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by

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Abstract

We derive plate theory for (possibly slightly stressed) heterogeneous multilayers in the regime of finite bending energies from three-dimensional elasticity theory by means of Γ-convergence. This extends results in [6, 19] to non-homogeneous materials. As expected from the homogeneous case we obtain a limiting energy functional depending on the second fundamental form of the plate surface. The effective elastic constants of the heterogeneous films will turn out to depend on the moments of the pointwise elastic constants of the materials.

1 Introduction

The derivation of effective theories for thin elastic structures is a classical problem in elasticity theory (see, e.g., the work of Euler, Kirchhoff, von Kármán [3, 12, 11] etc., also compare [16]). However, rigorous results deriving membrane, plate, rod or shell theories from three-dimensional elasticity have been obtained only recently (cf. [13, 14, 15, 5, 6, 7, 8, 9]). By now there has emerged a whole hierarchy of plate theories according to different scalings of the stored energy (cf. [7]). In these derivations one usually assumes the material of the elastic objects under consideration to be homogeneous, which in three-dimensional elasticity theory amounts to requiring that the stored energy function W, measuring the elastic energy

$$E(y) = \int_\Omega W(x, \nabla y(x))dx$$

of a body $\Omega \subset \mathbb{R}^3$ subject to a deformation $y : \Omega \to \mathbb{R}^3$, does not explicitly depend on x.

In their seminal paper [6] for much of the subsequent Γ-convergence results for effective theories, Friesecke, James and Müller derived Kirchhoff's plate theory for homogeneous materials from 3D-elasticity for bending dominated configurations. In the sequel these results have been extended in various directions. Up to now, however, it seems that the 'multilayer case' (cf. [6], page 1465) has remained open. This amounts to stored energy functions W which explicitly depend on x in the 'small film direction'. For multilayers it is natural to relax the requirement that $W(x, \cdot)$ be minimized precisely at $SO(3)$ slightly in order to include models for internally stressed films, e.g., epitaxially grown multilayers, stressed due to mismatching lattice constants. A first step in this direction was given in [20, 19] where an effective plate theory was derived for material mixings with possibly mismatching equilibria but equal elastic constants. Such an assumption is, e.g., satisfied for internal stresses within a monolayers caused by a temperature gradient.

It is not only mathematically interesting to discuss the more general case of heterogeneous multilayers, but also from the point of view of applications. If a stressed film is freed from the substrate, it will assume a geometrically non-trivial configuration in order to reduce its elastic energy. This phenomenon is used, e.g., in the waver-curvature measurement, where one tries to deduce material (mismatch) properties from measurements of the curved substrate. Another, recent application is the fabrication nanotubes (nanoscrolls, nanobelts, etc.) by growing bilayers of films with mismatching lattice constants and relieving them from the substrate (see, e.g., [21, 17]).

In the present paper we will derive a limiting energy functional for thin heterogeneous multilayers in the regime of finite bending energies (and thus give a solution to point (iv) in the list of open problems in [6]). Note that this is the appropriate regime for objects as nanotubes etc. mentioned above.

More precisely, assume that $\Omega_h = S \times (-h/2, h/2) \subset \mathbb{R}^3$, $S \subset \mathbb{R}^2$ a bounded convex domain, $h \ll 1$, is the reference configuration of a thin film. The elastic energy of a deformation $v : \Omega_h \to \mathbb{R}^3$ is given by

$$\int_{\Omega_h} W(z_3/h, \nabla v(z))dz.$$

Here $W : (-1/2, 1/2) \times \mathbb{R}^{3\times 3} \to \mathbb{R}$ is the stored energy function. The dependence on z_3 through z_3/h allows for considering multilayers made of laminated monolayers at fixed volume fraction. Changing variables to $x = (z_1, z_2, z_3/h)$ and defining y by $y(x', x_3) = v^{(h)}(x', hx_3)$, $x' = (x_1, x_2)$, the 3-dimensional energy functional is

$$\begin{aligned} E^{(h)}(v^{(h)}) &= \int_{\Omega_h} W(z_3, \nabla v^{(h)}(z))dz \\ &= h\int_{\Omega_1} W(x_3, \nabla' y(x), \frac{1}{h} y_{,3}(x))dx \ =: \ hI^h(y) \qquad (1) \end{aligned}$$

