

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1 Introduction

Multi-well energy functionals with higher-gradient dependence of form

$$\mathscr{I}(y) = \int_{\Omega} \psi(Dy(x)) + \varepsilon^2 |D^2 y(x)|^2 \; dx \tag{1.1}$$

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arise in models for crystallographic phase transitions including both elastic and interfacial energy. The function $\psi : \mathbb{R}^{n\times n}_{+} \to \mathbb{R}$ denotes the elastic energy density, where $\mathbb{R}^{n\times n}_{+}$ is the set of $n \times n$ real matrices with strictly positive determinant, and ψ is assumed to satisfy

(f) (*frame indifference*)
$\psi(F) = \psi(RF)$ for all $F \in \mathbb{R}^{n\times n}_{+}$ and all $R \in SO(n)$;
(m) (*multi-well structure*)
there exist matrices $U_1, U_2, \ldots U_k \in \mathbb{R}^{n\times n}_{+}$ with $U_j \notin SO(n)U_i$, $i \neq j$, such that $\psi(F) \geq 0$ for all $F \in \mathbb{R}^{n\times n}_{+}$, and $\psi(F) = 0 \Leftrightarrow F \in \cup_{1\leq i\leq k} SO(n)U_i$;
(n) (*non-interpenetration*)
$\psi(F) \to \infty$ as $\det F \to 0^+$.

We have in mind the elastic energy of a crystalline solid that has been cooled to a fixed temperature θ below a critical value θ_c at which the lattice structure minimizing the energy density ψ changes from a single high-symmetry phase (austenite) to several variants of a low-symmetry phase (martensite) (see Ball and James [7,8]). These low-symmetry energy-minimizing variants correspond to the matrices $U_1, \ldots U_k$ in (m).

The higher-gradient term $\varepsilon^2|D^2y|^2$ penalizes transitions between gradients Dy and is a simple candidate interfacial energy density (see Müller [24] and Conti and Schweizer [16], for example). A key benefit of the inclusion of this term in (1.1) is that the infimum of (1.1) over a given set of deformations y is typically attained, due to the compactness properties of minimizing sequences $\{y_n\}_{n=1}^{\infty}$ that result from the boundedness of $\int_\Omega |D^2y_n|^2\, dx$. This is in contrast to minimization of the purely elastic energy, when $\varepsilon = 0$, which often predicts infinitely fine oscillations between gradients because the infimum is not attained, but is better and better approximated by highly oscillatory gradients; see Ball and Carstensen [5]. Observed microstructures have a lengthscale and are thus not consistent with arbitrarily fine oscillations.

Here we study two additional consequences of inclusion of the higher-gradient term in (1.1). The first concerns the fate of the high-symmetry austenite phase, that globally minimizes ψ at super-critical temperatures, when the temperature is slightly sub-critical. Taking the reference configuration to be undistorted austenite at the critical temperature θ_c, the deformation corresponding to austenite at temperature θ is $\overline{y}(x) = \alpha(\theta)x + a$ for some $a \in \mathbb{R}^n$ and $\alpha(\theta) \in (0, \infty)$, with deformation gradient $\alpha(\theta)I$. When $\theta < \theta_c$, the matrix $\alpha(\theta)I$ is no longer a global minimizer of ψ. But it is reasonable to assume that ψ is a continuous function of temperature θ, and thus that given θ close to θ_c, $D\psi(\alpha(\theta)I) = 0$ and there exists $\nu > 0$ such that

$$D^2\psi(\alpha(\theta)I)(G, G) \geq \nu|G|^2 \quad \text{for all} \quad G = G^T; \tag{1.2}$$

(recall that the frame-indifference of ψ implies that $d^2\psi(e^{tK}\alpha(\theta)I)/dt^2 = 0$ when $t = 0$, so

$$D^2\psi(\alpha(\theta)I)(K, K) = 0 \quad \text{for all} \quad K = -K^T, \tag{1.3}$$

and hence (1.2) is the natural quadratic non-degeneracy condition on ψ at $\alpha(\theta)I$). See Fig. 1.

In Sect. 2, we address the question of whether (1.2) implies that $\overline{y}$ is a local minimizer of $\mathscr{I}$ with respect to a given norm $\|\cdot\|_X$; that is, whether or not

$$\mathscr{I}(y) \geq \mathscr{I}(\overline{y}) \quad \text{if} \quad \|y - \overline{y}\|_X \quad \text{is sufficiently small.} \tag{1.4}$$

When $\varepsilon = 0$, with no interfacial energy, the answer depends on the choice of norm $\|\cdot\|_X$. If $X = W^{1,\infty}(\Omega)$, the answer is yes; but the answer is no if $X = W^{1,p}(\Omega)$ or $L^p(\Omega)$ for

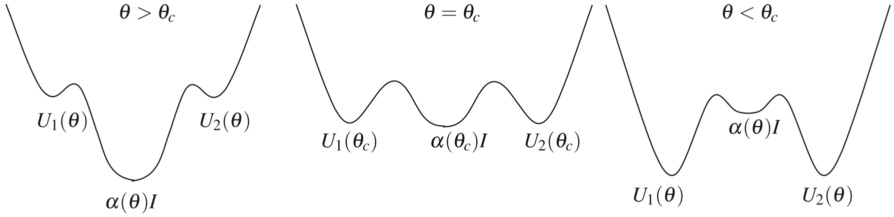

Fig. 1 One-dimensional cartoon of the dependence of ψ on θ when $k = 2$

any $1 \leq p < \infty$ (see Theorem 2.1). By contrast, when $\varepsilon > 0$, the presence of the interfacial energy allows us to show in Theorem 2.2 that $\overline{y}$ is a local minimizer of $\mathscr{I}$ in $L^1(\Omega)$. Note the comparison between this result and that in Ball et al. [6] on incompatibility-induced hysteresis, where similar local stability is proved in the absence of interfacial energy when the product phase is incompatible with the parent phase, provided the energy difference between the phases is small.

The second part of this article concerns interfaces between gradients lying in two energy wells $\mathrm{SO}(n)U_{i_0}$ and $\mathrm{SO}(n)U_{j_0}$, $j_0 \neq i_0$. Such interfaces are physically important and mathematically interesting. Their nature differs depending on the presence or absence of interfacial energy. When $\varepsilon = 0$, energy minimizing sequences typically involve surfaces across which the gradient Dy has jump discontinuities, giving sharp interfaces. In the simplest case, these sequences are comprised entirely of piecewise constant gradients, where each constant gradient lies in one of the energy wells $\mathrm{SO}(n)U_{i_0} \cup \mathrm{SO}(n)U_{j_0}$. When $\varepsilon > 0$, the surface-energy term $\varepsilon^2|D^2y|^2$ prohibits such jumps, and interfaces between wells must have some smoothness and thus non-zero width. Experiments show that in some materials, interfaces are not sharp but rather curve gradually through several atomic layers; see, for example, Manolikas, van Tendeloo and Amelinckx [22] and Salje [27]. Chrosch and Salje [14] and Salje et al. [28] give tables listing a measure of interface thickness for a variety of materials.

In Sects. 3–6, we investigate the structure, existence, and uniqueness of interfaces between wells in the presence of interfacial energy. The simplest form of an interface is planar and attention is focussed on such interfaces in this article. A deformation y corresponds to a planar interface if there exist a constant unit vector $N \in \mathbb{R}^n$, a function $\mathscr{F} : \mathbb{R} \to \mathbb{R}^{n\times n}$ and matrices $A \in \mathrm{SO}(n)U_{i_0}$ and $B \in \mathrm{SO}(n)U_{j_0}$ such that

$$Dy(x) = \mathscr{F}(x \cdot N), \tag{1.5}$$

and

$$\mathscr{F}(x \cdot N) \to A, B \tag{1.6}$$

as $x \cdot N \to -\infty, +\infty$. It is shown in Lemma 3.1 in Sect. 3 that conditions (1.5) and (1.6) in fact imply that the deformation gradient Dy has a rank-one structure,

$$Dy(x) = A + u(x \cdot N) \otimes N, \tag{1.7}$$

where $B = A + a \otimes N$ and u is a vector-valued function such that $u(s) \to 0, a$ as $s \to -\infty, \infty$. Note that (1.7) implies in particular that B must be rank-one connected to A if they are linked by a planar interface (and indeed, by certain more general interfaces—see also Lemma 3.2). The existence of planar-interface solutions y_0 to the Euler–Lagrange equations for the functional (1.1) is proved in Sect. 4 using minimization of a reduced functional formed by substituting the ansatz (1.7) into (1.1) together with a recent result of Alikakos and

Fusco [3]. Extra conditions on the elastic energy density ψ are needed to ensure that existence of such a planar interface between A and B is not prevented by the presence of additional equilibria; see Lemma 4.3, and also the following remark for a discussion of this requirement in cases of physical interest. The planar interface y_0 is shown to satisfy the full n-dimensional Euler–Lagrange equations for (1.1). We also give an example to illustrate that in general, the vector u arising in the gradient (1.7) of such a solution y_0 is not necessarily of the special form $u(x \cdot N) = \lambda(x \cdot N)a$ with λ a scalar-valued function, as is sometimes assumed; see, for example, Salje, Hayward and Lee [28]. A physical example of non-uniqueness (up to translation) within the class of planar interfaces is discussed in Sect. 5, based on the two martensite variants that minimize sub-critical temperature energy densities in orthorhombic to monoclinic phase transformations. Such non-uniqueness may be of interest in light of experimental observations that measurement of the thickness of an interface between two given lattice structures can vary between different regions of a material sample; see Shilo, Ravichandran and Bhattacharya [30], for example, where other possible mechanisms for the variation over a sample of interface width are discussed. Section 6 is devoted to deducing the existence of planar interfaces with additional symmetry under the assumption that the elastic energy density ψ satisfies material symmetry properties.

There is a lack of rigorous results on interfaces between wells for models described by (1.1). This article contains an initial study of some aspects of such interfaces, and it is clear that all sorts of questions remain. Foremost among these is a more complete understanding of the issue of uniqueness of interfaces, both within the class of planar interfaces, as in our discussion in Sect. 5, and within a class comprising some wider notion of interface not necessarily satisfying the ansatz (1.7). An example of a non-planar interface with profile periodic along the interface and energy strictly lower than the minimum energy of planar interfaces is presented in a similar setting, though without the frame-indifference assumption (f), in Conti, Fonseca and Leoni [15]; see also Jin and Kohn [20]. Curved interface solutions to certain elliptic equations and systems are constructed using variational methods by Rabinowitz and Stredulinsky [25,26] and by Schatzman [29], and it would be of interest to try to extend their ideas to the functional (1.1). Note that some of the proofs in [25,26,29] assume the existence of at least two "separated" planar interface solutions and so modification of these ideas to our setting would require an assumption of non-uniqueness of planar interfaces for (1.1).

We end the introduction with some brief remarks on the choice of interfacial energy dependence in (1.1). The term $\varepsilon^2|D^2y(x)|^2$ is simple, widely used, and yields lengthscales for microstructures, as mentioned above. Nevertheless, there are issues with how best to model interfacial energy and thus whether this is the most appropriate choice. Our assumption here is that the second-gradient term should penalize transitions and the coefficient of $|D^2y(x)|^2$ should therefore be positive. However, microscopic to macroscopic limit arguments using the Taylor expansion of the atomistic energy about a smooth deformation can yield higher-order gradient terms in which the coefficient of $|D^2y(x)|^2$ is either positive or negative, depending on the choice of atomic lattice and interaction potential in the microscopic model. This was observed explicitly in Bardenhagen and Triantafyllidis [10], who gave two-dimensional examples that illustrated both possibilities, and implicitly in Triantafyllidis and Bardenhagen [34], where conditions were imposed on parameters in a one-dimensional atomic interaction potential to ensure positivity of the coefficient of $|D^2y(x)|^2$ in the macroscopic limit. In a detailed study of such limiting processes, Blanc et al. [12] also discuss this sign question and give examples showing that both signs can arise in the one-dimensional case. A further issue is that only smooth interfaces are admissible for our energy. Ball and Mora-Corral [9] study a variety of models in which both smooth and sharp interfaces are allowed, motivated by experimental observations that interfaces in some materials are atomistically sharp, while in others the interface thickness extends over a number of atomic spacings. Another possible drawback of the term $\varepsilon^2|D^2y(x)|^2$ is that it is isotropic, and in some materials, an anisotropic interfacial energy might be more appropriate. The techniques used here should also yield results in the anisotropic case (see also Stefanopolous [31] for an extension of the work of Alikakos and Fusco [3] on the existence of interfaces to include a certain type of anisotropy.)

2 Local minimizers

For simplicity of notation, we take the reference configuration in this section to be undistorted austenite at a fixed sub-critical temperature $\theta < \theta_c$, instead of at θ_c itself. Thus in the notation of the Introduction, $\alpha(\theta) = 1$. We assume that $U_1, \ldots, U_k$ in the multi-well condition (m) are such that $I \notin \cup_{1\leq i\leq k}\mathrm{SO}(n)U_i$, so that

$$\psi(I) =: k > 0, \tag{2.1}$$

and that in addition to (m), the frame-indifference condition (f), and the non-interpenetration condition (n), ψ satisfies

$$D\psi(I) = 0, \tag{2.2}$$

and there exists $\nu > 0$ such that

$$D^2\psi(I)(G, G) \geq \nu|G|^2 \quad \text{for all} \quad G \in S^{n\times n}. \tag{2.3}$$

Here $S^{n\times n} = \{F \in \mathbb{R}^{n\times n} : F = F^T\}$ and $S_+^{n\times n} = \{F \in S^{n\times n} : F \in \mathbb{R}_+^{n\times n}\}$. The function ψ is defined only on $\mathbb{R}_+^{n\times n}$ to try to avoid interpenetration of matter and to prevent orientation reversal, and the non-interpenetration condition (n) , that

$$\psi(F) \to \infty \quad \text{as} \quad \det F \to 0^+,$$

ensures that $\det Dy(x) > 0$ for almost every $x \in \Omega$ if $\mathscr{I}(y) < \infty$. Suppose also that

$$\psi \in C^2(\mathbb{R}_+^{n\times n}, \mathbb{R}). \tag{2.4}$$

Recall from the polar decomposition theorem that each $F \in \mathbb{R}_+^{n\times n}$ can be written in a unique way as $F = RU$, where $R \in \mathrm{SO}(n)$ and $U =: \sqrt{F^TF}$ is positive-definite and symmetric, and that

$$|U - I| \leq |F - S| \quad \text{for all } S \in \mathrm{SO}(n), \tag{2.5}$$

where $|F|^2 := \mathrm{tr}(F^TF)$.

We begin with the case $\varepsilon = 0$, when there is no interfacial energy in (1.1).

Theorem 2.1 *Let $\Omega \subset \mathbb{R}^n$ be bounded and open and $\bar{y} : \Omega \to \mathbb{R}^n$ be defined by $\bar{y}(x) = Rx + a$ for some constant $R \in SO(n)$ and $a \in \mathbb{R}^n$. Suppose that $\varepsilon = 0$ and ψ in (1.1) satisfies (f), (m), (n) and (2.1)–(2.4). Then*

(a) *$\bar{y}$ is a local minimizer of $\mathscr{I}$ in $W^{1,\infty}(\Omega, \mathbb{R}^n)$;*
(b) *if there exist $a, N, b, m \in \mathbb{R}^n$, with N, m non-parallel unit vectors, $\lambda \in (0, 1)$ and $A \in SO(n)U_1$, $B \in SO(n)U_2$ such that*

$$B = A + a \otimes N \tag{2.6}$$

and

$$R - A = -b \otimes m + \lambda a \otimes N, \tag{2.7}$$

then $\overline{y}$ is not a local minimizer of $\mathscr{I}$ in $W^{1,p}(\Omega, \mathbb{R}^n)$, $1 \le p < \infty$.

Proof

(a) Let $U \in S_+^{n\times n}$ be close enough to I so that $\det(I + t(U - I)) > 0$, and so $\psi(I + t(U - I)) < \infty$, for all $t \in (-1/2, 3/2)$. Then it follows from (2.2), (2.3) and Taylor's Theorem applied to $t \mapsto \psi(I + t(U - I))$ that there exist $\delta, \sigma > 0$ such that

$$\psi(U) \ge \psi(I) + \sigma|U - I|^2 \quad \text{whenever} \quad |U - I| < \delta. \tag{2.8}$$

This, together with (2.5), yields that

$$\mathscr{I}(y) \ge \mathscr{I}(\overline{y}) + \sigma \int_\Omega \left|\sqrt{Dy^T Dy} - I\right|^2 dx, \tag{2.9}$$

provided $y \in W^{2,2}(\Omega)$ and $\|y - \overline{y}\|_{W^{1,\infty}(\Omega)} < \delta$, since $|\sqrt{Dy^T Dy} - I| \le |Dy - R| < \delta$ for such y, and $\psi(Dy) = \psi(\sqrt{Dy^T Dy})$.