for $y \in W^{1,2}(\Omega_1; \mathbb{R}^3)$. Here ∇' denotes the planar gradient (∂_1, ∂_2). To incorporate mismatch of energy wells we introduce $W_0 : (-1/2, 1/2) \times \mathbb{R}^{3\times 3} \to \mathbb{R}$ and assume that

$$W(x_3, F) = W^{(h)}(x_3, F) = W_0(x_3, F(\mathrm{Id} + hB^{(h)}(x_3))) \qquad (2)$$

for some $B^{(h)} : (-1/2, 1/2) \to \mathbb{R}^{3\times 3}$. As we will see, the scaling $|hB^{(h)}| = \mathcal{O}(h)$ will precisely lead to non-trivial energy configurations at finite bending energies.

For multilayers we have to make sure that the usual assumptions on the pointwise energy densities $W(x_3, \cdot)$ are satisfied uniformly.

Assumption 1.1 *We will assume that W given by (2) satisfies the following hypotheses.*

(i) For almost all $t \in (-1/2, 1/2)$, $W_0(t, \cdot)$ is continuous on $\mathbb{R}^{3\times 3}$ and C^2 in a neighborhood of $SO(3)$ which does not depend on t. For all $F \in \mathbb{R}^{3\times 3}$, $W(\cdot, F) \in L^\infty((-1/2, 1/2); \mathbb{R})$.

(ii) If $Q_3(t, \cdot)$ denotes the Hessian of $W_0(t, \cdot)$ at Id, then $t \mapsto Q_3(t, \cdot)$ belongs to $L^\infty((-1/2, 1/2); \mathbb{R}^{9\times 9})$. Furthermore,

$$\omega(s) := \operatorname*{ess\,sup}_{-1/2<t<1/2} \sup_{|F|\leq s} |W_0(t, \mathrm{Id} + F) - \frac{1}{2} Q_3(t, F)|$$

shall satisfy $s^{-2}\omega(s) \to 0$ as $s \to 0$.

(iii) Frame indifference: There exists $C > 0$ such that for a.e. $t \in (-1/2, 1/2)$,

$$W_0(t, F) = W_0(t, RF)$$

for all $F \in \mathbb{R}^{3\times 3}$ and all $R \in SO(3)$.

(iv) Energy well: For a.e. $t \in (-1/2, 1/2)$, $W(t, F) = 0$ if $F \in SO(3)$ and

$$\operatorname*{ess\,inf}_{-1/2<t<1/2} W_0(t, F) \geq C\, dist^2(F, SO(3))$$

for all $F \in \mathbb{R}^{3\times 3}$.

(v) $B^{(h)} \to B$ in $L^\infty((-1/2, 1/2), \mathbb{R}^{3\times 3})$ as $h \to 0$.

In contrast to the homogeneous case, the proof of our central Γ-convergence result requires a thorough understanding of the geometry of isometric immersions of $\mathbb{R}^2$ into $\mathbb{R}^3$. The basic results in this direction where obtained by Pakzad in [18] and are reviewed and slightly extended in Section 2.

In Section 3 we first prove compactness of sequences of deformations with finite bending energy, i.e., sequences satisfying $\sup_h I^h(y^{(h)}) < \infty$. This is quite easily achieved by a comparison with homogeneous films whose flat reference configuration is stress free. The main result of this paper is Theorem 3.2, where the convergence of the functionals $h^{-2}I^h$ is investigated. The lower bound in this Γ-convergence result can be obtained by a modification of the corresponding result for monolayers (see [6]), and we do not re-derive all the steps contained in that paper. Rather we focus on the parts of the derivation that differ from [6]. Similar as in [6] we obtain an integral expression for the energy in terms of the second fundamental form of the film surface. The relevant quadratic form can be computed from the first moments of the pointwise quadratic forms of Kirchhoff's plate theory (see Proposition 3.5 for a precise statement). However, the reference state is not a state of minimal energy any more; the thin film can reduce energy by rolling up.

The most interesting part is to prove the upper bound in the Γ-limit. We have to provide test functions with almost optimal energy. To construct these test functions we have to prove a representation result for matrix valued functions on the two-dimensional film domain in terms of symmetrized gradients and the second fundamental form of the film surface, see Lemma 3.3. In the proof of this lemma one is led to a system of two first order partial differential equations. Using the results of Pakzad (cf. [18]) on the developability of $W^{2,2}$ isometric immersions, we can give an explicit formula for its solution.