(b) Since Ω is bounded, there exists $x_0 \in \partial\Omega$ such that $x \cdot m < x_0 \cdot m$ for all $x \in \Omega$. Let $\Gamma_\gamma = \Omega \cap \{x : x_0 \cdot m - \gamma < x \cdot m < x_0 \cdot m\}$ with $x_0 \in \partial\Gamma_\gamma$. Since Ω is open, there exists γ_j such that

$$|\Gamma_{\gamma_j}| = \frac{1}{j} \tag{2.10}$$

whenever j is sufficiently large, where $|\cdot|$ here denotes n-dimensional Lebesgue measure. Then for such j, define $y_j : \Omega \to \mathbb{R}^n$ by

$$y_j(x) = \begin{cases} \overline{y}(x), & x \in \Omega \setminus \Gamma_{\gamma_j}, \\ z_j(x), & x \in \Gamma_{\gamma_j}, \end{cases} \tag{2.11}$$

where z_j is such that

(i) $y_j \in C(\Omega, \mathbb{R}^n) \cap W^{1,\infty}(\Omega, \mathbb{R}^n)$;
(ii) there exist constant matrices $D^\pm$ such that $Dz_j \in \{A, B, D^\pm\}$ *a.e.* for every j;
(iii) $|\{x : Dz_j \ne A, B\}| \le 1/j^2$;
(iv) $\det Dz_j > 0$ *a.e.*.

That such z_j exist is a consequence of conditions (2.6) and (2.7), which ensure that the laminate construction in the proof of Theorem 3 in Ball and James [7] can be used. Note that property (ii) implies the existence of $M, C > 0$ such that $\psi(Dz_j) \le M$ for every j, and

$$\|\overline{y} - y_j\|_{W^{1,p}(\Omega)} \le C|\Gamma_{\gamma_j}| = \frac{C}{j} \to 0 \quad \text{as} \quad j \to \infty.$$

Now since $\psi(A) = \psi(B) = 0$,

$$\int_{\Gamma_{\gamma_j}} \psi(Dz_j)dx = \int_{\{x:Dz_j(x)\ne A,B\}} \psi(Dz_j)dx \le \frac{M}{j^2},$$

and hence, using (2.1) and (2.10), we have

$$\begin{aligned}\mathscr{I}(\overline{y}) - \mathscr{I}(y_j) &= \int_{\Gamma_{\gamma_j}} \psi(D\overline{y}) - \psi(Dy_j)dx \\ &= \int_{\Gamma_{\gamma_j}} kdx - \int_{\{x:Dz_j(x)\neq A,B\}} \psi(Dz_j)dx \\ &\geq \frac{k}{j} - \frac{M}{j^2},\end{aligned}$$

which is positive for j sufficiently large. □

Remark (2.6) and (2.7) are compatibility conditions for the existence of a classical interface between austenite and finely-twinned martensite. Such an interface enables the energy of austenite, $\overline{y}$, to be reduced by introducing a small martensitic plate. This is the idea behind the construction of y_j in the proof of Theorem 2.1. These conditions are known to hold in cases of physical interest (see, for example, Bhattacharya [11]). For example, for a cubic-tetragonal transition with $n = 3$, the matrices U_1 and U_2 can be taken to be diag(η_2, η_1, η_1) and diag (η_1, η_2, η_1) for some $\eta_1, \eta_2 > 0$ and Ball and James [7, Figure 5] give conditions on η_1, η_2 under which such an austenite-martensite interface is possible.

When $\varepsilon > 0$ and interfacial energy is present, the following, much stronger, local stability result holds.

Theorem 2.2 *Let $\Omega \subset \mathbb{R}^n$ be bounded, open and connected with Lipschitz boundary $\partial\Omega$, and $\overline{y} : \Omega \to \mathbb{R}^n$ be defined by $\overline{y}(x) = Rx + a$ for some constant $R \in SO(n)$ and $a \in \mathbb{R}^n$. Suppose that $\varepsilon > 0$ and ψ in (1.1) satisfies (f), (m), (n) and (2.1)–(2.4). Then there exist $\delta > 0, \sigma > 0$ such that*

$$\mathscr{I}(y) \geq \mathscr{I}(\overline{y}) + \sigma \int_{\Omega} \left(\left| \sqrt{Dy^T Dy} - I \right|^2 + |D^2 y|^2 \right) dx, \tag{2.12}$$

for any $y \in W^{2,2}(\Omega, \mathbb{R}^n)$ with $\mathscr{I}(y) < \infty$ and $\|y - \overline{y}\|_{L^1(\Omega,\mathbb{R}^n)} < \delta$. In particular, $\overline{y}$ is a local minimizer in $L^1(\Omega)$.

Proof Assume throughout that $y \in W^{2,2}(\Omega, \mathbb{R}^n)$ and $\mathscr{I}(y) < \infty$, so that $\det Dy > 0$ and $\sqrt{Dy^T Dy}$ is well-defined almost everywhere. We establish (2.12) via two arguments, depending on the value of $\int_\Omega |D^2 y|^2$. A standard contradiction proof, such as in Morrey [23] or Evans [17, §5.8.1], gives the following Poincaré-type inequality that is exploited in both cases: for every $\eta > 0$, there exists c_η such that for every $y \in W^{2,2}(\Omega, \mathbb{R}^n)$,

$$\int_{\Omega} |Dy|^2 \, dx \leq \eta \int_{\Omega} |D^2 y|^2 \, dx + c_\eta \left(\int_{\Omega} \left| y - ⨍ y \right| \, dx \right)^2, \tag{2.13}$$

where $⨍ y := \frac{1}{|\Omega|} \int_\Omega y$. Since $\int_\Omega \left| y - ⨍ y \right| \, dx \leq 2 \int_\Omega |y| \, dx$, it is then immediate that there exists $\tilde{c}_\eta$ such that

$$\int_{\Omega} |Dy|^2 \, dx \leq \eta \int_{\Omega} |D^2 y|^2 \, dx + \tilde{c}_\eta \left(\int_{\Omega} |y| \, dx \right)^2. \tag{2.14}$$

We first treat the case when $\int_\Omega |D^2y|^2$ is larger than a critical value L (to be specified in (2.24) below). Let the constant $c_1 > 0$, the existence of which is guaranteed by (2.14), be such that

$$\int_\Omega |Dy|^2\,dx \le c_1\left[\int_\Omega |D^2y|^2\,dx + \left(\int_\Omega |y|\,dx\right)^2\right] \quad \text{for all} \quad y, \tag{2.15}$$

and the constant $d_1 > 0$ be such that

$$\left(\int_\Omega |y|\,dx\right)^2 \le d_1, \tag{2.16}$$

whenever $\|y - \overline{y}\|_{L^1(\Omega)} < 1$. Then (2.15) and (2.16) give that for such y,

$$\int_\Omega |Dy|^2\,dx \le c_1\left(d_1 + \int_\Omega |D^2y|^2\,dx\right), \tag{2.17}$$

and since

$$\left|\sqrt{Dy^TDy} - I\right|^2 = |Dy|^2 - 2\mathrm{tr}\sqrt{Dy^TDy} + n \le |Dy|^2 + n, \tag{2.18}$$

because $\sqrt{Dy^TDy}$ is positive-definite and so $\mathrm{tr}\sqrt{Dy^TDy} > 0$, it follows that for every $\sigma > 0$,

$$\sigma\left(\int_\Omega \left|\sqrt{Dy^TDy} - I\right|^2 + |D^2y|^2\,dx\right) \le \sigma\left(c_1d_1 + n\,|\Omega| + (1 + c_1)\int_\Omega |D^2y|^2\,dx\right). \tag{2.19}$$

Now

$$\mathscr{I}(y) \ge \varepsilon^2 \int_\Omega |D^2y|^2\,dx, \tag{2.20}$$

since $\psi \ge 0$ by (m), and (2.1) gives that

$$\mathscr{I}(\overline{y}) = k|\Omega|. \tag{2.21}$$

Hence

$$\varepsilon^2\int_\Omega |D^2y|^2\,dx \ge k|\Omega| + \sigma\left(c_1d_1 + n|\Omega| + (1 + c_1)\int_\Omega |D^2y|^2\,dx\right), \tag{2.22}$$

implies that

$$\mathscr{I}(y) \ge \mathscr{I}(\overline{y}) + \sigma\left(\int_\Omega |\sqrt{Dy^TDy} - I|^2 + |D^2y|^2\,dx\right), \tag{2.23}$$

by (2.19), (2.20) and (2.21). So now fix $\sigma > 0$ sufficiently small that $\varepsilon^2 - \sigma(1+c_1) > 0$ and define the critical value

$$L = \frac{k|\Omega| + \sigma(c_1 d_1 + n|\Omega|)}{\varepsilon^2 - \sigma(1+c_1)}. \tag{2.24}$$

Then (2.22), and thus (2.23), hold for this choice of σ provided that y satisfies $\|y-\overline{y}\|_{L^1(\Omega)} \leq 1$ and

$$\int_\Omega |D^2 y|^2 \, dx \geq L. \tag{2.25}$$

Now suppose y is such that $\int_\Omega |D^2 y|^2 \, dx \leq L$, where L is defined by (2.24). Let $\delta_1 > 0$. Then (2.14) with $\eta = \delta_1^2/2L$, applied to $y - \overline{y}$, gives that

$$\int_\Omega |Dy - R|^2 \, dx \leq \frac{\delta_1^2}{2L} \int_\Omega |D^2 y|^2 \, dx + c(\delta_1) \left(\int_\Omega |y - \overline{y}| \, dx \right)^2 \tag{2.26}$$

for a constant $c(\delta_1) > 0$ independent of y. So $\|y - \overline{y}\|_{L^1(\Omega)} < \delta_1/\sqrt{2c(\delta_1)}$ implies

$$\int_\Omega |Dy - R|^2 \, dx \leq \delta_1^2, \tag{2.27}$$

and hence, since $|\sqrt{Dy^T Dy} - I| \leq |Dy - R|$ by (2.5), it follows that

$$\int_\Omega \left| \sqrt{Dy^T Dy} - I \right|^2 \, dx \leq \delta_1^2. \tag{2.28}$$

So in this case, y being close to $\overline{y}$ in $L^1(\Omega)$ implies that $\sqrt{Dy^T Dy}$ is close to I in $L^2(\Omega)$. This will allow us to reduce the problem to one of local minimizers in $S^{n\times n}$, and then to use conditions (2.2) and (2.3), together with Theorem 2.1 in Taheri [33], to establish (2.12). In order to appeal to [33], we will introduce below a suitable auxiliary function $\bar{\psi}$, defined on all of $\mathbb{R}^{n\times n}$ instead of only on $\mathbb{R}^{n\times n}_+$, that agrees with ψ on a neighbourhood of I in $\mathbb{R}^{n\times n}$. First note that denoting $\sqrt{Dy(x)^T Dy(x)}$ by $U(x)$, (2.28) can be rewritten as

$$\|U - I\|_{L^2(\Omega)} < \delta_1. \tag{2.29}$$

Identify $S^{n\times n}$ with $\mathbb{R}^{n(n+1)/2}$. Then note that it follows from, for example, the proof of Lemma 6.1 in Ball [4], that there exists $\rho > 0$ such that the derivative $D_F \hat{U}$ of the mapping $\hat{U}(F) = \sqrt{F^T F}$ from $\mathbb{R}^{n\times n}_+$ to $S^{n\times n}_+$ satisfies

$$|D_F \hat{U}(F) \cdot G| \leq \rho |G| \quad \text{for every} \quad F \in \mathbb{R}^{n\times n}_+ \quad \text{and} \quad G \in \mathbb{R}^{n\times n}. \tag{2.30}$$

Hence the derivative $DU(x)$ of the mapping $x \mapsto U(x) = \hat{U}(Dy(x))$ satisfies

$$\begin{aligned} |DU(x)|^2 &= |D_F \hat{U}(Dy(x)) \cdot D^2 y(x)|^2 \\ &\leq \rho^2 |D^2 y(x)|^2. \end{aligned} \tag{2.31}$$

Now by (n), we can choose $\mu > 0$ such that, with k as in (2.1),

$$\psi(M) \geq \max\{1, k + \tfrac{1}{2}\} \quad \text{if } \det M \leq \mu. \tag{2.32}$$

Let $\eta \in C^\infty(\mathbb{R}, \mathbb{R})$ be a non-decreasing function such that

$$\eta(s) = \begin{cases} 0 & \text{if } s \le \mu/2; \\ 1 & \text{if } s \ge \mu, \end{cases} \tag{2.33}$$

and for $F \in \mathbb{R}^{n\times n}$, define

$$\bar{\psi}(F) = \begin{cases} \eta(\det F)\psi(F) & \text{if } \det F \ge \mu/2; \\ 0 & \text{if } \det F \le \mu/2. \end{cases} \tag{2.34}$$

Then

(i) $\bar{\psi} \in C^2(\mathbb{R}^{n\times n}, \mathbb{R})$, since $\psi \in C^2(\mathbb{R}^{n\times n}_+, \mathbb{R})$;
(ii) $\bar{\psi}(F) \le \psi(F)$ for all $F \in \mathbb{R}^{n\times n}$, which is immediate from (2.34) since $\psi \ge 0$;
(iii) for F in a sufficiently small neighbourhood of I, $\bar{\psi}(F) = \psi(F)$, since $\det F$ is then close to $\det I = 1$, and hence

$$\bar{\psi}(I) = \psi(I), \quad D\bar{\psi}(I) = D\psi(I), \quad D^2\bar{\psi}(I) = D^2\psi(I). \tag{2.35}$$

Properties (i) and (ii) of $\bar{\psi}$, together with (2.31), then ensure that

$$\mathscr{I}(y) \ge \hat{\mathscr{I}}(U) + \frac{\varepsilon^2}{2}\int_\Omega |D^2 y|^2\,dx, \tag{2.36}$$

where $\hat{\mathscr{I}} : W^{1,2}(\Omega, S^{n\times n}) \to \mathbb{R}$ is defined by

$$\hat{\mathscr{I}}(U) = \int_\Omega \bar{\psi}(U) + \frac{\varepsilon^2}{2\rho^2}|DU|^2\,dx. \tag{2.37}$$

We will deduce the required estimate (2.12) from (2.36) by applying [33, Theorem 2.1] to $\hat{\mathscr{I}}$. First note that (2.2), (2.3) and (2.35) give that I is a local minimum of $\bar{\psi}$ with

$$D^2\bar{\psi}(I)(G,G) \ge \nu|G|^2 \quad \text{for all } \; G \in S^{n\times n},$$

and hence for $G \in W^{1,2}(\Omega; S^{n\times n})$,

$$\int_\Omega D\bar{\psi}(I)G\,dx = 0, \tag{2.38}$$

and

$$\begin{aligned}\int_\Omega D^2\bar{\psi}(I)(G,G) + \frac{\varepsilon^2}{\rho^2}|DG|^2\,dx &\ge \int_\Omega \nu|G|^2 + \frac{\varepsilon^2}{\rho^2}|DG|^2\,dx \\ &\ge \hat{\nu}\|G\|^2_{W^{1,2}},\end{aligned} \tag{2.39}$$

for some $\hat{\nu} > 0$. It thus follows immediately from [33, Theorem 2.1] that there exist $\sigma_1 > 0$ and $\delta_1 > 0$ such that

$$\begin{aligned}\hat{\mathscr{I}}(U) - \hat{\mathscr{I}}(I) &\ge \sigma_1\|U - I\|^2_{W^{1,2}} \\ &= \sigma_1 \int_\Omega |U - I|^2 + |DU|^2\,dx,\end{aligned} \tag{2.40}$$

whenever $\|U - I\|_{L^2} < \delta_1$. Take $\delta_1, \sigma_1 > 0$ as in (2.40) and let $\delta = \delta_1/\sqrt{2c(\delta_1)}$, with $c(\delta_1)$ as in (2.26). Estimates (2.29), (2.40) and (2.36) then yield that

$$\mathscr{I}(y) \geq \mathscr{I}(\overline{y}) + \sigma_1 \int_\Omega \left| \sqrt{Dy^T Dy} - I \right|^2 dx + \frac{\varepsilon^2}{2} \int_\Omega |D^2 y|^2 \, dx, \tag{2.41}$$

whenever $\|y - \overline{y}\|_{L^1(\Omega)} < \delta$ and $\int_\Omega |D^2 y|^2 \, dx \leq L$. The result (2.12) is now a consequence of (2.23) and (2.41). □

3 Structure of interfaces

The planar interface conditions (1.5) and (1.6) imply that Dy has a rank-one structure.

Lemma 3.1 *Let $\mathscr{F} \in W^{1,1}_{loc}(\mathbb{R}; \mathbb{R}^{n\times n})$ satisfy (1.5) and (1.6). Then there exist a constant vector $a \in \mathbb{R}^n$ and a function $u : \mathbb{R} \to \mathbb{R}^n$ such that*

$$u(s) \to 0, a \quad \text{as} \quad s \to -\infty, \infty, \tag{3.1}$$

and for all $x \in \mathbb{R}^n$,

$$\mathscr{F}(x \cdot N) = A + u(x \cdot N) \otimes N; \tag{3.2}$$

in particular,

$$B = A + a \otimes N, \tag{3.3}$$

and so B is rank-one connected to A.