In section 4 we consider convergence of the rescaled strain in the spirit of [6] and discuss the geometry of energy minimizers with free boundary conditions analogous to [19]. This yields an ansatz free justification of calculations of minimal energy configurations used in the physics literature, where so far (mostly linear) three-dimensional elasticity theory is used to describe the energy of such objects (cf., e.g., [10], [22]), and in order to discuss the geometry of energy minimizers one uses appropriate ansatz functions and optimizes with respect to certain parameters (e.g., radius, winding direction for nanoscrolls).

Finally, in Section 5 we give a specific example of the applicability of our results and discuss the size of nanoscrolls that were fabricated by Paetzeldt et. al., see [17]. The calculations of the radii of optimal energy are in good agreement with the measured values.

2 The geometry of isometric immersions

As in the homogeneous setting the class of plate deformations with finite bending energy will turn out to coincide with the set of (Sobolev-) isometric immersions of S into $\mathbb{R}^3$

$$\mathcal{A} := \{u \in W^{2,2}(S;\mathbb{R}^3) : \nabla u \in O(2,3) \text{ a.e.}\}. \tag{3}$$

To prove our main Γ-limit result for x_3-dependent stored energy functions, we have to study this class of functions more thoroughly. In particular, we will need a slightly refined version of the following density result for smooth maps in $\mathcal{A}$, first proved by Pakzad in [18].

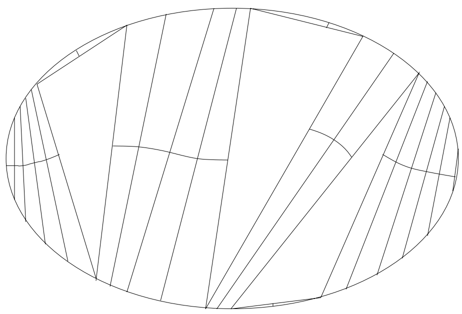
Theorem 2.1 (cf. [18]) *C^2-maps are $W^{2,2}$-strongly dense in $\mathcal{A}$.*

The main purpose of this section is to collect some of the results of [18] that will be used in the sequel and to indicate how the approximation scheme can be modified to show that indeed C^∞-maps are strongly dense in $\mathcal{A}$. In fact, only minor changes in the proofs of [18] are necessary, so we will not repeat all the arguments here, but rather focus on describing their modifications and refer the reader to [18] for more details.

Suppose u lies in $\mathcal{A}$, and denote by II its second fundamental form, i.e., $\mathrm{II}_{ij} = u_{,i} \cdot (u_{,1} \wedge u_{,2})_{,j}$. Then II is singular, and there exists $f_u \in W^{1,2}$ such that $\nabla f_u = \mathrm{II}$. We call $\gamma : [0, l] \to S$, parameterized by arclength, a *leading curve* if it is orthogonal to the inverse images of f_u on regions where f_u is not constant. We denote by κ and ν the curvature and unit normal, respectively, i.e., $\gamma'' = \kappa\nu$. In fact, κ must be bounded, hence $\gamma \in W^{2,\infty}$. A subdomain $S' \subset S$ is said to be covered by a curve γ if

$$S' \subset \{\gamma(t) + s\nu(t) : s \in \mathbb{R}, t \in [0, l]\}.$$

As shown in [18], S can be partitioned into so-called bodies and arms. Here a *body* is a connected maximal subdomain on which u is affine and whose boundary contains more than two segments inside S. An *arm* is a maximal subdomain $S(\gamma)$ covered by some leading curve γ. The boundary segments $S \cap (\gamma(t) + \mathbb{R}\nu(t))$, $t \in \{0, l\}$, are referred to as the *free hands* of the arm $S(\gamma)$.