Proof Assume without loss of generality that $N = e_1$, so that $x \cdot N = e_1$, and define $\phi \in C_0^\infty(\mathbb{R}^n)$ by

$$\phi(x) = \prod_{p=1}^{n} \phi^p(x_p), \quad x = (x_1, \ldots, x_n) \in \mathbb{R}^n,$$

where $\phi^p \in C_0^\infty(\mathbb{R})$ for each $1 \leq p \leq n$, and $\int_\mathbb{R} \phi^p = 1$ for each $2 \leq p \leq n$. Now $Dy(x) = \mathscr{F}(x_1)$ is a gradient, so for each $1 \leq i, j, k \leq n$ we have

$$\int_{\mathbb{R}^n} \mathscr{F}_{ij}(x_1)\phi_{,k}(x) \, dx = \int_{\mathbb{R}^n} \mathscr{F}_{ik}(x_1)\phi_{,j}(x) \, dx, \tag{3.4}$$

and hence

$$\int_{\mathbb{R}^n} \mathscr{F}_{ij}(x_1)(\phi^k)'(x_k) \left(\prod_{p\neq k} \phi^p(x_p) \right) dx = \int_{\mathbb{R}^n} \mathscr{F}_{ik}(x_1)(\phi^j)'(x_j) \left(\prod_{p\neq j} \phi^p(x_p) \right) dx,$$

so that

$$\int_\mathbb{R} \delta_{1k} \mathscr{F}_{ij}(x_1)(\phi^1)'(x_1) \, dx_1 = \int_\mathbb{R} \delta_{1j} \mathscr{F}_{ik}(x_1)(\phi^1)'(x_1) \, dx_1,$$

since $\int_{\mathbb{R}} \phi^p = 1$ for $p \geq 2$, and hence

$$\int_{\mathbb{R}} \left[\delta_{1k}\mathscr{F}_{ij}(x_1) - \delta_{1j}\mathscr{F}_{ik}(x_1)\right](\phi^1)'(x_1)\,dx_1 = 0.$$

It then follows, by the du Bois–Reymond lemma, that there exist constants C_{ijk} such that

$$\delta_{1k}\mathscr{F}_{ij}(x_1) - \delta_{1j}\mathscr{F}_{ik}(x_1) = C_{ijk} \quad \text{for all} \quad x_1 \in \mathbb{R}, \tag{3.5}$$

which when $k = 1$ gives

$$\mathscr{F}_{ij}(x_1) = C_{ij1} + \mathscr{F}_{i1}(x_1)\delta_{1j}, \quad x_1 \in \mathbb{R}. \tag{3.6}$$

Now (3.6) and (1.6) give that

$$A_{ij} = C_{ij1} + A_{i1}\delta_{1j}, \;\; B_{ij} = C_{ij1} + B_{i1}\delta_{1j}, \quad \text{for} \quad 1 \leq i, j \leq n, \tag{3.7}$$

and hence

$$B_{ij} = A_{ij} + (B_{i1} - A_{i1})\delta_{1j},$$

so that

$$B = A + a \otimes e_1,$$

where

$$a = (B - A)e_1 \in \mathbb{R}^n. \tag{3.8}$$

Equation (3.6) and the first equation in (3.7) also yield that

$$\mathscr{F}_{ij}(x_1) = A_{ij} + (\mathscr{F}_{i1}(x_1) - A_{i1})\delta_{1j},$$

and so

$$\mathscr{F}(x_1) = A + u(x_1) \otimes e_1,$$

where $u : \mathbb{R} \to \mathbb{R}^n$ is given by $u(s) = (\mathscr{F}(s) - A)e_1$. It follows from (1.6) and (3.8) that $u(s) \to 0, a$ as $s \to -\infty, \infty$. □

A deformation $y : \mathbb{R}^n \to \mathbb{R}^n$ having gradient satisfying (1.5) and (1.6) must be of form

$$y(x) = Ax + U(x \cdot N), \tag{3.9}$$

where $U : \mathbb{R} \to \mathbb{R}^n$ and $U' = u$, since (3.2) yields that $D(y(x) - Ax - U(x \cdot N)) = 0$ for such y.

It is in fact not necessary to assume the one-dimensional form (1.5) to obtain that B must be rank-one connected to A. The next lemma can be proved by a rescaling argument, the details of which we omit, and was first established in an unpublished manuscript of K. Huang.

Lemma 3.2 *Suppose that $y \in L^1_{\text{loc}}(\mathbb{R}^n, \mathbb{R}^n)$ and there exist $A, B \in \mathbb{R}^{n\times n}$ and a unit vector $N \in \mathbb{R}^n$ such that*

(i) $Dy \in L^\infty(\mathbb{R}^n, \mathbb{R}^{n\times n})$;

(ii) $Dy(jx) \to \begin{cases} A \text{ if } \; x \cdot N < 0, \\ B \text{ if } \; x \cdot N > 0, \end{cases} \quad$ *as* $j \to \infty$ *for a.e.* $x \in \mathbb{R}^n$.

Then there exists $a \in \mathbb{R}^n$ such that

$$B = A + a \otimes N.$$

Note that condition (i) in Lemma 3.2 is necessary; the function $y : \mathbb{R}^2 \to \mathbb{R}^2$ given by

$$y(x_1, x_2) = \begin{pmatrix} \ln(\cosh x_1) - \frac{x_1}{2} \\ x_2 \, (\tanh x_1 + \frac{1}{2}) \end{pmatrix},$$

satisfies

$$Dy(jx_1, jx_2) = \begin{pmatrix} \tanh jx_1 - \frac{1}{2} & 0 \\ jx_2 \operatorname{sech}^2 jx_1 & \tanh jx_1 + \frac{1}{2} \end{pmatrix}$$

$$\to \begin{pmatrix} -\frac{3}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix} \text{or} \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{3}{2} \end{pmatrix} \quad \text{as} \quad j \to \infty,$$

depending on whether $x_1 < 0$ or $x_1 > 0$.

4 Existence of planar interfaces

Substitution of the ansatz (3.2) into the energy (1.1) leads naturally to a reduced energy functional of form

$$\mathscr{J}(u) = \int_{\mathbb{R}} \psi(A + u(s) \otimes N) + \varepsilon^2 |u'(s)|^2 \; ds, \tag{4.1}$$

since N is a unit vector, and so

$$|D^2 y(x)|^2 = y_{i,\alpha\beta} y_{i,\alpha\beta} = u_i'(x \cdot N) u_i'(x \cdot N) N_\alpha N_\alpha N_\beta N_\beta = |u'(x \cdot N)|^2.$$

We will seek a planar interface solution y to the Euler–Lagrange equations for the original functional (1.1) by minimizing the reduced functional (4.1) among a class of $u : \mathbb{R} \to \mathbb{R}^n$ satisfying (3.1). There are two main steps: first, to obtain a solution to the Euler–Lagrange equations for the reduced problem (4.1), and second, to show that, via (3.2), this in fact yields a solution of the Euler–Lagrange equations of the original problem (1.1).

The problem of minimizing functionals of the form

$$\mathscr{E}(u) = \int_{\mathbb{R}} W(u(s)) + \varepsilon^2 |u'(s)|^2 \, ds \tag{4.2}$$

among vector-valued $u : \mathbb{R} \to \mathbb{R}^n$ connecting two minima of the potential W was first addressed as a side-issue by Sternberg [32], where critical points of (4.2) are obtained via minimization of the related functional

$$\inf_{\gamma(-1)=\alpha, \gamma(1)=\beta} \int_{-1}^{1} \sqrt{W(\gamma(t))} |\gamma'(t)| \, dt \tag{4.3}$$

among suitable parametrised curves $\gamma : [-1, 1] \to \mathbb{R}^n$ connecting minima a and b of W. There are also a number of later articles [1,3,13,29] in which the existence of a minimizer for (4.2) in some class of u is addressed directly via minimization of (4.2) under various hypotheses on the potential W. In particular, conditions are needed on the form of W close to the minima a and b in order to obtain compactness properties of minimizing sequences. A recent paper of Alikakos and Fusco [3] uses a constrained minimization argument to establish the existence of a minimizing connection under non-degeneracy conditions on the minima of

W that are notably weaker than those in previous work, which typically required quadratic behaviour of W close to the minima a and b.

We exploit [3] to obtain an existence result for our reduced functional (4.1). The following theorem is proved in [3, Theorems 3.1, 3.2]. Assumption (ii) is a mild non-degeneracy condition on the behaviour of W near the minima of W. Here and in the following, we use the usual notation $S^{n-1} := \{u \in \mathbb{R}^n : |u| = 1\}$.

Theorem 4.1 (Alikakos and Fusco [3]) *Suppose $W : \mathbb{R}^n \to \mathbb{R}$ is a C^2-function such that*

(i) *there exist $a^- \neq a^+$ such that $W(a^\pm) = 0$ and $W(u) > 0$ for all $u \in \mathbb{R}^n$, $u \neq a^\pm$;*
(ii) *there exists $r_0 \in (0, |a^+ - a^-|)$ such that each of the maps $r \mapsto W(a^+ + r\xi)$, $r \mapsto W(a^- + r\xi)$ has a strictly positive derivative for every $r \in (0, r_0)$ and for each $\xi \in S^{n-1}$;*
(iii) $\liminf_{|u|\to\infty} W(u) > 0$.

Let $\mathscr{C}$ be the set

$$\mathscr{C} := \left\{ u \in W^{1,2}_{loc}(\mathbb{R}, \mathbb{R}^n) : \lim_{s\to-\infty} u(s) = a^-, \lim_{s\to\infty} u(s) = a^+ \right\}. \tag{4.4}$$

Then there exists $u_0 \in \mathscr{C}$ such that

$$\mathscr{E}(u_0) = \inf_{u\in\mathscr{C}} \mathscr{E}(u), \tag{4.5}$$

where $\mathscr{E}$ is as defined in (4.2).

To use Theorem 4.1 to obtain an existence result for the reduced problem (4.1), we need some preliminary lemmas. The first concerns the fact that, since the stored energy function ψ is defined on $\mathbb{R}^{n\times n}_+$, we are interested in vectors $u : \mathbb{R} \to \mathbb{R}^n$ for which $\det(A + u(s) \otimes N) > 0$ for all $s \in \mathbb{R}$.

Lemma 4.2 *Let $\psi : \mathbb{R}^{n\times n}_+ \to \mathbb{R}$ satisfy the conditions (f), (m) and (n) on frame indifference, multi-well structure and non-interpenetration given in the Introduction. Suppose that $A \in SO(n)U_{i_0}$ and $B \in SO(n)U_{j_0}$, $i_0 \neq j_0$ are such that $B = A + a \otimes N$ for some $a, N \in \mathbb{R}^n$ with $a \neq 0$ and $|N| = 1$. Define the open half-space*

$$\mathscr{H} := \{u \in \mathbb{R}^n : 1 + u \cdot A^{-T} N > 0\} \subset \mathbb{R}^n. \tag{4.6}$$

Then

(i) $\det(A + u \otimes N) > 0 \Leftrightarrow u \in \mathscr{H}$,
$\det(A + u \otimes N) = 0 \Leftrightarrow u \in \partial\mathscr{H}$;
(ii) $\psi(A + u \otimes N) \to \infty$ *as* $u \to \partial\mathscr{H}$.

Proof The fact that

$$\det(A + u \otimes N) = \det A \det(I + u \otimes A^{-T} N) = \det A(1 + u \cdot A^{-T} N),$$

yields (i), and (ii) is then an immediate consequence of condition (n). □

With $\mathscr{H}$ as in Lemma 4.2, we now define $W : \mathscr{H} \to [0, \infty)$ by

$$W(u) = \psi(A + u \otimes N); \tag{4.7}$$

by Lemma 4.2(ii),

$$W(u) \to \infty \quad \text{as} \quad u \to \partial\mathscr{H}. \tag{4.8}$$

The next lemma concerns the minima of $W(u)$. It involves an interplay between the rank-one structure (3.2) and the frame-indifference of the function ψ in (4.1).

Lemma 4.3 *Let ψ, A, B, a, N and $\mathscr{H}$ be as in the statement of Lemma 4.2. Suppose in addition that A, N and the U_i, $1 \le i \le k$, in (m) are such that*

$$A + b \otimes N \notin \cup_{\substack{1\le i\le k,\\ i\neq i_0, j_0}} SO(n)U_i \quad \text{for all} \ \ b \in \mathscr{H}. \tag{4.9}$$

Then

$$W(0) = W(a) = 0 \ \ \text{and} \ \ W(u) > 0 \ \ \text{for all} \ \ u \in \mathscr{H} \ \ \text{with} \ \ u \notin \{0, a\}.$$

Proof Note first that $W(u) = \psi(A + u \otimes N) \ge 0$ for all $u \in \mathscr{H}$, and $W(u) = 0$ if and only if $A + u \otimes N \in \cup_{1\le i\le k}\mathrm{SO}(n)U_i$. By condition (4.9), $A + u \otimes N \notin \cup_{\substack{1\le i\le k,\\ i\neq i_0, j_0}} \mathrm{SO}(n)U_i$ for any $u \in \mathscr{H}$. If $A+u\otimes N \in \mathrm{SO}(n)U_{i_0} = \mathrm{SO}(n)A$, then $u = 0$, since A is not rank-one connected to any element of $\mathrm{SO}(n)A$. Likewise, if $A+u\otimes N = B+(u-a)\otimes N \in \mathrm{SO}(n)U_{j_0} = \mathrm{SO}(n)B$, then $u - a = 0$, since B is not rank-one connected to any element of $\mathrm{SO}(n)B$. Hence $W(u) = 0 \Leftrightarrow u \in \{0, a\}$, as required. □

Remark Condition (4.9) ensures that even if ψ has more than two energy-minimizing wells, the function W has only two zeroes. This is important because, in general, the existence of more than two zeroes of W can result in the non-existence of connections between a given pair of zeroes. See, for example, Alama et al. [1], Alikakos et al. [2], Alikakos and Fusco [3], Stefanopolous [31], and also Fife and McLeod [18] and Volpert et al. [35]. The condition (4.9) holds in particular for the martensite wells in a cubic to tetragonal transition, when $k = 3$ and $U_1 = \mathrm{diag}(\eta_2, \eta_1, \eta_1)$, $U_2 = \mathrm{diag}(\eta_1, \eta_2, \eta_1)$ and $U_3 = \mathrm{diag}(\eta_1, \eta_1, \eta_2)$. For each $k \in \{2, 3\}$, $U_1 + a \otimes N \in \mathrm{SO}(3)U_k$ if and only if either

$$a = \frac{\sqrt{2}(\eta_k^2 - \eta_1^2)}{\eta_1^2 + \eta_k^2}(-\eta_k e_1 + \eta_1 e_k), \quad N = \frac{1}{\sqrt{2}}(e_1 + e_k), \tag{4.10}$$

or

$$a = \frac{\sqrt{2}(\eta_k^2 - \eta_1^2)}{\eta_1^2 + \eta_k^2}(-\eta_k e_1 - \eta_1 e_k), \quad N = \frac{1}{\sqrt{2}}(e_1 - e_k), \tag{4.11}$$

where e_i, $i \in \{1, 2, 3\}$, denotes the standard unit vector in direction x_i. It clearly follows from (4.10) and (4.11) that if N is such that $U_1 + a \otimes N \in \mathrm{SO}(3)U_2$ for some $a \in \mathbb{R}^3$, then $U_1 + u \otimes N \notin \mathrm{SO}(3)U_3$ for any $u \in \mathbb{R}^3$.

But (4.9) does not, alas, hold in general. A counterexample, which was pointed out to us by Bhattacharya, is given by a special choice of lattice parameters in the martensite wells in a cubic to orthorhombic transition, when $k = 6$. With the first three variants U_1, U_2 and U_3 of the six variants $U_1, \ldots, U_6$ taken to be

$$U_1 = \begin{pmatrix} \beta & 0 & 0 \\ 0 & \frac{\alpha+\gamma}{2} & \frac{\alpha-\gamma}{2} \\ 0 & \frac{\alpha-\gamma}{2} & \frac{\alpha+\gamma}{2} \end{pmatrix}, \quad U_2 = \begin{pmatrix} \beta & 0 & 0 \\ 0 & \frac{\alpha+\gamma}{2} & \frac{\gamma-\alpha}{2} \\ 0 & \frac{\gamma-\alpha}{2} & \frac{\alpha+\gamma}{2} \end{pmatrix}, \quad U_3 = \begin{pmatrix} \frac{\alpha+\gamma}{2} & 0 & \frac{\alpha-\gamma}{2} \\ 0 & \beta & 0 \\ \frac{\alpha-\gamma}{2} & 0 & \frac{\alpha+\gamma}{2} \end{pmatrix},$$

where $\alpha, \beta, \gamma > 0$ and $\gamma > \alpha$, it is shown in Hane [19] that there exists a rank-one connection between U_1 and $\mathrm{SO}(3)U_2$ with $N = e_3$, and also a rank-one connection between U_1 and $\mathrm{SO}(3)U_3$ with

$$N = \frac{(2\beta^2 - \alpha^2 - \gamma^2)(e_1 + e_2) + 2(\gamma^2 - \alpha^2)e_3}{\sqrt{8\beta^2(\beta^2 - \alpha^2 - \gamma^2) + 6\alpha^4 - 4\alpha^2\gamma^2 + 6\gamma^4}}.$$

Hence if

$$2\beta^2 - \alpha^2 - \gamma^2 = 0, \tag{4.12}$$

the normal $N = e_3$ arises in rank-one connections both between U_1 and $SO(3)U_2$ and between U_1 and $SO(3)U_3$. Note, however, that experimental values of α, β and γ typically satisfy $\alpha, \gamma \geq 1$ and $\beta < 1$ (see Bhattacharya [11, Table 4.2]), for which (4.12) is impossible.

It is of interest to establish whether or not (4.9) is in some sense generic. The following lemma gives a sufficient condition for the non-degeneracy (4.9) to hold in the case when $n = 3$ and the matrices $\{U_i\}_{i=1}^k$ in (m) satisfy additional conditions that are implied by imposing cubic material symmetry (see Sect. 6) on ψ.

Lemma 4.4 *Suppose that the matrices $U_1, U_2, \ldots U_k \in \mathbb{R}_+^{3\times 3}$ in the multi-well structure (m) are symmetric, $|U_1|^2 = |U_2|^2 = \cdots = |U_k|^2$, and*

$$\operatorname{cof}(U_{j_0}^2 - U_{i_0}^2) \cdot (U_l^2 - U_{i_0}^2) \neq 0 \tag{4.13}$$

for some $i_0, j_0 \in \{1, \ldots, k\}$, $i_0 \neq j_0$, and all $l \in \{1, \ldots, k\} \setminus \{i_0, j_0\}$. Then condition (4.9) is satisfied with $A = U_{i_0}$ and $N \in \mathbb{R}^3$ such that $A + a \otimes N \in SO(3)U_{j_0}$ for some $a \in \mathbb{R}^3$.

Proof Suppose not. Then there exist $j_0, l \in \{1, \ldots, k\} \setminus \{i_0\}$, $j_0 \neq l$, $N \in \mathbb{R}^3$ with $|N| = 1$, and $a, b \in \mathbb{R}^3$ such that

$$U_{i_0} + a \otimes N \in SO(3)U_{j_0} \quad \text{and} \quad U_{i_0} + b \otimes N \in SO(3)U_l.$$

Since U_{j_0} and U_l are symmetric, there exist vectors $c, d \in \mathbb{R}^3$ such that

$$\begin{aligned} U_{j_0}^2 - U_{i_0}^2 &= c \otimes N + N \otimes c, \\ U_l^2 - U_{i_0}^2 &= d \otimes N + N \otimes d, \end{aligned}$$

and as $|U_{j_0}| = |U_l| = |U_{i_0}|$, taking the trace of these equalities implies that

$$c \cdot N = 0, \quad d \cdot N = 0. \tag{4.14}$$

Now for each $\mu \in \mathbb{R}$, the matrix

$$\mu(U_l^2 - U_{i_0}^2) + (U_{j_0}^2 - U_{i_0}^2) = (\mu d + c) \otimes N + N \otimes (\mu d + c)$$

has rank two, since $\mu d + c$ and N are orthogonal for every μ, and thus

$$\det[\mu(U_l^2 - U_{i_0}^2) + (U_{j_0}^2 - U_{i_0}^2)] = 0 \quad \text{for all } \mu \in \mathbb{R}. \tag{4.15}$$

The left-hand side of (4.15) is a polynomial in μ, and the coefficient of μ, given by the derivative of the left-hand side evaluated when $\mu = 0$, must be zero. Hence

$$\operatorname{cof}(U_{j_0}^2 - U_{i_0}^2) \cdot (U_l^2 - U_{i_0}^2) = 0,$$

which contradicts (4.13). □

Note that in the cubic to orthorhombic transition, (4.13) holds for $i_0 = 1$, $j_0 = 2$ and $l = 3$ if and only if the lattice parameters α, β and γ do not satisfy equation (4.12), because

$$\operatorname{cof}(U_2^2 - U_1^2) = \begin{pmatrix} -(\alpha^2 - \gamma^2)^2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

and

$$U_3^2 - U_1^2 = \frac{1}{2}\begin{pmatrix} -(2\beta^2-\alpha^2-\gamma^2) & 0 & \alpha^2-\gamma^2 \\ 0 & 2\beta^2-\alpha^2-\gamma^2 & -(\alpha^2-\gamma^2) \\ \alpha^2-\gamma^2 & -(\alpha^2-\gamma^2) & 0 \end{pmatrix},$$

so that

$$\begin{aligned} \operatorname{cof}(U_2^2 - U_1^2)\cdot(U_3^2 - U_1^2) &= \frac{(\alpha^2-\gamma^2)^2(2\beta^2-\alpha^2-\gamma^2)}{2} \\ &= 0 \Leftrightarrow 2\beta^2-\alpha^2-\gamma^2 = 0, \end{aligned}$$

since $\alpha \neq \gamma$.

We conclude this remark on condition (4.9) by noting that Alama et al. [1] and Alikakos and Fusco [3] (see also [31]) show that a sufficient condition for the existence of a connection between two given zeroes a_1 and a_2 of W in the presence of a third zero a_3 is that

$$e_{12} < e_{13} + e_{32}, \tag{4.16}$$

where e_{ij} denotes the minimal energy of a connection between a_i and a_j. Symmetry conditions on the function W can ensure that (4.16) is satisfied; see, for example, Stefanopolous [31], and also Bronsard et al. [13]. However, in spite of physically realistic ψ having material-symmetry properties in addition to frame-indifference (f), it is not clear that for such ψ, the function $W(\cdot) = \psi(A + \cdot \otimes N)$ satisfies sufficient symmetry to ensure that (4.16) is typically satisfied if (4.9) fails, essentially because imposing the ansatz $A + u \otimes N$ partially breaks the symmetry of ψ. An illustration of this is given by the fact that in the cubic to orthorhombic example given above, the vectors a and b in the two rank-one connections $U_1 + a \otimes e_3 \in \mathrm{SO}(3)U_2$ and $U_1 + b \otimes e_3 \in \mathrm{SO}(3)U_3$ do not have the same length and thus cannot be related by a rotation (see Hane [19] for details).

The next lemma addresses the fact that Theorem 4.1 cannot be applied directly using W defined in (4.7); W is only defined on a half-space $\mathscr{H}$ and blows-up at the boundary $\partial\mathscr{H}$. To overcome this difficulty, we will show, under an additional condition on the behaviour of $\psi(A + u \otimes N)$ when $A + u \otimes N$ is close to $\partial\mathscr{H}$, that minimizing sequences for (4.1) stay away from $\partial\mathscr{H}$, and then construct a modified function $\hat{W}$ which will be used to prove an existence result for (4.1).

Lemma 4.5 *Let A, B, a, N and $\mathscr{H}$ be as in Lemma 4.2 and a convex open set $\Omega \subset \mathbb{R}^n$ be such that*

$$\mathscr{H} \subset \Omega \subset \mathbb{R}^n, \tag{4.17}$$

(*with non-strict inclusion,* i.e. $\Omega = \mathscr{H}$ *or* $\mathbb{R}^n$ *permitted*). *Suppose that* $\tilde{W} : \Omega \to [0, \infty)$ *has the property that there exists* $\nu_0 > 0$ *such that* $\det A > \nu_0$, $\det(A + a \otimes N) > \nu_0$, *and*

$$\left.\frac{d}{dt}\tilde{W}(u + tA^{-T}N)\right|_{t=0} < 0 \tag{4.18}$$

whenever $u \in \Omega$ *and* $\det(A + u \otimes N) < \nu_0$. *Define*

$$\tilde{\mathscr{C}} := \{u \in W^{1,2}_{loc}(\mathbb{R}, \Omega) : \lim_{s\to-\infty} u(s) = 0,\ \lim_{s\to\infty} u(s) = a\}, \tag{4.19}$$

$$\tilde{\mathscr{C}}_{\nu_0} := \{u \in \tilde{\mathscr{C}} : \det(A + u(s) \otimes N) \geq \nu_0 \ \ \textit{for all} \ \ s \in \mathbb{R}\}, \tag{4.20}$$

and

$$\tilde{\mathscr{E}}(u) := \int_{\mathbb{R}} \tilde{W}(u(s)) + \varepsilon^2 |u'(s)|^2 \, ds, \quad u \in \tilde{\mathscr{C}}. \tag{4.21}$$

Then

(i)

$$\inf_{u \in \tilde{\mathscr{C}}} \tilde{\mathscr{E}}(u) = \inf_{u \in \tilde{\mathscr{C}}_{\nu_0}} \tilde{\mathscr{E}}(u); \tag{4.22}$$

(ii) *if* $u_0 \in \tilde{\mathscr{C}}$ *is such that*

$$\tilde{\mathscr{E}}(u_0) = \inf_{\tilde{\mathscr{C}}} \tilde{\mathscr{E}}(u), \tag{4.23}$$

then $u_0 \in \tilde{\mathscr{C}}_{\nu_0}$.

Proof Let $u \in \tilde{\mathscr{C}}$ with $\det(A + u(s) \otimes N) < \nu_0$ for some $s \in \mathbb{R}$. We will show that there exists $\hat{u} \in \tilde{\mathscr{C}}_{\nu_0}$ with $\tilde{\mathscr{E}}(\hat{u}) < \tilde{\mathscr{E}}(u)$, from which both (i) and (ii) follow immediately.

Note that

$$\det(A + u \otimes N) = \nu_0 \Leftrightarrow 1 + u \cdot A^{-T} N = \frac{\nu_0}{\det A} =: \tilde{\nu}_0.$$

Define $\hat{u} \in \tilde{\mathscr{C}}_{\nu_0}$ by

$$\hat{u}(s) = \begin{cases} u(s) & \text{if } \det(A + u(s) \otimes N) \geq \nu_0; \\ u(s) + \left(\dfrac{-1 + \tilde{\nu}_0 - u(s) \cdot (A^{-T} N)}{|A^{-T} N|^2} \right) A^{-T} N & \text{if } \det(A + u(s) \otimes N) < \nu_0. \end{cases} \tag{4.24}$$

If $\det(A + u(s) \otimes N) < \nu_0$ then $\det(A + \hat{u}(s) \otimes N) = \nu_0$, and since $u(s) \cdot A^{-T} N < -1 + \tilde{\nu}_0 = \hat{u}(s) \cdot A^{-T} N$ it thus follows that

$$\tilde{W}(\hat{u}(s)) < \tilde{W}(u(s)).$$

Also

$$\begin{aligned} |\hat{u}'(s)|^2 &= |u'(s)|^2 + \frac{(u'(s) \cdot A^{-T} N)^2}{|A^{-T} N|^2} - 2 \frac{(u'(s) \cdot A^{-T} N)^2}{|A^{-T} N|^2} \\ &= |u'(s)|^2 - \frac{(u'(s) \cdot A^{-T} N)^2}{|A^{-T} N|^2} \\ &\leq |u'(s)|^2. \end{aligned}$$

Hence

$$\tilde{\mathscr{E}}(\hat{u}) < \tilde{\mathscr{E}}(u),$$

as required. □

Our main existence theorem is the following.

Theorem 4.6 *Let* ψ, A, B, a, N *and* $\mathscr{H}$ *be as in the statement of Lemma 4.3. Suppose that* ψ *also satisfies*

(i) $\psi \in C^2(\mathbb{R}^{n\times n}_+, \mathbb{R})$;
(ii) *there exists* $r_0 \in (0, |a|)$ *such that each of the maps* $r \mapsto \psi(A + r\xi \otimes N)$ *and* $r \mapsto \psi(B + r\xi \otimes N)$ *has a strictly positive derivative for every* $r \in (0, r_0)$ *and for each* $\xi \in S^{n-1}$;
(iii) $\liminf_{|u|\to\infty} \psi(A + u \otimes N) > 0$;
(iv) *there exists* $\nu_0 \in (0, \min\{\det A, \det B\})$ *such that*

$$\frac{d}{dt}\psi(A + u \otimes N + tA^{-T}N \otimes N)\Big|_{t=0} < 0$$

whenever $u \in \mathscr{H}$ *and* $\det(A + u \otimes N) < \nu_0$.

Let $\mathscr{C} = \{u \in W^{1,2}_{loc}(\mathbb{R}, \mathscr{H}) : \lim_{s\to-\infty} u(s) = 0, \lim_{s\to\infty} u(s) = a\}$. *Then there exists* $u_0 \in \mathscr{C}$ *such that*

$$\mathscr{J}(u_0) = \inf_{u\in\mathscr{C}} \mathscr{J}(u), \tag{4.25}$$

where $\mathscr{J}$ *is as defined in (4.1).*

Proof Let $W : \mathscr{H} \to \mathbb{R}$ be defined as in (4.7), $\mathscr{E}$ be defined as in (4.2) with this choice of W, and $\tilde{\nu}_0 = \nu_0/\det A$. We will extend W to a function $\hat{W} : \mathbb{R}^n \to \mathbb{R}$ by "stretching" the part of W close to $\partial\mathscr{H}$. First let $f : \mathbb{R} \to (-1, \infty)$ be such that

(i) $f \in C^2(\mathbb{R}, (-1, \infty))$;
(ii) $f(s) = s$ for all $s \geq -1 + \tilde{\nu}_0$;
(iii) $f(s) \to -1$ as $s \to -\infty$;
(iv) $f'(s) > 0$ for all $s \in \mathbb{R}$.

Then for all $u \in \mathbb{R}^N$,

$$\det\left(A + \left(u + \frac{f(u\cdot A^{-T}N) - u\cdot A^{-T}N}{|A^{-T}N|^2}A^{-T}N\right)\otimes N\right) = \det A(1 + f(u\cdot A^{-T}N)),$$

and hence

$$\det\left(A + \left(u + \frac{f(u\cdot A^{-T}N) - u\cdot A^{-T}N}{|A^{-T}N|^2}A^{-T}N\right)\otimes N\right) > 0, \tag{4.26}$$

and

$$\begin{aligned}\det\left(A + \left(u + \frac{f(u\cdot A^{-T}N) - u\cdot A^{-T}N}{|A^{-T}N|^2}A^{-T}N\right)\otimes N\right) < \nu_0 \\ \Leftrightarrow \det(A + u \otimes N) < \nu_0.\end{aligned} \tag{4.27}$$

From (4.26), we can define $\hat{W} : \mathbb{R}^n \to \mathbb{R}$ as

$$\hat{W}(u) := W\left(u + \left(\frac{f(u\cdot A^{-T}N) - u\cdot A^{-T}N}{|A^{-T}N|^2}\right)A^{-T}N\right), \quad u \in \mathbb{R}^n.$$

Then $\hat{W} \in C^2(\mathbb{R}^n, \mathbb{R})$ and satisfies

(i) $\hat{W}(u) = W(u)$ whenever $\det(A + u \otimes N) \geq \nu_0$;
(ii) $\hat{W}(u) \geq 0$ for all $u \in \mathbb{R}^n$;
(iii) $\hat{W}(u) = 0$ if and only if $u \in \{0, a\}$, by Lemma 4.3 and (4.27);
(iv) $\liminf_{|u|\to\infty} \hat{W}(u) > 0$.