Lemma 2.2 (cf. [18], Lemmas 3.3 and 3.4) *The set of mappings which allow for a partition of S into a finite number of bodies and arms is $W^{2,2}$-strongly dense in $\mathcal{A}$.*

The approximation by smooth isometric immersions consists of first approximating u on covered domains (linearly near the free hands) and then patching together the different pieces appropriately. We only need to consider arms. So suppose $S(\gamma) \subset S$ is covered by γ. We can transform coordinates according to

$$\Phi_\gamma : S(l, s_-^\gamma, s_+^\gamma) \to S(\gamma), \quad \Phi_\gamma(t, s) = \gamma(t) + s\nu(t),$$

where

$$\begin{aligned} S(l, s_-^\gamma, s_+^\gamma) &:= \{(t, s) \in [0, l] \times \mathbb{R} : \gamma(t) + s\nu(t) \in S(\gamma)\} \\ &= \{(t, s) \in [0, l] \times \mathbb{R} : s_-^\gamma < s < s_+^\gamma\}. \end{aligned}$$

Consider the Darboux frame $(\mathbf{t}, \mathbf{v}, \mathbf{n})$ of $\tilde{\gamma} = u \circ \gamma$ in $u(S)$ with

$$\begin{cases} \mathbf{t} := \tilde{\gamma}', \\ \mathbf{v} := \nabla u(\nu), \\ \mathbf{n} := \mathbf{t} \times \mathbf{v}, \end{cases} \quad \text{and} \quad \begin{cases} \mathbf{t}' = \kappa_g \mathbf{v} + \kappa_n \mathbf{n}, \\ \mathbf{v}' = -\kappa_g \mathbf{t} + \tau_g \mathbf{n}, \\ \mathbf{n}' = -\kappa_n \mathbf{t} - \tau_g \mathbf{v}. \end{cases}$$

For a given curve $\tilde{\gamma}$ with frame $(\mathbf{t}, \mathbf{v}, \mathbf{n})$ the basic observation is that the surface u satisfying

$$u(\Phi_\gamma(t, s)) = \tilde{\gamma}(t) + s\mathbf{v}(t)$$

is an isometry if and only if $\kappa_g = \kappa$ and $\tau_g = 0$. In order to construct $u_m \in C^2 \cap \mathcal{A}$ such that $u_m \to u$ in $W^{2,2}$, Pakzad approximates γ by curves γ_m with continuous curvature κ_m and κ_n by continuous $\kappa_{n;m}$. The original frame is then approximated by solutions of

$$\begin{pmatrix} \mathbf{t}_m' \\ \mathbf{v}_m' \\ \mathbf{n}_m' \end{pmatrix} = \begin{pmatrix} 0 & \kappa_m & \kappa_{n;m} \\ -\kappa_m & 0 & 0 \\ -\kappa_{n;m} & 0 & 0 \end{pmatrix} \begin{pmatrix} \mathbf{t}_m \\ \mathbf{v}_m \\ \mathbf{n}_m \end{pmatrix},$$

and finally u_m is defined by $u_m(\Phi_{\gamma_m}(t, s)) = \tilde{\gamma}_m(t) + s\mathbf{v}_m(t)$, possibly extended by a linear map.

To guarantee smoothness of u_m, it suffices to assure that κ_m and $\kappa_{n;m}$ are smooth. It is not hard to see that κ_m can be chosen in C^∞, vanishing near its starting and final point. Now set

$$\tilde{\kappa}_{n;m}(t) := \psi(m(t - l_m^*))\sqrt{\frac{\varphi_m}{\varphi}(t)}g_m(t)$$

for some cut-off function ψ, some $g_m \to \kappa_n$ a.e., vanishing near 0, and φ_m, φ as defined in [18]. In [18], $\kappa_{n;m}$ is defined to be $\tilde{\kappa}_{n;m}$. Clearly we may assume that g_m be smooth. However, $\sqrt{\varphi_m/\varphi}$ can only be guaranteed to be continuous. But still we can choose $\kappa_{n;m}$ C^∞-smooth with $|\kappa_{n;m}| \leq \tilde{\kappa}_{n;m}$ and $\kappa_{n;m} - \tilde{\kappa}_{n;m} \to 0$ uniformly on $[0, l]$. Note that this is an admissible choice in the sense that Propositions 3.3 and 3.4 of [18], showing that u_m is an isometry approximating u, still apply.

Having matched the approximations on different arms and bodies smoothly, applying a dilation argument as in the proof of [18], Proposition 3.1, we may even assume that $\varphi_m \geq \rho_m > 0$ and u_m is smooth up to the boundary. Summarizing, this shows the following.

Proposition 2.3 *We say that $u \in \mathcal{A}_0$ if u is a $C^\infty(\overline{S})$-smooth isometric immersion which allows for a finite partition of S into bodies and arms, and u is affine on the bodies and in a neighborhood of the free hands of the arms. Then $\mathcal{A}_0$ is $W^{2,2}$-strongly dense in $\mathcal{A}$.*

For later use we finally infer from [18] (also compare the proof of Theorem 3.2 in [19]) that on covered domains $S(\gamma)$ the second fundamental form II can be written as

$$\mathrm{II}(\Phi_\gamma(t, s)) = \frac{\lambda(t)}{1 - s\kappa(t)}\mu(t) \otimes \mu(t),$$

where $\mu = d\gamma/dt$. If $u \in \mathcal{A}_0$, then there exists $\rho > 0$ such that $1 - s\kappa(t) \geq \rho > 0$ wherever $\mathrm{II} \neq 0$.

3 Plate theory for stressed multilayers

In this section we prove our main Γ-limit result deriving plate theory for heterogeneous multilayers from three-dimensional elasticity theory. Throughout we will assume that the energy functional I^h defined in (1) with stored energy density W satisfies Assumption 1.1.

The following compactness result is a direct consequence of the corresponding result for homogeneous W proven in [6].

Theorem 3.1 *(Compactness) Suppose a sequence $(y^{(h)}) \subset W^{1,2}(\Omega; \mathbb{R}^3)$ has finite bending energy, i.e.,*

$$\limsup_{h \to \infty} \frac{1}{h^2} I^h(y^{(h)}) < \infty.$$

Then $\nabla_h y^{(h)} := (\nabla' y^{(h)}, \frac{1}{h} y_3^{(h)})$ is precompact in $L^2(\Omega)$ as $h \to 0$: there exists a subsequence (not relabeled) such that

$$\nabla_h y^{(h)} \to (\nabla' y, b) \quad \text{in } L^2(\Omega_1) \text{ as } h \to 0,$$

$(\nabla' y, b) \in SO(3)$ *a.e. Furthermore,* $(\nabla' y, b) \in H^1(\Omega)$ *is independent of* x_3.

Proof. Note that by Assumptions 1.1 (iv) and (v), $\operatorname{dist}^2(F, SO(3))$ is bounded by

$$2 \operatorname{dist}^2 \left(F(\mathrm{Id} + hB^{(h)}(t)), SO(3) \right) + 2 \left| FhB^{(h)}(t) \right|^2 \leq C \left(W(t, F) + |F|^2 h^2 \right)$$

for a.e. $t \in (-1/2, 1/2)$ and all $F \in \mathbb{R}^{3\times3}$. But then

$$\operatorname{dist}^2(F, SO(3)) \leq C \left(W(t, F) + h^2 \right).$$

So if $h^{-2} I^h(y^{(h)})$ is bounded, then

$$\int_{\Omega_1} \operatorname{dist}^2(\nabla_h y^{(h)}(x), SO(3)) \leq C \left(\int_{\Omega_1} W(x_3, \nabla_h y^{(h)}(x)) + h^2 \right) \leq Ch^2.$$

The claim therefore directly follows from the homogeneous case (cf. [6]). □

Recall the definition of $\mathcal{A}$ from (3). We view $\mathcal{A}$ as a set of functions on Ω_1, independent of x_3. To be consistent with the terminology used in elasticity theory, the surface normal to $y \in \mathcal{A}$ is denoted by $b = y_{,1} \wedge y_{,2}$.

Depending on $Q_3(t, \cdot)$, the Hessian of $W_0(t, \cdot)$ at the identity, we define a relaxed quadratic form on 2×2-matrices by

$$Q_2(t, F) := \min_{c \in \mathbb{R}^3} Q_3(t, \hat{F} + c \otimes e_3) = \min_{c \in \mathbb{R}^3} Q_3 \left(t, \hat{F} + \frac{c \otimes e_3 + e_3 \otimes c}{2} \right),$$

where $\hat{F}$ is the 3×3-matrix $\sum_{i,j=1}^2 F_{ij} e_i \otimes e_j$. Furthermore define $\bar{Q}_2 : \mathbb{R}^{2\times2} \to \mathbb{R}_+$ (independent of t) by

$$\bar{Q}_2(F) := \min_{A \in \mathbb{R}^{2\times2}} \int_{-1/2}^{1/2} Q_2(t, A + tF + \check{B}(t)) dt,$$

where $\check{B}$ is derived from B by omitting the last row and the last column. Since $Q_2(t, \cdot)$ vanishes on antisymmetric matrices for a.e. t, we may replace $\mathbb{R}^{2\times2}$ by $\mathbb{R}^{2\times2}_{\mathrm{sym}}$ and $\check{B}$ by $\frac{1}{2}(\check{B}^T + \check{B})$ in this definition. Note that $\bar{Q}_2$ is a quadratic function of F.