It thus follows from Theorem 4.1 that there exists $u_0 \in \hat{\mathscr{C}} := \{u \in W^{1,2}_{loc}(\mathbb{R}, \mathbb{R}^n) : \lim_{s\to-\infty} u(s) = 0, \lim_{s\to\infty} u(s) = a\}$ such that

$$\hat{\mathscr{E}}(u_0) = \inf_{u\in\hat{\mathscr{C}}} \hat{\mathscr{E}}(u),$$

where

$$\hat{\mathscr{E}}(u) := \int_{\mathbb{R}} \hat{W}(u(s)) + \varepsilon^2 |u'(s)|^2 \, ds, \quad u \in \hat{\mathscr{C}}.$$

Now let $u \in \mathbb{R}^n$ be such that $\det(A + u \otimes N) < \nu_0$ and define

$$z^*(t) := \frac{f(u \cdot A^{-T}N + t|A^{-T}N|^2) - u \cdot A^{-T}N}{|A^{-T}N|^2}, \quad t \in \mathbb{R}.$$

Then $\hat{W}(u + tA^{-T}N) = W\left(u + z^*(t)A^{-T}N\right)$, and by (4.27), $\det(A + (u + z^*(0)A^{-T}N) \otimes N) < \nu_0$. So

$$\begin{aligned}
\frac{d}{dt}\hat{W}(u + tA^{-T}N)\Big|_{t=0} &= \frac{d}{dz}W(u + zA^{-T}N)\Big|_{z=z^*(0)} \frac{dz^*}{dt}\Big|_{t=0} \\
&= \frac{d}{dz}W(u + zA^{-T}N)\Big|_{z=z^*(0)} f'(u \cdot A^{-T}N + t|A^{-T}N|^2)\Big|_{t=0} \\
&= f'(u \cdot A^{-T}N) \frac{d}{dz}W(u + zA^{-T}N)\Big|_{z=z^*(0)} \\
&< 0,
\end{aligned}$$

by condition (iv) on $\psi(A + u \otimes N + tA^{-T}N \otimes N) = W(u + tA^{-T}N)$ in the statement of the theorem. Hence it follows from Lemma 4.5 applied with $\Omega = \mathbb{R}^n$, $\tilde{W} = \hat{W}$ and $\tilde{\mathscr{C}}_{\nu_0} = \hat{\mathscr{C}}_{\nu_0} := \{u \in \hat{\mathscr{C}} : \det(A + u \otimes N) \geq \nu_0\}$ that

$$\inf_{u\in\hat{\mathscr{C}}} \hat{\mathscr{E}}(u) = \inf_{u\in\hat{\mathscr{C}}_{\nu_0}} \hat{\mathscr{E}}(u),$$

and that

$$u_0 \in \hat{\mathscr{C}}_{\nu_0}.$$

On the other hand, Lemma 4.5 applied with $\Omega = \mathscr{H}$ yields that

$$\inf_{u\in\mathscr{C}} \mathscr{E}(u) = \inf_{u\in\mathscr{C}_{\nu_0}} \mathscr{E}(u),$$

where $\mathscr{C}_{\nu_0} := \{u \in \mathscr{C} : \det(A + u(s) \otimes N) \geq \nu_0$ for all $s \in \mathbb{R}\}$, again using condition (iv) in the statement of the theorem. Since $W(u) = \hat{W}(u)$ for all u with $\det(A + u \otimes N) \geq \nu_0$, it follows that

$$\inf_{u\in\hat{\mathscr{C}}} \hat{\mathscr{E}}(u) = \inf_{u\in\hat{\mathscr{C}}_{\nu_0}} \hat{\mathscr{E}}(u) = \inf_{u\in\mathscr{C}_{\nu_0}} \mathscr{E}(u) = \inf_{u\in\mathscr{C}} \mathscr{E}(u),$$

and hence

$$\mathscr{E}(u_0) = \inf_{u\in\mathscr{C}} \mathscr{E}(u). \qquad \square$$

The next two lemmas show that conditions (ii) and (iv) in Theorem 4.6 hold for a reasonably large class of ψ.

Lemma 4.7 *Define* $\psi : \mathbb{R}^{n\times n}_+ \to \mathbb{R}$ *by*

$$\psi(F) := h(\det F) + g(F),$$

where

(i) $h \in C^2((0,\infty),\mathbb{R})$ *and* $h'(z) \to -\infty$ *as* $z \to 0^+$*;*
(ii) $g \in C^2(\mathbb{R}^{n\times n}_+,\mathbb{R})$ *and* $Dg(F)$ *is bounded on* $\{F \in \mathbb{R}^{n\times n}_+ : \det F < \nu\}$ *for some* $\nu > 0$.

Then there exists $\nu_0 > 0$ *such that*

$$\frac{d}{dt}\psi(A + (u + tA^{-T}N)\otimes N)\Big|_{t=0} < 0$$

whenever $0 < \det(A + u\otimes N) < \nu_0$*; that is,* ψ *satisfies condition (iv) in Theorem 4.6.*

Proof First note that $\det(A + (u + tA^{-T}N)\otimes N) = \det A(1 + (u + tA^{-T}N)\cdot A^{-T}N)$, and hence

$$\frac{d}{dt}\det(A + (u + tA^{-T}N)\otimes N) = \det A|A^{-T}N|^2.$$

So

$$\begin{aligned}&\frac{d}{dt}\psi(A + (u + tA^{-T}N)\otimes N)\Big|_{t=0}\\ &\quad= h'(\det(A + u\otimes N))\det A|A^{-T}N|^2 + Dg(A + u\otimes N)N\cdot A^{-T}N < 0\end{aligned}$$

if $\det(A + u\otimes N)$ is sufficiently small, since $Dg(A + u\otimes N)$ is bounded and $h'(\det(A + u\otimes N)) \to -\infty$ as $\det(A + u\otimes N) \to 0$. □

Lemma 4.8 *Let* $A \in \mathbb{R}^{n\times n}_+$ *and* $\psi \in C^2(\mathbb{R}^{n\times n}_+,\mathbb{R})$ *be such that* $\psi(M) \geq \psi(A)$ *whenever* $|M - A| \leq \delta$ *for some* $\delta > 0$*, let the frame-indifference condition (f) hold, and suppose there exists* $\gamma > 0$ *such that*

$$D^2\psi(A)(GA, GA) \geq \gamma|G|^2 \quad \textit{for all} \quad G \in S^{n\times n}. \tag{4.28}$$

Then given $N \in \mathbb{R}^n$*, there exists* $r_0 > 0$ *such that for each* $\xi \in S^{n-1}$*, the map* $r \mapsto \psi(A + r\xi\otimes N)$ *has a strictly positive derivative for every* $r \in (0, r_0)$*; that is, condition (ii) in Theorem 4.6 is satisfied at* A*.*

Proof Note first that for each $t \in \mathbb{R}$ and $K \in \mathbb{R}^{n\times n}$ with $K^T = -K$,

$$\frac{\partial\psi}{\partial F_{i\alpha}}(e^{Kt}A) = 0, \tag{4.29}$$

since $D\psi(RA) = 0$ for all $R \in \mathrm{SO}(n)A$. Then differentiating (4.29) with respect to t and setting $t = 0$ yields that

$$\frac{\partial^2\psi}{\partial F_{j\beta}F_{i\alpha}}(A)K_{jl}A_{l\beta} = 0, \tag{4.30}$$

and hence for any $G, K \in \mathbb{R}^{n\times n}$ with $G^T = G$ and $K^T = -K$,

$$\begin{aligned}&D^2\psi(A)((G + K)A, (G + K)A)\\ &\quad= D^2\psi(A)(KA, KA) + 2D^2\psi(A)(KA, GA) + D^2\psi(A)(GA, GA)\\ &\quad= D^2\psi(A)(GA, GA)\\ &\quad\geq \gamma|G|^2.\end{aligned} \tag{4.31}$$

In particular, given $N \in \mathbb{R}^n$ and $\xi \in S^{n-1}$, taking $G = \frac{1}{2}[\xi \otimes A^{-T}N + A^{-T}N \otimes \xi]$ and $K = \frac{1}{2}[\xi \otimes A^{-T}N - A^{-T}N \otimes \xi]$ gives $G + K = \xi \otimes A^{-T}N$ and $(G+K)A = \xi \otimes N$. Since

$$|G|^2 = \frac{1}{2}[|\xi|^2|A^{-T}N|^2 + (\xi \cdot (A^{-T}N))^2] \\ \geq \frac{1}{2}|A^{-T}N|^2,$$

it follows from (4.31) that

$$D^2\psi(A)(\xi \otimes N, \xi \otimes N) \geq \frac{\gamma}{2}|A^{-T}N|^2 \quad \text{for all} \quad \xi \in \mathbb{R}^n, \ |\xi| = 1. \tag{4.32}$$

Now since $u = 0$ is a local minimum of $\psi(A + u \otimes N)$,

$$\begin{aligned} &\frac{d}{dt}\psi(A + t\xi \otimes N)\bigg|_{t=t_0} \\ &= \frac{d}{dt}\psi(A + t\xi \otimes N)\bigg|_{t=t_0} - \frac{d}{dt}\psi(A + t\xi \otimes N)\bigg|_{t=0} \\ &= t_0 D^2\psi(A + \tau(\xi)\xi \otimes N)(\xi \otimes N, \xi \otimes N) \quad \text{for some} \quad \tau(\xi) \in (0, t_0) \\ &= t_0[D^2\psi(A)(\xi \otimes N, \xi \otimes N) \\ &\quad + \{D^2\psi(A + \tau(\xi)\xi \otimes N) - D^2\psi(A)\}(\xi \otimes N, \xi \otimes N)] \\ &\geq t_0 \left[\frac{\gamma}{2}|A^{-T}N|^2 + \{D^2\psi(A + \tau(\xi)\xi \otimes N) - D^2\psi(A)\}(\xi \otimes N, \xi \otimes N)\right] \\ &\geq t_0 \frac{\gamma}{4}|A^{-T}N|^2 \end{aligned}$$

when $t_0 \leq r_0$ for some $r_0 > 0$ independent of ξ, by (4.32) and the continuity of $D^2\psi$ at A. □

Remark Condition (ii) in Theorem 4.6 is a very mild growth condition at the minima and allows the wells to be much "flatter" than the condition in Lemma 4.8. Lemma 4.10 below shows that (ii) is also satisfied under natural growth conditions on $\psi(F)$ in terms of $\text{dist}(F, \text{SO}(n)A)$ and $\text{dist}(F, \text{SO}(n)B)$ when F is close to $\text{SO}(n)A$ and $\text{SO}(n)B$, respectively. The key is the following lemma, which shows that the degeneracy from the frame-indifference condition (f) is counteracted by the rank-one ansatz (3.2). Underlying the proof is the fact that the rank-one cone $\{I + u \otimes N : u \in \mathbb{R}^n\}$ is transversal to the tangent space to $\text{SO}(n)$ at the identity I, which consists of all skew-symmetric perturbations of I.

Lemma 4.9 *Let $N \in \mathbb{R}^n$ be a unit vector and $G \in \mathbb{R}^{n \times n}$ be invertible. Then there exists $\kappa > 1$ such that for all $u \in \mathbb{R}^n$,*

$$|u| \leq \kappa \, dist\,(G + u \otimes N, SO(n)G) \leq \kappa|u|. \tag{4.33}$$

Proof The second inequality in (4.33) is immediate. Suppose, for contradiction, that for each $j \in \mathbb{N}$ there exists $u^{(j)} \in \mathbb{R}^n$ such that

$$|u^{(j)}| \geq j \quad \text{dist}(G + u^{(j)} \otimes N, \text{SO}(n)G). \tag{4.34}$$

Let $R^{(j)} \in \text{SO}(n)$ be such that

$$\text{dist}(G + u^{(j)} \otimes N, \text{SO}(n)G) = |G + u^{(j)} \otimes N - R^{(j)}N|,$$

and choose $c > 0$ so that $|FG| \geq c|F|$ for all $F \in \mathbb{R}^{n\times n}$. Then (4.34) implies that

$$\begin{aligned} |u^{(j)}| &\geq j|G + u^{(j)} \otimes N - R^{(j)}N| \\ &= j|(I - R^{(j)} + u^{(j)} \otimes G^{-T}N)G| \\ &\geq jc|I - R^{(j)} + u^{(j)} \otimes G^{-T}N|, \end{aligned} \tag{4.35}$$

and hence

$$\frac{|u^{(j)}|}{j} \geq c\left||u^{(j)}||G^{-T}N| - |I - R^{(j)}|\right|, \tag{4.36}$$

from which it follows that $u^{(j)}$ is bounded independently of j. There thus exist $u \in \mathbb{R}^n$, $R \in \mathrm{SO}(n)$ and subsequences of $\{u^{(j)}\}_{j=1}^{\infty}$ and $\{R^{(j)}\}_{j=1}^{\infty}$, not relabelled, such that

$$u^{(j)} \to u \quad \text{and} \quad R^{(j)} \to R \quad \text{as} \quad j \to \infty.$$

Moreover,

$$I - R + u \otimes G^{-T}N = 0, \tag{4.37}$$

by (4.35), and hence $u = 0$ and $R = I$, since the only matrix in $\mathrm{SO}(n)$ to which I is rank-one connected is I itself. It also follows from (4.35) that

$$\frac{1}{jc} \geq \left|\frac{I - R^{(j)}}{|u^{(j)}|} + \frac{u^{(j)}}{|u^{(j)}|} \otimes N\right|, \tag{4.38}$$

and hence $\dfrac{I - R^{(j)}}{|u^{(j)}|}$ is bounded independently of j. So there exist $K \in \mathbb{R}^{n\times n}$, $y \in \mathbb{R}^n$ with $|y| = 1$, and further subsequences of $\{u^{(j)}\}_{j=1}^{\infty}$ and $\{R^{(j)}\}_{j=1}^{\infty}$, again not relabelled, such that

$$\frac{I - R^{(j)}}{|u^{(j)}|} \to K \quad \text{and} \quad \frac{u^{(j)}}{|u^{(j)}|} \to y \quad \text{as} \quad j \to \infty, \tag{4.39}$$

and, by (4.38), y and K satisfy

$$-y \otimes N = K. \tag{4.40}$$

Now it follows from (4.39) and the fact that $R^{(j)} \to I$ as $j \to \infty$ that

$$\frac{(R^{(j)})^T(I - R^{(j)})}{|u^{(j)}|} \to K \quad \text{as} \quad j \to \infty, \tag{4.41}$$

whereas (4.39) also yields that

$$\frac{(R^{(j)})^T(I - R^{(j)})}{|u^{(j)}|} = \frac{-(I - R^{(j)})^T}{|u^{(j)}|} \to -K^T \quad \text{as} \quad j \to \infty. \tag{4.42}$$

So $K = -K^T$, by (4.41) and (4.42); that is, K is a skew-symmetric matrix. But this contradicts (4.40), since $|y| = 1$ and a non-zero rank-one matrix cannot be skew-symmetric. □

Lemma 4.10 *Let ψ, a, N, A and B be as in Lemma 4.2. Suppose further that there exist $\mu > 0$, $0 < \alpha < \beta$ and $p \in \mathbb{N}$ with $p \geq 2$ such that ψ is a C^p-function, and for each $G \in \{A, B\}$,*

$$\alpha \, dist^p(F, SO(n)G) \leq \psi(F) \leq \beta \, dist^p(F, SO(n)G), \tag{4.43}$$

if $F \in \mathbb{R}^{n\times n}_+$ *is such that* $dist(F, SO(n)G) \le \mu$. *Then condition (ii) in Theorem 4.6 is satisfied for this choice of* ψ.

Proof Fix $G \in \{A, B\}$ and define a mapping $f : S^{n-1} \times [0,\infty) \to \mathbb{R}$ by

$$f(\xi, r) := \psi(G + r\xi \otimes N).$$

Then it follows from (4.43) and Lemma 4.9 that there exists $\kappa > 1$ such that for all $\xi \in S^{n-1}$ and $r \in [0, \mu)$,

$$\frac{\alpha}{\kappa^p} r^p \le f(\xi, r) \le \beta r^p. \tag{4.44}$$

Since Taylor's theorem gives that for all $r \in [0, \mu)$ and $\xi \in S^{n-1}$,

$$f(\xi, r) = \sum_{k=0}^{p-1} \frac{\partial^k f}{\partial r^k}(\xi, 0)\frac{r^k}{k!} + \frac{\partial^p f}{\partial r^p}(\xi, \theta_{r,\xi})\frac{r^p}{p!}, \quad \theta_{r,\xi} \in (0, r), \tag{4.45}$$

it follows from (4.44) that for each $\xi \in S^{n-1}$,

$$\frac{\partial^k f}{\partial r^k}(\xi, 0) = 0, \quad 0 \le k \le p-1, \quad \text{and} \quad \frac{\partial^p f}{\partial r^p}(\xi, 0) \ge \frac{\alpha p!}{\kappa^p}. \tag{4.46}$$

Now $\frac{\partial^p f}{\partial r^p}(\cdot,\cdot)$ is uniformly continuous on $S^{n-1} \times [0, \mu]$, so there exists $r_0 \in (0, \mu)$ such that

$$\left|\frac{\partial^p f}{\partial r^p}(\xi, r) - \frac{\partial^p f}{\partial r^p}(\xi, 0)\right| \le \frac{\alpha p!}{2\kappa^p} \quad \text{for all} \quad (\xi, r) \in S^{n-1} \times [0, r_0]. \tag{4.47}$$

Then application of Taylor's Theorem with integral form of the remainder to $\frac{\partial f}{\partial r}(\xi, r)$ gives that for each $\xi \in S^{n-1}$,

$$\begin{aligned}
\frac{\partial f}{\partial r}(\xi, r) &= \sum_{k=0}^{p-2} \frac{\partial^{k+1} f}{\partial r^{k+1}}(\xi, 0)\frac{r^k}{k!} + \int_0^r \frac{(r-t)^{p-2}}{(p-2)!}\frac{\partial^p f}{\partial r^p}(\xi, t)\, dt \\
&= \int_0^r \frac{(r-t)^{p-2}}{(p-2)!}\frac{\partial^p f}{\partial r^p}(\xi, t)\, dt, \quad \text{by (4.46)}, \\
&= \int_0^r \frac{(r-t)^{p-2}}{(p-2)!}\left[\frac{\partial^p f}{\partial r^p}(\xi, 0) + \frac{\partial^p f}{\partial r^p}(\xi, t) - \frac{\partial^p f}{\partial r^p}(\xi, 0)\right] dt \\
&\ge \int_0^r \frac{(r-t)^{p-2}}{(p-2)!}\left[\frac{\alpha p!}{\kappa^p} - \frac{\alpha p!}{2\kappa^p}\right] dt \quad \text{if} \quad r \in [0, r_0], \quad \text{by} \quad \text{(4.46) and (4.47)}, \\
&= \frac{\alpha p!}{2(p-2)!\kappa^p}\frac{r^{p-1}}{p-1} \\
&> 0.
\end{aligned}$$

□

It remains to establish that the function u_0 given by (4.25) yields a solution of the Euler–Lagrange equations of the original functional (1.1).