Theorem 3.2 *(Γ-limit) The functionals $h^{-2} I^h$ Γ-converge to I^0 in $W^{1,2}$ (with respect to the strong and the weak topology) as $h \to 0$:*

(i) If $y^{(h)} \rightharpoonup y$ in $W^{1,2}$ as $h \to 0$, then

$$\liminf_{h \to 0} I^h(y^{(h)}) \geq I^0(y).$$

(ii) For all $y \in W^{1,2}$ there exists a sequence $y^{(h)} \to y$ in $W^{1,2}$ as $h \to 0$ such that

$$\lim_{h \to 0} I^h(y^{(h)}) = I^0(y).$$

The two-dimensional limiting energy functional I^0 is given by

$$I^0(y) = \begin{cases} \frac{1}{2}\int_S \bar{Q}_2(\mathrm{II})dx & \text{for } y \in \mathcal{A}, \\ \infty & \text{else,} \end{cases}$$

where II *is the second fundamental form of y.*

By our definition of $\bar{Q}_2$, a proof of the lower bound (i) can be given following along the lines of the corresponding results for homogeneous materials (cf. [6] and [19]).

Proof of Theorem 3.2 (i). In the proof of Theorem 3.1 we noted that sequences $(y^{(h)})$ with bounded energy converging to y satisfy

$$\int_{\Omega_1} \mathrm{dist}^2(\nabla_h y^{(h)}, SO(3)) \le Ch^2.$$

As shown in [6], one therefore can construct a piecewise constant approximation $R^{(h)} : S'_h \subset S \to SO(3)$ to $\nabla_h y^{(h)}$ such that (for a subsequence)

$$G^{(h)}(x', x_3) = \frac{R^{(h)}(x')^T \nabla_h y^{(h)}(x', x_3) - \mathrm{Id}}{h} \rightharpoonup G \qquad \text{in } L^2.$$

($G^{(h)}$ is extended by 0 outside $S'_h \times (-1/2, 1/2)$.) If $\check{G}$ denotes the 2×2-matrix obtained by ommiting the third row and third column of G, it is further shown that

$$\check{G}(x', x_3) = \check{G}(x', 0) + x_3 \mathrm{II}(x'), \quad \mathrm{II} = (\nabla' y)^T \nabla' b,$$

and

$$\chi_h G^{(h)} \rightharpoonup G \quad \text{in } L^2(\Omega_1),$$

where χ_h is the characteristic function of the set $S'_h \cap \{|G^{(h)}(x)| \le h^{-1/2}\}$.

It remains to estimate the energy in terms of G. This is done in analogy to [6] and [19] by a careful Taylor-expansion of $W_0(x_3, \cdot)$ around the identity. By Assumptions 1.1 (iii) and (ii),

$$\begin{aligned} \frac{1}{h^2}\int_{\Omega_1} W(x_3, \nabla_h y^{(h)})dx \;&\ge\; \frac{1}{h^2}\int_{\Omega_1} \chi_h W_0\left(x_3, (R^{(h)})^T \nabla_h y^{(h)}(\mathrm{Id} + hB^{(h)})\right)dx \\ &=\; \frac{1}{h^2}\int_{\Omega_1} \chi_h W_0\left(x_3, \mathrm{Id} + hA^{(h)}\right)dx \\ &\ge\; \int_{\Omega_1} \frac{1}{2} Q_3\left(x_3, \chi_h A^{(h)}\right) - \frac{1}{h^2}\chi_h \omega\left(|hA^{(h)}|\right)dx \end{aligned}$$

with $A^{(h)} = G^{(h)} + (R^{(h)})^T \nabla_h y^{(h)} B^{(h)} \rightharpoonup G + B$. (Note that $|hA^{(h)}| \le C\sqrt{h}$ on $\{\chi \neq 0\}$.) Using lower semicontinuity and $Q_3(x_3, F) \ge Q_2(x_3, \check{F})$, we find by integrating over x_3 that