Proposition 4.11 *Let u_0 be given by (4.25). Then*

(a) $u_0 \in C^3(\mathbb{R}, \mathbb{R}^n)$ *and satisfies the Euler–Lagrange equations for (4.1),*

$$-2\varepsilon^2 u_0''(s) + \nabla W(u_0(s)) = 0, \quad s \in \mathbb{R}, \tag{4.48}$$

where $W(u) := \psi(A + u \otimes N)$;

(b) *if* $y_0(x) = Ax + U_0(x \cdot N)$, $x \in \mathbb{R}^n$, *where* $U_0'(s) = u_0(s)$, $s \in \mathbb{R}$, *then*

$$Dy_0(x) := A + u_0(x \cdot N) \otimes N$$

and y_0 *satisfies the Euler–Lagrange equations of (1.1),*

$$-\operatorname{div} D_F \psi(Dy) + 2\varepsilon^2 \Delta^2 y = 0. \tag{4.49}$$

(The system (4.49) can be written in component form using the summation convention as

$$-\left(\frac{\partial \psi}{\partial F_{i\alpha}}(Dy)\right)_{,\alpha} + 2\varepsilon^2 y_{i,\alpha\alpha\beta\beta} = 0, \quad 1 \le i \le n,$$

where $_{,\alpha}$ denotes differentiation with respect to x_α, the αth component of $x \in \mathbb{R}^n$. Note that these are the Euler–Lagrange equations for (1.1) if allowed smooth variations ϕ of y are such that both ϕ and $D\phi$ vanish on the boundary of the domain.)

Proof (a) This is standard. (b) Note first that

$$\nabla W(u) = D_F \psi(A + u \otimes N) \cdot N, \tag{4.50}$$

and so (4.48) gives that

$$-2\varepsilon^2 u_0''(s) + D_F \psi(A + u_0(s) \otimes N) \cdot N = 0, \quad s \in \mathbb{R}, \tag{4.51}$$

which can be written in component form as

$$-2\varepsilon^2 {u_0}_i''(s) + \frac{\partial \psi}{\partial F_{i\alpha}}(A + u_0(s) \otimes N) N_\alpha = 0, \quad s \in \mathbb{R}, \tag{4.52}$$

where $1 \le i \le n$. Since $u_0 \in C^3(\mathbb{R}, \mathbb{R}^n)$, we can then differentiate (4.52) once with respect to s to get that for each $1 \le i \le n$,

$$-2\varepsilon^2 {u_0}_i'''(s) + \frac{\partial}{\partial F_{j\beta}}\left(\frac{\partial \psi}{\partial F_{i\alpha}}(A + u_0(s) \otimes N)\right) {u_0}_j'(s) N_\beta N_\alpha = 0, \quad s \in \mathbb{R}. \tag{4.53}$$

Now if y_0 is such that $Dy_0 = A + u_0(x \cdot N) \otimes N$, then ${y_0}_{i,\alpha} = A_{i\alpha} + {u_0}_i(x \cdot N) N_\alpha$. So

$$\begin{aligned} {y_0}_{i,\alpha\alpha\beta\beta} &= {u_0}_i'''(x \cdot N) N_\alpha N_\alpha N_\beta N_\beta \\ &= {u_0}_i'''(x \cdot N), \end{aligned} \tag{4.54}$$

since $|N| = 1$, and

$$\left(\frac{\partial \psi}{\partial F_{i\alpha}}(Dy_0)\right)_{,\alpha} = \frac{\partial}{\partial F_{j\beta}}\left(\frac{\partial \psi}{\partial F_{i\alpha}}(A + u_0(x \cdot N) \otimes N)\right) {u_0}_j'(x \cdot N) N_\alpha N_\beta. \tag{4.55}$$

It thus follows from (4.54), (4.55), and (4.53) applied with $s = x \cdot N$, that (4.49) holds for such y_0, as required. □

We finish this section by remarking that one might attempt to obtain a solution to the Euler–Lagrange equations (4.49) using the alternative, simpler ansatz

$$Dy(x) = A + \lambda(x \cdot N)a \otimes N, \tag{4.56}$$

where $B := A + a \otimes N$ and $\lambda : \mathbb{R} \to \mathbb{R}$ is such that $\lambda(s) \to 0, 1$ as $s \to -\infty, \infty$. Substitution of the ansatz (4.56) into (1.1) leads to an energy of the form

$$\mathscr{K}(\lambda) := \int_{\mathbb{R}} \psi(A + \lambda(s)a \otimes N) + \varepsilon^2 |a|^2 \lambda'(s)^2 \, ds, \tag{4.57}$$

since $|N|$ is a unit vector, and so

$$|D^2 y(x \cdot N)|^2 = y_{i,\alpha\beta} y_{i,\alpha\beta} = \lambda'(x \cdot N)^2 a_i a_i N_\alpha N_\alpha N_\beta N_\beta = \lambda'(x \cdot N)^2 |a|^2.$$

Suppose, for simplicity, that $\psi(F) = 0$ if and only if $F \in \mathrm{SO}(n)A \cup \mathrm{SO}(n)B$. It is straightforward to show that $\psi(A + \lambda a \otimes N) \in \mathrm{SO}(n)A \cup \mathrm{SO}(n)B$ if and only if $\lambda \in \{0, 1\}$. So under suitable conditions on ψ, to ensure that conditions (ii) and (iii) hold, Theorem 4.1 with $n = 1$ and $W(y) := \psi(A + ya \otimes N)$ yields the existence of a function $\lambda_0 \in \mathscr{D} = \{\lambda \in W^{1,2}_{loc}(\mathbb{R}, \mathbb{R}) : \lambda(s) \to 0, 1 \quad \text{as} \quad s \to -\infty, \infty\}$ such that

$$\mathscr{K}(\lambda_0) = \inf_{\lambda \in \mathscr{D}} \mathscr{K}(\lambda).$$

Arguments analogous to those in the proof of Proposition 4.11 (a) yield that $\lambda_0 \in C^3(\mathbb{R}, \mathbb{R})$ and satisfies the (single) Euler–Lagrange equation for (4.57), namely

$$-2\varepsilon^2 |a|^2 \lambda_0''(s) + \frac{\partial \psi}{\partial F_{i\alpha}}(A + \lambda_0(s)a \otimes N) a_i N_\alpha = 0, \quad s \in \mathbb{R}. \tag{4.58}$$

This, however, is not enough to ensure that $Dy_0(x) := A + \lambda_0(x \cdot N)a \otimes N$ satisfies the system of Euler–Lagrange equations (4.49). Differentiation of (4.58) with respect to s and substitution of $s = x \cdot N$ gives that

$$\begin{aligned} &-2\varepsilon^2 |a|^2 \lambda_0'''(x \cdot N) \\ &+ \frac{\partial}{\partial F_{j\beta}} \left(\frac{\partial \psi}{\partial F_{i\alpha}}(A + \lambda_0(x \cdot N)a \otimes N) \right) a_i N_\alpha a_j N_\beta \lambda_0'(x \cdot N) = 0, \quad x \cdot N \in \mathbb{R}. \end{aligned} \tag{4.59}$$

But for $Dy_0(x) := A + \lambda_0(x \cdot N)a \otimes N$ to satisfy the system of Euler–Lagrange equations (4.49), we need that for each $1 \leq i \leq n$,

$$-2\varepsilon^2 a_i \lambda_0'''(x \cdot N) + \frac{\partial}{\partial F_{j\beta}} \left(\frac{\partial \psi}{\partial F_{i\alpha}}(A + \lambda_0(x \cdot N)a \otimes N) \right) a_j N_\beta N_\alpha \lambda_0'(x \cdot N) = 0$$

for all $x \cdot N \in \mathbb{R}$, which does not follow from (4.59) in general.

Of course, supplementary conditions can be imposed on ψ to ensure that the full system of Euler–Lagrange equations is satisfied. For instance, let $\{e_a, \xi^1, \ldots, \xi^{n-1}\} \subset S^{n-1}$ be an orthonormal basis for $\mathbb{R}^n$ with $e_a = a/|a|$, and given $u \in \mathbb{R}^n$, write $u = u_a e_a + \sum_{j=1}^{n-1} \mu_j \xi^j$, $u_a, \mu_1, \ldots, \mu_{n-1} \in \mathbb{R}$. In these co-ordinates, the Euler–Lagrange equations (4.48) become

$$-2\varepsilon^2 u_a'' + \frac{\partial}{\partial u_a} \psi(A + u \otimes N) = 0, \tag{4.60}$$

and

$$-2\varepsilon^2 \mu_j'' + \frac{\partial}{\partial \mu_j} \psi(A + u \otimes N) = 0, \quad j \in 1, \ldots, n-1. \tag{4.61}$$

Now suppose that, for each $u \in \mathbb{R}^n$,

$$\psi(A + u \otimes N) \geq \psi(A + u_a e_a \otimes N). \tag{4.62}$$

Then $\frac{d}{dt}\psi(A+(u+t\xi)\otimes N)|_{t=0} = 0$ whenever $u = \lambda a, \lambda \in \mathbb{R}$ and $\xi \in \{\xi^1, \ldots, \xi^{n-1}\}$. Thus Eq. (4.61) automatically hold for any smooth function $u : \mathbb{R} \to \mathbb{R}^n$ of form $u(s) = \lambda(s)a$, $s \in \mathbb{R}$, $\lambda(s) \in \mathbb{R}$, and so in particular, for $u_0(s) = \lambda_0(s)a$, $s \in \mathbb{R}$, where λ_0 satisfies (4.58). Since (4.58) also implies (4.60), condition (4.62) therefore guarantees that the full system of Euler–Lagrange equations is satisfied. An example of a function ψ for which (4.62), (f), (m), (n) and material symmetry all hold is given by modifying the construction in (5.7) and (5.15) in Sect. 5 by replacing the function h illustrated in Fig. 3 by any $h \in C^\infty(\mathbb{R}, \mathbb{R})$ with $h(0) = 1$ and $h(s) \geq 1$ for all $s \in \mathbb{R}$, such as $h \equiv 1$, for instance. But (4.62) is rather restrictive in general, and may not hold for physically realistic choices of ψ.

We give an example of a simple stored energy function ψ, inspired by a toy model of Kružík [21], for which there are no solutions of (4.48) with $u(s) = \lambda(s)a$ for all $s \in \mathbb{R}$. Let $\delta > 0$ and

$$A = I - \delta e_3 \otimes e_1, \quad B = I + \delta e_3 \otimes e_1$$

so that

$$B = A + a \otimes N \quad \text{with} \quad a = 2\delta e_3, \; N = e_1.$$

Note that the set $\mathrm{SO}(3)A \cup \mathrm{SO}(3)B$ corresponds precisely to the two variants of martensite that minimize an energy density ψ at sub-critical temperature in an orthorhombic to monoclinic phase transformation; see Ball and James [8]. Define $\psi : \mathbb{R}^{n\times n}_+ \to \mathbb{R}$ so that

$$\psi(F) = \left|F^T F - A^T A\right|^2 \left|F^T F - B^T B\right|^2$$

for F in a neighbourhood of the set $\{F \in \mathbb{R}^{n\times n} : F = A + \lambda a \otimes N, \lambda \in [0, 1]\}$. Then the ansatz

$$F = A + u \otimes N = \begin{pmatrix} 1+u_1 & 0 & 0 \\ u_2 & 1 & 0 \\ u_3 - \delta & 0 & 1 \end{pmatrix} \Rightarrow F^T F$$

$$= \begin{pmatrix} (u_1+1)^2 + u_2^2 + (u_3-\delta)^2 & u_2 & u_3 - \delta \\ u_2 & 1 & 0 \\ u_3 - \delta & 0 & 1 \end{pmatrix},$$

and routine calculation yields that

$$\begin{aligned} \psi(A + u \otimes N) = {} & \left(2u_2^2 + 2u_3^2 + [u_1^2 + u_2^2 + u_3^2 + 2(u_1 - \delta u_3)]^2\right) \\ & \times \left(2u_2^2 + 2(u_3 - 2\delta)^2 + [u_1^2 + u_2^2 + u_3^2 + 2(u_1 - \delta u_3)]^2\right), \end{aligned}$$

from which it follows that

$$\frac{\partial}{\partial u_1}\psi(A + u \otimes N)\bigg|_{u_1=0, u_2=0} = 8u_3(u_3 - 2\delta)\left(u_3^2 + (u_3 - 2\delta)^2 + (u_3^2 - 2\delta u_3)^2\right).$$

This expression is a non-trivial polynomial in u_3, so only vanishes for a discrete set of values of u_3 and cannot equal zero for all $u_3 \in (0, 2\delta)$. Hence the Euler–Lagrange equations of (4.1), namely

$$-2\varepsilon^2 u_i'' + \frac{\partial}{\partial u_i}\psi(A + u \otimes N) = 0, \quad i = 1, 2, 3,$$

are not satisfied for any $u : \mathbb{R} \to \mathbb{R}^3$ with $u_1 \equiv 0, u_2 \equiv 0$ and $u_3(\xi) \to 0, 2\delta$ as $\xi \to -\infty, \infty$. There is thus no solution of the Euler–Lagrange equations for u of the form $u(s) = \lambda(s)a = \lambda(s)2\delta e_3$, and so no interface between A and B with $Dy(x) = A + \lambda(x \cdot N)a \otimes N$.

Remark Salje [27] has studied the thickness of a twin boundary in $NdGaO_3$ by rotating the sample linearly between extreme positions in which the two variants are in focus (i.e. along the arc of the great circle joining the two extreme positions). In intermediate positions the two variants are out of focus and the interface is in focus, thus enabling its thickness to be estimated. Our results imply that in general u might not be a multiple of a, so that intermediate rotations not on the great circle might lead to different in-focus areas in the twin boundary. Chrosch and Salje [14] and Salje et al. [28] estimate interface thickness by fitting to experimental data obtained by diffraction methods a theoretical interface profile, derived under the assumption that the gradient has the one-dimensional form (4.56). Again, since (4.56) may not hold in general, it would be interesting to explore alternative methods of analysing the data.

5 Uniqueness and non-uniqueness of planar interfaces

Assume throughout this section that A, B, a, N and ψ are as in the statement of Theorem 4.6; in particular, that $B = A + a \otimes N$. We investigate the uniqueness of solutions of the Euler–Lagrange equations (4.48) in the class

$$\mathscr{S} = \{u \in C^3(\mathbb{R}, \mathbb{R}^n);\, u(s) \to 0, a \text{ as } s \to -\infty, \infty\};$$

note that if $u \in W^{1,2}_{loc}(\mathbb{R}, \mathbb{R}^n)$ satisfies the weak Euler–Lagrange equations for (4.1), then $u \in C^3(\mathbb{R}, \mathbb{R}^n)$ and satisfies (4.48). Of course, any solution u of (4.48) yields a one-parameter family of solutions, $u(\cdot + \tau)$ for all $\tau \in \mathbb{R}$, and our interest is in uniqueness *modulo* such translation.

When $n = 1$, strong uniqueness properties hold in the class of all solutions of (4.48) in $\mathscr{S}$. This is in part due to the maximum principle, which does not hold for (4.48) for general n. These properties in fact follow from well-known uniqueness and stability results for travelling-front solutions $u(x, t) = w(x - ct)$ of reaction-diffusion equations of the form $u_t = u_{xx} + f(u)$ when f is of so-called "bistable" type, having stable equilibria 0 and a to which $w(x - ct)$ tends as $x - ct \to -\infty, \infty$ respectively. The fact that $W(0) = W(a)$ here means that $f = W'$ satisfies $\int_0^a f(u)\, du = 0$, and so the speed c of travelling fronts must actually be zero. A precise statement is the following.

Proposition 5.1 (Fife and McLeod [18]) *Let $W \in C^2(\mathbb{R}, \mathbb{R})$ be such that $W(0) = W(a) = 0$ for some $a > 0$, $W(u) > 0$ for $u \notin \{0, a\}$,*

$$W'(u) < 0 \text{ when } u < 0 \quad \text{and} \quad W'(u) > 0 \text{ when } u > a, \tag{5.1}$$

and

$$W'(u) \geq 0 \quad \text{for } u > 0 \quad \text{close to } 0, \quad W'(u) \leq 0 \quad \text{for } u < a \text{ close to } a.$$

Then up to translation, there is at most one solution $u \in C^2(\mathbb{R}, \mathbb{R})$ of the equation

$$u''(s) - W'(u(s)) = 0, \quad s \in \mathbb{R}, \tag{5.2}$$

with $u(s) \to 0, a$ as $s \to -\infty, \infty$, respectively.

We next give a physical example, with $n = 3$, of non-uniqueness of solutions of (4.48) within the subset of $\mathscr{S}$ consisting of global minimizers of (4.1). Some of the ideas in this construction are due to S. Müller. Note that examples of non-uniqueness when $n = 2$ can be devised using a similar approach. As in the toy model at the end of Sect. 4, we again base our construction on the two martensite variants that minimize subcritical-temperature energy densities in orthorhombic to monoclinic phase transformations. Let $\delta > 0$ and

$$A = I - \delta e_3 \otimes e_1, \quad B = I + \delta e_3 \otimes e_1,$$

so that

$$B = A + a \otimes N, \quad \text{where} \quad a = 2\delta e_3, \ N = e_1.$$

We will construct a density ψ with the energy wells $SO(3)A \cup SO(3)B$ that, in addition to the frame-indifference (f) and non-interpenetration (n) conditions, satisfies the orthorhombic material symmetry property:

$$\psi(FQ) = \psi(F) \quad \text{for all} \quad F \in \mathbb{R}^{n\times n}_{+} \text{ and all } Q \in \mathscr{P} := \cup_{i=0,\ldots,3}\{Q_i\}, \tag{5.3}$$

where

$$Q_0 = I \text{ and } Q_i = -I + 2e_i \otimes e_i, \quad i = 1, \ldots, 3. \tag{5.4}$$

Here $\mathscr{P}$ is the orthorhombic group, consisting of the identity together with rotations of π about each of the three co-ordinate axes.

Now let ψ in the reduced functional (4.1) be defined by

$$\psi(F) = \sum_{i=0}^{3} \hat{\psi}(Q_i^T F^T F Q_i), \quad F \in \mathbb{R}^{3\times 3}_{+}, \tag{5.5}$$

where Q_i are as in (5.4) and $\hat{\psi}$ is to be specified below. It is straightforward to check that both the frame-indifference condition (f) and the orthorhombic symmetry property (5.3) are automatically satisfied by ψ for any choice of $\hat{\psi}$. To define $\hat{\psi} : S^{3\times 3}_{+} \to \mathbb{R}$, first note that given $C \in S^{3\times 3}_{+}$, there exist unique $c_1, c_2, \ldots, c_6 \in \mathbb{R}$ such that

$$\begin{aligned} C = I &+ c_1[e_1 \otimes e_1] + c_2[e_2 \otimes e_1 + e_1 \otimes e_2] + c_3[e_3 \otimes e_1 + e_1 \otimes e_3] \\ &+ c_4[e_2 \otimes e_2] + c_5[e_3 \otimes e_3] + c_6[e_2 \otimes e_3 + e_3 \otimes e_2], \end{aligned} \tag{5.6}$$

and then let

$$\hat{\psi}(C) = \frac{1}{4}\left\{g(c_3)h(c_2) + q(c_1 + 1 - c_2^2 - c_3^2)^2 + c_2^2 + c_4^2 + c_5^2 + c_6^2 + p(\det C)\right\}, \tag{5.7}$$

where

(i) $q \in C^\infty(\mathbb{R}, \mathbb{R})$ is a non-decreasing function such that

$$q(s) = \begin{cases} -1 + \sqrt{s} & \text{if} \quad s \geq \gamma; \\ -1 \leq q(s) \leq -1 + \sqrt{s} & \text{if} \quad 0 \leq s \leq \gamma; \\ -1 & \text{if} \quad s \leq 0, \end{cases}$$

for some $0 < \gamma << 1$ (see Fig. 2);

(ii) the function $g \in C^\infty(\mathbb{R}, \mathbb{R})$ is such that $g(w) = g(-w)$ for all $w \in \mathbb{R}$, $g(-\delta) = g(\delta) = 0$, $g'(-\delta) = g'(\delta) = 0$, $g''(-\delta) > 0$, $g''(\delta) > 0$, and $g(w) > 0$ for $w \notin \{-\delta, \delta\}$ (see Fig. 2);

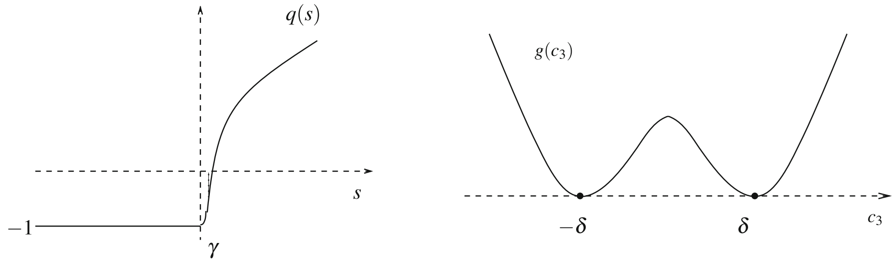

Fig. 2 Forms of the functions q and g

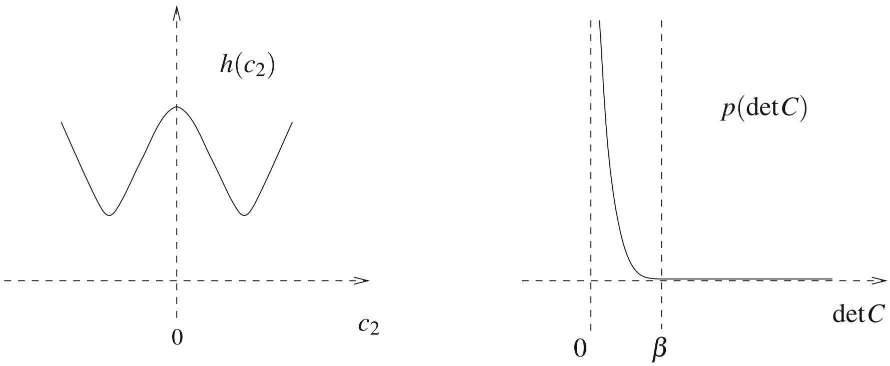

Fig. 3 Forms of the functions h and p

(iii) the function $h \in C^{\infty}(\mathbb{R}, \mathbb{R})$ is such that $h(w) > 0$ and $h(w) = h(-w)$ for all $w \in \mathbb{R}$, $h(w) \to \infty$ as $|w| \to \infty$, $h(0) = 1$, $h'(0) = 0$ and $h''(0) = -k$ for some (large) positive constant k, to be chosen later (see Fig. 3);

(iv) there exists $0 < \beta << 1$ such that the function $p \in C^{\infty}((0, \infty), \mathbb{R})$ satisfies $p(w) = 0$ for $w \geq \beta$, p is decreasing on $(0, \beta)$, and $p(w) \to \infty$ as $w \to 0$ (see Fig. 3).

Then $\hat{\psi}(C) \geq 0$ for all $C \in S_{+}^{3\times 3}$ and $\hat{\psi}(C) \to \infty$ as $\det C \to 0$. Hence, by (5.5) and the fact that $\det(Q_i F^T F Q_i^T) = (\det F)^2$, $\psi(F) \geq 0$ for all $F \in \mathbb{R}_{+}^{3\times 3}$ and $\psi(F) \to \infty$ as $\det F \to 0$. So the non-interpenetration condition (n) is satisfied.

The rank-one ansatz (3.2) here becomes

$$A + u \otimes N = I - \delta e_3 \otimes e_1 + u \otimes e_1$$

where $u(\xi) \to 0, 2\delta e_3$ as $\xi \to -\infty, \infty$. It is convenient to work with

$$\tilde{u} = u - \delta e_3 \in \mathbb{R}^3, \tag{5.8}$$

where $\tilde{u}(\xi) \to -\delta e_3, +\delta e_3$ as $\xi \to -\infty, \infty$; using $\tilde{u}$ rather than u simplifies the symmetry formulae in the following, and there is clearly an immediate correspondence between the existence of $\tilde{u}$ and of u. Note also that

$$\det(I + \tilde{u} \otimes e_1) = 1 + \tilde{u} \cdot e_1 = 1 + \tilde{u}_1 (= 1 + u_1),$$

so that

$$\det(I + \tilde{u} \otimes e_1) > 0 \Leftrightarrow 1 + \tilde{u}_1 > 0.$$

Now if $F = I + \tilde{u} \otimes e_1$ with $\det F > 0$, then

$$\begin{aligned} F^T F &= I + \tilde{u} \otimes e_1 + e_1 \otimes \tilde{u} + |\tilde{u}|^2 e_1 \otimes e_1 \\ &= I + (\tilde{u}_1 e_1 + \tilde{u}_2 e_2 + \tilde{u}_3 e_3) \otimes e_1 + e_1 \otimes (\tilde{u}_1 e_1 + \tilde{u}_2 e_2 + \tilde{u}_3 e_3) \\ &\quad + (\tilde{u}_1^2 + \tilde{u}_2^2 + \tilde{u}_3^2) e_1 \otimes e_1 \\ &= I + (2\tilde{u}_1 + \tilde{u}_1^2 + \tilde{u}_2^2 + \tilde{u}_3^3) e_1 \otimes e_1 + \tilde{u}_2 [e_2 \otimes e_1 + e_1 \otimes e_2] \\ &\quad + \tilde{u}_3 [e_3 \otimes e_1 + e_1 \otimes e_3]. \end{aligned} \tag{5.9}$$

Taking $C = F^T F$ in (5.6) then gives

$$c_1 = (\tilde{u}_1 + 1)^2 + \tilde{u}_2^2 + \tilde{u}_3^2 - 1, \quad c_2 = \tilde{u}_2, \quad c_3 = \tilde{u}_3 \quad \text{and} \quad c_4 = c_5 = c_6 = 0,$$

and hence for such F,

$$\hat{\psi}(F^T F) = \frac{1}{4} \left\{ g(\tilde{u}_3) h(\tilde{u}_2) + q((\tilde{u}_1 + 1)^2)^2 + \tilde{u}_2^2 + p((1 + \tilde{u}_1)^2) \right\}. \tag{5.10}$$

From the definition of q and the fact that $1 + \tilde{u}_1 > 0$, it follows that

$$q((\tilde{u}_1 + 1)^2) = -1 + \sqrt{(\tilde{u}_1 + 1)^2} = \tilde{u}_1 \quad \text{if} \quad (\tilde{u}_1 + 1)^2 \geq \gamma, \tag{5.11}$$

and

$$-1 \leq q((\tilde{u}_1 + 1)^2) \leq \tilde{u}_1 \leq -1 + \sqrt{\gamma} \quad \text{if} \quad 0 \leq (\tilde{u}_1 + 1)^2 \leq \gamma. \tag{5.12}$$

In particular, if $(\tilde{u}_1 + 1)^2 \geq \gamma$, then

$$\hat{\psi}(F^T F) = \frac{1}{4} \left\{ g(\tilde{u}_3) h(\tilde{u}_2) + \tilde{u}_1^2 + \tilde{u}_2^2 + p((1 + \tilde{u}_1)^2) \right\}. \tag{5.13}$$

To deduce the form of $\psi(F)$ for $F = I + \tilde{u} \otimes e_1$, note first that for each $i, j = 1, 2, 3$,

$$Q_i e_j = (-I + 2e_i \otimes e_i) e_j = -e_j + 2(e_i \cdot e_j) e_i = \begin{cases} e_j & \text{if } i = j; \\ -e_j & \text{if } i \neq j, \end{cases}$$

and so for each $F = I + \tilde{u} \otimes e_1$,

$$\begin{aligned}
&Q_1^T F^T F Q_1\\
&\quad = I + [(\tilde{u}_1+1)^2 + \tilde{u}_2^2 + \tilde{u}_3^2 - 1] e_1\otimes e_1 - \tilde{u}_2[e_2\otimes e_1 + e_1\otimes e_2]\\
&\qquad -\tilde{u}_3[e_3\otimes e_1 + e_1\otimes e_3];\\
&Q_2^T F^T F Q_2\\
&\quad = I + [(\tilde{u}_1+1)^2 + \tilde{u}_2^2 + \tilde{u}_3^2 - 1] e_1\otimes e_1 - \tilde{u}_2[e_2\otimes e_1 + e_1\otimes e_2]\\
&\qquad +\tilde{u}_3[e_3\otimes e_1 + e_1\otimes e_3];\\
&Q_3^T F^T F Q_3\\
&\quad = I + [(\tilde{u}_1+1)^2 + \tilde{u}_2^2 + \tilde{u}_3^2 - 1] e_1\otimes e_1 + \tilde{u}_2[e_2\otimes e_1 + e_1\otimes e_2]\\
&\qquad -\tilde{u}_3[e_3\otimes e_1 + e_1\otimes e_3].
\end{aligned}$$

Since the expression in (5.10) is invariant under replacing $\tilde{u}_2$ by $-\tilde{u}_2$ and/or $\tilde{u}_3$ by $-\tilde{u}_3$, it follows that for $F = I + \tilde{u}\otimes e_1$,

$$\hat{\psi}(F^T F) = \hat{\psi}(Q_i^T F^T F Q_i), \quad i = 1,2,3, \tag{5.14}$$

and hence (5.5) implies that $\psi(I + \tilde{u}\otimes e_1)$ in the reduced functional (4.1) is given by the formula

$$\begin{aligned}
\psi(F) &= 4\hat{\psi}(F^T F)\\
&= g(\tilde{u}_3)h(\tilde{u}_2) + q((\tilde{u}_1+1)^2)^2 + \tilde{u}_2^2 + p((1+\tilde{u}_1)^2) &(5.15)\\
&= g(\tilde{u}_3)h(\tilde{u}_2) + \tilde{u}_1^2 + \tilde{u}_2^2 + p((1+\tilde{u}_1)^2) \quad \text{if} \quad (\tilde{u}_1+1)^2 \geq \gamma. &(5.16)
\end{aligned}$$

Next observe that the energy wells of ψ, when $\psi(F) = 0$, occur precisely when $F \in \mathrm{SO}(3)A \cup \mathrm{SO}(3)B$. To see this, note first that given $C \in S_+^{3\times 3}$,

$$\hat{\psi}(C) = \frac{1}{4}\{g(c_3)h(c_2) + q(c_1 + 1 - c_2^2 - c_3^2)^2 + c_2^2 + c_4^2 + c_5^2 + c_6^2 + p(\det C)\} = 0$$

if and only if

$$g(c_3) = 0 \Leftrightarrow c_3 = \pm\delta, \quad c_2 = c_4 = c_5 = c_6 = 0, \quad \det C \geq \beta,$$

and

$$\begin{aligned}
q(c_1 + 1 - c_2^2 - c_3^2) = 0 &\Leftrightarrow \sqrt{c_1 + 1 - c_2^2 - c_3^2} = 1\\
&\Leftrightarrow c_1 = \delta^2.
\end{aligned}$$

It follows that C is of the form

$$\begin{aligned}
C &= I + \delta^2[e_1\otimes e_1] \pm \delta[e_3\otimes e_1 + e_1\otimes e_3]\\
&= F^T F \quad \text{where} \quad F = I + \tilde{u}\otimes e_1 \text{ with } \tilde{u} = \pm\delta e_3. &(5.17)
\end{aligned}$$

Now given $C = F^T F$ with $\det F > 0$, there exists unique $U \in S_+^{3\times 3}$ with $\det U > 0$ such that $F = RU$ for some $R \in \mathrm{SO}(3)$, and so the matrix F is determined uniquely, up to a rotation, by C. Since $\det C = (\det F)^2 = 1 > \beta$ for $F = I \pm \delta e_3\otimes e_1$, we thus have

$$\hat{\psi}(F^T F) = 0 \Leftrightarrow F = R(I \pm \delta e_3\otimes e_1) \quad \text{for some} \quad R \in \mathrm{SO}(3),$$

and

$$\psi(F) = 0 \Leftrightarrow F = R(I \pm \delta e_3\otimes e_1) \quad \text{for some} \quad R \in \mathrm{SO}(3),$$

because (5.14) holds for $F = R(I \pm \delta e_3 \otimes e_1)$, $R \in SO(3)$, and so $\hat{\psi}(F^T F) = 0 \Leftrightarrow \hat{\psi}(Q_i^T F^T F Q_i) = 0$ for each $i = 1, 2, 3$. Thus the multi-well structure (m) is satisfied with $k = 2$. Note that there being exactly two energy wells means that condition (4.9) in Lemma 4.3 is trivially satisfied.

Now define

$$\begin{aligned}\eta(\tilde{u}_1, \tilde{u}_2, \tilde{u}_3) &:= g(\tilde{u}_3)h(\tilde{u}_2) + q((\tilde{u}_1 + 1)^2)^2 + \tilde{u}_2^2 + p((\tilde{u}_1 + 1)^2)\\ &= \psi(I + \tilde{u} \otimes e_1).\end{aligned} \tag{5.18}$$

Then

$$\eta(\tilde{u}_1, \tilde{u}_2, \tilde{u}_3) = 0 \Leftrightarrow (\tilde{u}_2, \tilde{u}_2, \tilde{u}_3) = (0, 0, -\delta) \quad \text{or} \quad (0, 0, \delta),$$

and, since $q((\tilde{u}_1 + 1)^2)^2 = \tilde{u}_1^2$ and $p((\tilde{u}_1 + 1)^2) = 0$ when $(\tilde{u}_1 + 1)^2 \geq \max\{\gamma, \beta\}$, it is easy to see that

$$D^2\eta(0, 0, -\delta) > 0 \quad \text{and} \quad D^2\eta(0, 0, \delta) > 0,$$

which ensures that the non-degeneracy condition (ii) in Theorem 4.6 is satisfied by ψ.