$$\begin{aligned} \liminf_{h\to 0} \frac{1}{h^2}\int_{\Omega_1} W(x_3, \nabla_h y^{(h)})dx \;&\ge\; \frac{1}{2}\int_{\Omega_1} Q_3\left(x_3, G(x) + B(x_3)\right)dx \\ \ge\; \frac{1}{2}\int_{\Omega_1} Q_2\left(x_3, \check{G}(x', 0) + x_3\mathrm{II}(x') + \check{B}(x_3)\right)dx& \\ \ge\; \frac{1}{2}\int_S \bar{Q}_2\left(\mathrm{II}(x')\right)dx'.& \end{aligned}$$

$\square$

The proof of Theorem 3.2 (ii), i.e., the construction of recovery sequences for I^0 can not be adapted in a straightforward manner from [6] or [19]. Our test functions need to contain additional terms. The main new technical ingredient is the following representation result for matrix valued functions.

Lemma 3.3 *Suppose $y \in \mathcal{A}_0$. Let $A \in C^\infty(\overline{S}; \mathbb{R}^{2\times 2}_{\mathrm{sym}})$ be a smooth function taking values in the symmetric 2×2-matrices such that $A \equiv 0$ in a neighborhood of $\{\mathrm{II} = 0\}$. Then there exist smooth functions $g_1, g_2, \alpha \in C^\infty(\overline{S}; \mathbb{R})$ such that*

$$A = \nabla_{\mathrm{sym}}\, g + \alpha \mathrm{II},$$

where $\nabla_{\mathrm{sym}}\, g$ denotes the symmetrized gradient $\frac{1}{2}(\nabla^T + \nabla)$ of $g = (g_1, g_2)^T$. In addition, g and α can be chosen vanishing on $\{\mathrm{II} = 0\}$.

Proof. On bodies (where $\mathrm{II} \equiv 0$, cf. Section 2) we let $g_1 \equiv g_2 \equiv \alpha \equiv 0$. On a covered domain $S(\gamma)$ we can introduce variables t, s such that y is of the form

$$y(x_1, x_2) = y(\Phi_\gamma(t, s)) = \tilde{\gamma}(t) + s\mathbf{v}(t),$$

where t is arclength of $\tilde{\gamma}$, and

$$\mathrm{II}(x_1, x_2) = \mathrm{II}(\Phi_\gamma(t, s)) = \lambda(t, s)\mu(t) \otimes \mu(t),$$

where $\lambda(t, s) = \lambda(t)/(1 - s\kappa(t))$, μ is the unit vector $d\gamma/dt$ and $\mathbf{v} = \nabla u \cdot \nu$, $\nu = \mu^\perp$, see Section 2.

If $\lambda(t) = 0$, we set $g_1(\Phi_\gamma(t, s)) = g_2(\Phi_\gamma(t, s)) = \alpha(\Phi_\gamma(t, s)) = 0$. Now suppose $\lambda(t) \neq 0$ for $t_1 < t < t_2$ and consider the matrices

$$F_1 = \frac{1}{|\mathrm{II}|}\begin{pmatrix} \mathrm{II}_{22} & -\mathrm{II}_{12} \\ -\mathrm{II}_{12} & \mathrm{II}_{11} \end{pmatrix}, \quad F_2 = \frac{1}{\sqrt{2}|\mathrm{II}|}\begin{pmatrix} 2\mathrm{II}_{12} & \mathrm{II}_{22} - \mathrm{II}_{11} \\ \mathrm{II}_{22} - \mathrm{II}_{11} & -2\mathrm{II}_{12} \end{pmatrix}.$$

Also define $F_3 = \mathrm{II}/|\mathrm{II}|$. Then for every fixed (t, s), (F_1, F_2, F_3) forms an orthonormal basis of $\mathbb{R}^{2\times 2}_{\mathrm{sym}}$ and we have to find $g = (g_1, g_2)$ and α such that the three equations

$$F_i : \nabla_{\mathrm{sym}}\, g + F_i : \alpha\mathrm{II} = F_i : A, \quad i = 1, 2, 3,$$

are satisfied.