Application of Theorem 4.1 with $n = 1$ and $W(y) := \eta(0, 0, y)$, $y \in \mathbb{R}$, yields the existence of a minimizer $\overline{u}$ of (4.1) among

$$\mathscr{S}_0 := \{\tilde{u} \in C^2(\mathbb{R}, \mathbb{R}^3) : \tilde{u}_1(s) \equiv 0, \tilde{u}_2(s) \equiv 0, \tilde{u}_3(s) \to -\delta, \delta \text{ as } s \to -\infty, \infty\}.$$

Since

$$\frac{\partial \eta}{\partial \tilde{u}_1}(0, 0, \tilde{u}_3) = 4q(1)q'(1) + 2p'(1) = 0 \quad \text{and} \quad \frac{\partial \eta}{\partial \tilde{u}_2}(0, 0, \tilde{u}_3) = g(\tilde{u}_3)h'(0) = 0$$

for all $\tilde{u}_3 \in \mathbb{R}$, $\overline{u} \in \mathscr{S}_0$ is also a solution of the full system of three Euler–Lagrange equations for (4.1). In fact, the proof of Proposition 5.1 yields that $\overline{u}$ is up to translation the unique such solution in $\mathscr{S}_0$, and that $\overline{u}_3'(s) > 0$ for all $s \in \mathbb{R}$.

We will show that $\overline{u}$ is not a global minimizer of (4.1) in

$$\tilde{\mathscr{S}} = \{\tilde{u} \in C^3(\mathbb{R}, \mathbb{R}^3); \tilde{u}(s) \to -\delta e_3, \delta e_3 \text{ as } s \to -\infty, \infty\}$$

when the parameter k in the definition of the function h is sufficiently large. The second variation at $\overline{u}$, acting on variations $\phi(s) = \phi_2(s)e_2$, is given by

$$\begin{aligned}\delta^2 \mathscr{J}(\overline{u})(\phi, \phi) &= \int_{\mathbb{R}} \frac{\partial^2 \eta}{\partial \tilde{u}_2^2}(0, 0, \overline{u}_3(s))\phi_2^2(s) + 2\varepsilon^2 \dot{\phi}_2^2(s)\, ds\\ &= \int_{\mathbb{R}} [2 + g(\overline{u}_3(s))h''(0)]\phi_2^2(s) + 2\varepsilon^2 \dot{\phi}_2^2(s)\, ds\\ &= \int_{\mathbb{R}} [2 - kg(\overline{u}_3(s))]\phi_2^2(s) + 2\varepsilon^2 \dot{\phi}_2^2(s)\, ds.\end{aligned}$$

Now choose an interval $[-M, M]$. For $s \in [-M, M]$,

$$\frac{\partial^2 \eta}{\partial \tilde{u}_2^2}(0, 0, \overline{u}_3(s)) = 2 - kg(\overline{u}_3(s)) \leq 2 - kg_0,$$

where $g_0 := \min_{s\in[-M,M]} g(\overline{u}_3(s)) > 0$. So k can then be chosen large enough that there exists $\phi_2 : \mathbb{R} \to \mathbb{R}$ with $\mathrm{supp}\phi_2 \subset\subset [-M, M]$ and

$$\delta^2 \mathscr{J}(\overline{u})(\phi, \phi) \leq \int_{\mathbb{R}} (2 - kg_0)\phi_2^2 + 2\varepsilon^2\dot{\phi}_2^2\, ds < 0. \tag{5.19}$$

Thus $\overline{u}$ is not a global minimizer of $\mathscr{J}$ in $\tilde{\mathscr{S}}$.

Since Theorem 4.6 ensures a global minimizer of $\mathscr{J}$ in $\tilde{\mathscr{S}}$ does exist, this yields non-uniqueness of solutions to the Euler–Lagrange equations of $\mathscr{J}$ in $\tilde{\mathscr{S}}$. In fact, the choice of the function ψ here ensures that there must also be non-uniqueness in the class of global minimizers. To see this, note first that the form (5.18) of $\psi(I + \tilde{u} \otimes e_1)$ implies that if $\tilde{u} \in \tilde{\mathscr{S}}$ with $\tilde{u}_1 \not\equiv 0$ and $\tilde{u}_0 = 0e_1 + \tilde{u}_2 e_2 + \tilde{u}_3 e_3$, then $\mathscr{J}(\tilde{u}_0) < \mathscr{J}(\tilde{u})$. Hence any global minimizer $\tilde{u}$ of $\mathscr{J}$ in $\tilde{\mathscr{S}}$ has $\tilde{u}_1 \equiv 0$, and, by (5.19), $\tilde{u}_2 \not\equiv 0$. Since $\eta(\tilde{u}_1, \tilde{u}_2, \tilde{u}_3) = \eta(\tilde{u}_1, -\tilde{u}_2, \tilde{u}_3)$, it follows that there must be at least two global minimizers, since there must be such a minimizer with non-zero $\tilde{u}_2$ dependence, and a second can be constructed by replacing $\tilde{u}_2$ by $-\tilde{u}_2$.

Remark Note that Alikakos et al. [2] study the issue of uniqueness in the case $n = 2$, using complex-function theory to investigate solutions of the Euler–Lagrange equations connecting minima of $W(u)$, for a class of W in the general functional (4.2). Attention is focussed on potentials of form $W(u) = |f(u_1 + iu_2)|^2$, where $f : \mathbb{C} \to \mathbb{C}$. Multiple connections are constructed for certain potentials with f meromorphic, whereas it is proved that there is up to translation at most one connection when f is holomorphic.

6 Interfaces between martensitic variants in cubic to tetragonal transformations

In this section, we use material symmetry to show that there are interfaces with symmetry properties between martensite variants in cubic to tetragonal transformations. Let $n = 3$, and suppose that the elastic energy density $\psi \in C^2(\mathbb{R}^{3\times3}_+; \mathbb{R})$ satisfies (f) and (n) together with the cubic material symmetry property

$$\psi(FQ) = \psi(F) \text{ for all } F \in \mathbb{R}^{3\times3} \quad \text{and}$$
$$Q \in P^{24} = \{\text{rotations of a cube to itself}\} \subset \mathrm{SO}(3),$$

and that the multi-well condition (m) is satisfied with $k = 3$ and

$$U_1 = \mathrm{diag}(\eta_2, \eta_1, \eta_1), \quad U_2 = \mathrm{diag}(\eta_1, \eta_2, \eta_1), \quad U_3 = \mathrm{diag}(\eta_1, \eta_1, \eta_2),$$

for some $\eta_1, \eta_2 > 0$. The matrices U_1, U_2 and U_3 correspond to the three variants of the low-symmetry phase, martensite, that minimize the energy density at such a sub-critical temperature. Recall from the remark following Lemma 4.3 that condition (4.9) is satisfied in this case.

We will concentrate on interfaces between $A = U_1$ and $B = A + a \otimes N \in \mathrm{SO}(3)U_2$. By an interface we understand a solution $u \in C^3(\mathbb{R}, \mathbb{R}^3)$ of the Euler–Lagrange equations (4.48) with $u(s) \to 0, a$ as $s \to -\infty, \infty$, which is not necessarily a global or even local minimizer of (4.1). For concreteness, we focus on the case

$$a = \frac{\sqrt{2}(\eta_2^2 - \eta_1^2)}{\eta_1^2 + \eta_2^2}(-\eta_2 e_1 + \eta_1 e_2), \quad N = \frac{1}{\sqrt{2}}(e_1 + e_2).$$

Proposition 6.1 *Let A, a, N and ψ be as above. Then there exists a solution $u \in C^3(\mathbb{R}, \mathbb{R}^3)$ to the Euler–Lagrange equations* (4.48) *with $u(s) \to 0, a$ as $s \to -\infty, \infty$ such that*

(i) $u_3 \equiv 0$;
(ii) *$\{u(s) : s > 0\}$ is given by the reflection of $\{u(s) : s < 0\}$ in the perpendicular bisector in the $\{u_3 \equiv 0\}$-plane of the straight line joining* 0 *to a.*

Proof First note that

$$QAQ^T = A,$$

for $Q = -e_1 \otimes e_1 - e_2 \otimes e_2 + e_3 \otimes e_3$, which is a rotation of an origin-centred cube to itself. Since the frame-indifference (f) and material symmetry assumptions then give

$$\psi(A + u \otimes N) = \psi(Q(A + u \otimes N)Q^T),$$

and $QN = -N$, it thus follows that

$$\psi(A + u \otimes N) = \psi(A - Qu \otimes N) \quad \text{for all} \quad u = u_1e_1 + u_2e_2 + u_2e_3 \in \mathbb{R}^3. \tag{6.1}$$

Also, since $-Qu = u_1e_1 + u_2e_2 - u_3e_3$, differentiating with respect to u_3 yields

$$\frac{\partial \psi}{\partial F_{3\alpha}}(A + u \otimes N) \quad N_\alpha = -\frac{\partial \psi}{\partial F_{3\alpha}}(A - Qu \otimes N) \quad N_\alpha = -\frac{\partial \psi}{\partial F_{3\alpha}}(A + u \otimes N)N_\alpha,$$

if $u \in C^2(\mathbb{R}, \mathbb{R}^3)$ has $u_3 \equiv 0$. Hence the Euler–Lagrange equation for u_3,

$$2\varepsilon^2 u_3'' = \frac{\partial \psi}{\partial F_{3\alpha}}(A + u \otimes N)N_\alpha, \tag{6.2}$$

is satisfied for *any* function $u \in C^2(\mathbb{R}, \mathbb{R}^3)$ with $u_3 \equiv 0$. Now applying the existence theory in Sect. 3 to the functional

$$\int_{\mathbb{R}} \psi(A + (u_1e_1 + u_2e_2 + 0e_3) \otimes N)) + \varepsilon^2 |u_1'e_1 + u_2'e_2 + 0e_3|^2 \, ds, \tag{6.3}$$

implies the existence of $\hat{u} = \hat{u}_1e_1 + \hat{u}_2e_2 + 0e_3 \in C^2(\mathbb{R}, \mathbb{R}^3)$ that minimizes (6.3) among

$$\mathscr{C}_z = \{u \in W^{1,2}_{loc}(\mathbb{R}, \mathbb{R}^3) : u_3 \equiv 0, \; u(s) \to 0, a \text{ as } s \to -\infty, \infty\}$$

and is such that

$$2\varepsilon^2 \hat{u}_1'' = \frac{\partial \psi}{\partial F_{1\alpha}}(A + \hat{u} \otimes N) \; N_\alpha, \quad 2\varepsilon^2 \hat{u}_2'' = \frac{\partial \psi}{\partial F_{2\alpha}}(A + \hat{u} \otimes N) \; N_\alpha.$$

In particular, there is an interface, $\hat{u}$, with $u_3 \equiv 0$, and so (i) holds.

We next show that there is at least one such interface $\hat{u}$ that satisfies both (i) and (ii). The key is the fact that

$$\hat{Q} U_1 \hat{Q}^T = U_2, \tag{6.4}$$

where $\hat{Q} = e_2 \otimes e_1 + e_1 \otimes e_2 - e_3 \otimes e_3$ is a rotation of π about the axis $\frac{1}{\sqrt{2}}(e_1 + e_2)$, which maps an origin-centred cube to itself. Now a routine calculation shows that

$$A + a \otimes N = RU_2 = R\hat{Q}A\hat{Q}^T, \tag{6.5}$$

where $A = U_1$ and $R \in \mathrm{SO}(3)$ is given by

$$R = \frac{2\eta_1\eta_2}{\eta_1^2 + \eta_2^2}(e_1 \otimes e_1 + e_2 \otimes e_2) + \frac{\eta_1^2 - \eta_2^2}{\eta_1^2 + \eta_2^2}(e_1 \otimes e_2 - e_2 \otimes e_1) + e_3 \otimes e_3. \tag{6.6}$$

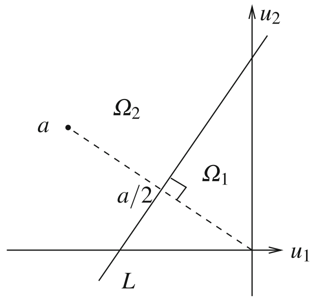

Fig. 4 The line L and the point a in the $\{u_3 = 0\}$-plane

Equations (6.4) and (6.5) together yield that for each $u \in \mathbb{R}^3$,

$$\begin{aligned} R\hat{Q}(A + u \otimes N)\hat{Q}^T &= R\hat{Q}A\hat{Q}^T + R\hat{Q}u \otimes \hat{Q}N \\ &= A + a \otimes N + R\hat{Q}u \otimes N \\ &= A + (a + R\hat{Q}u) \otimes N, \end{aligned}$$

since $\hat{Q}N = N$. It then follows from (f) and the cubic symmetry property that for all $u \in \mathbb{R}^3$,

$$\psi(A + u \otimes N) = \psi(A + (a + R\hat{Q}u) \otimes N), \tag{6.7}$$

and hence

$$W(u) = W(a + R\hat{Q}u),$$

where W is, as usual, defined by (4.7).

To see the effect of this symmetry more clearly, note first that if $v \in \mathbb{R}^3$ is such that $a + R\hat{Q}v = v$, then for all $u \in \mathbb{R}^3$,

$$\begin{aligned} W(v + u) &= W(a + R\hat{Q}v + R\hat{Q}u) \\ &= W(v + R\hat{Q}u). \end{aligned} \tag{6.8}$$

Now straightforward calculations show that

$$a + R\hat{Q}v = v \Leftrightarrow v \text{ lies on the line } L = \left\{ v{:}v_3 = 0 \text{ and } \eta_1 v_2 - \eta_2 v_1 = \frac{1}{\sqrt{2}}(\eta_2^2 - \eta_1^2) \right\}, \tag{6.9}$$

$$R\hat{Q}u = -u \Leftrightarrow u_1 e_1 + u_2 e_2 = \lambda a \quad \text{for some} \quad \lambda \in \mathbb{R}, \quad \text{and} \tag{6.10}$$

$$R\hat{Q}u = u \Leftrightarrow u_3 = 0 \quad \text{and} \quad (u_1 e_1 + u_2 e_2) \cdot a = 0. \tag{6.11}$$

So (6.8) yields in particular that

$$W(v + u) = W(v - u), \tag{6.12}$$

whenever $v \in L$ and $u = \lambda a$ for some $\lambda \in \mathbb{R}$. The line L is the perpendicular bisector of the line between 0 and a in the $\{u_3 \equiv 0\}$-plane, and $u \mapsto a + R\hat{Q}u$ reflects $u = u_1 e_1 + u_2 e_2$ in L. We label the two halves of the $\{u_3 = 0\}$-plane by Ω_1 and Ω_2, as in Fig. 4.

It follows from (6.12) that there is a minimizer $\tilde{u}$ of (6.3) among $\mathscr{C}_z$ with the additional properties that $\tilde{u}(-s)$ is the reflection in L of $\tilde{u}(s)$ for each $s \in \mathbb{R}$, and

$$\tilde{u}(s) \in \Omega_1 \cup L \quad \text{for} \quad s < 0, \quad \tilde{u}(0) \in L, \quad \tilde{u}(s) \in \Omega_2 \cup L \quad \text{for} \quad s > 0. \tag{6.13}$$

To see this, consider an element $u \in \mathscr{C}_z$ of a minimizing sequence for (6.3). It can be supposed without loss of generality that

(i) $u(0) \in L$ and $u(s) \in \Omega_2$ for $s > 0$;
(ii) $u(s) \in L \cup \Omega_1$ for $s < 0$.

Property (i) is immediate because $u(s) \to 0, a$ as $s \to -\infty, \infty$ and (6.3) is invariant under translation of u. That (ii) can be assumed is a consequence of (6.12): a segment with $u(s_1), u(s_2) \in L$ and $u(s) \in \Omega_2$ for $s_1 < s < s_2 \leq 0$ can be reflected in L without altering the value of (6.3) or changing the fact that $u \in \mathscr{C}_z$. Now if

$$\int_{-\infty}^{0} \psi(A + (u_1 e_1 + u_2 e_2 + 0e_3) \otimes N)) + \varepsilon^2 |u_1' e_1 + u_2' e_2 + 0e_3|^2 \, ds$$
$$\leq \int_{0}^{\infty} \psi(A + (u_1 e_1 + u_2 e_2 + 0e_3) \otimes N)) + \varepsilon^2 |u_1' e_1 + u_2' e_2 + 0e_3|^2 \, ds, \quad (6.14)$$

we can, without increasing (6.3), replace $u(s)$ for $s > 0$ by the reflection of $u(-s)$ in L, since $u(-s) \to 0$ as $s \to \infty$ and thus its reflection in L tends to a as $s \to \infty$. If the opposite inequality holds in (6.14), we can replace $u(s)$ for $s < 0$ by the reflection of $u(-s)$ in L. So in both cases, $u(-s)$ is the reflection of $u(s)$ in L for all $s \in \mathbb{R}$. Hence this, together with (6.13), also holds for a minimizer $\tilde{u}$ of (6.3) among $\mathscr{C}_z$. Since such a minimizer $\tilde{u} \in C^3(\mathbb{R}, \mathbb{R}^3)$, by Proposition 4.11 (a), the curve $\tilde{u}$ must be perpendicular to L at $\tilde{u}(0)$. □

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