The first two of these equations read

$$\begin{aligned} \mathrm{II}_{22} g_{1,1} - \mathrm{II}_{12}(g_{1,2} + g_{2,1}) + \mathrm{II}_{11} g_{2,2} &= |\mathrm{II}| F_1 : A, \\ 2\mathrm{II}_{12} g_{1,1} + (\mathrm{II}_{22} - \mathrm{II}_{11})(g_{1,2} + g_{2,1}) - 2\mathrm{II}_{12} g_{2,2} &= \sqrt{2}|\mathrm{II}| F_2 : A. \end{aligned}$$

Writing the left hand sides as

$$-\lambda\mu_2(-\mu_2 g_{1,1} + \mu_1 g_{1,2}) + \lambda\mu_1(-\mu_2 g_{2,1} + \mu_1 g_{2,2}) = \lambda\mu^\perp \cdot \partial_{\mu^\perp} g,$$

respectively,

$$\begin{aligned} &-\lambda\mu_1(-\mu_2 g_{1,1} + \mu_1 g_{1,2}) - \lambda\mu_2(-\mu_2 g_{2,1} + \mu_1 g_{2,2}) \\ &+\lambda\mu_2(\mu_1 g_{1,1} + \mu_2 g_{1,2}) - \lambda\mu_1(\mu_1 g_{2,1} + \mu_2 g_{2,2}) \\ &= -\lambda\mu \cdot \partial_{\mu^\perp} g - \lambda\mu^\perp \cdot \partial_\mu g, \end{aligned}$$

with $\lambda = \lambda(t,s)$ and absorbing the (definite) sign of $\lambda = \pm|\mathrm{II}|$ into A, we arrive at

$$\begin{aligned} \mu^\perp \cdot \partial_{\mu^\perp} g &= F_1 : A, \\ -\mu \cdot \partial_{\mu^\perp} g - \mu^\perp \cdot \partial_\mu g &= \sqrt{2} F_2 : A. \end{aligned}$$

Changing variables to (t,s) yields $\partial_{\mu^\perp} = \partial_s$ and $\partial_\mu = (1-s\kappa)^{-1}\partial_t$, where κ is the curvature of γ. Define $u = (u_1, u_2)$ by $u_1 = \mu \cdot g$, $u_2 = \mu^\perp \cdot g$ (i.e., $g = u_1 \mu + u_2 \mu^\perp$). Then the above system is equivalent to

$$\begin{aligned} u_{2,s} &= F_1 : A, \\ -u_{1,s} - \frac{\kappa}{1-s\kappa} u_1 - \frac{1}{1-s\kappa} u_{2,t} &= \sqrt{2} F_2 : A. \end{aligned}$$

Since $y \in \mathcal{A}_0$, this is a linear differential equation with bounded and smooth coefficients for u on $S(l, s_-^\gamma, s_+^\gamma)$, and we can find a solution by first solving the first equation for u_2 and then the second one for u_1. For definiteness we choose initial conditions at $s = 0$ requiring that $u(t, s = 0) = 0$.

To finish the proof we have to make sure that also the third equation (for $i = 3$) is satisfied. But this is trivial. Just choose α such that

$$\frac{1}{|\mathrm{II}|} F_3 : \nabla_{\mathrm{sym}}\, g + \alpha = \frac{1}{|\mathrm{II}|} F_3 : A.$$

Note that this way we obtain a C^∞-solution u on $\overline{S(\gamma)}$ since A and g vanish on lines $\{t = \text{const.}\}$ near $\lambda(t) = 0$. For the same reason we can patch together solutions on two arms or an arm and a body since near the free hands of an arm and on all of a body u is affine, i.e., $\mathrm{II} \equiv 0$, whence $g_1 = g_2 = \alpha = 0$. $\square$

Remark. The proof also gives bounds of the form

$$\|g\|_{W^{k,p}}, \|\alpha\|_{W^{k,p}} \le C \|A\|_{W^{k+1,p}}$$

with $C = C(k,p,y)$, $1 \le p \le \infty$. In fact it is easy to verify that u calculated above is given explicitly by

$$\begin{aligned} u_2(t,s) &= \int_0^s (F_1 : A)(t, s') ds', \\ u_1(t,s) &= (1 - s\kappa(t)) \int_0^s \left(\frac{-\int_0^{s'} \frac{\partial}{\partial t}(F_1 : A)(t, s'') ds''}{(1 - s'\kappa(t))^2} - \frac{\sqrt{2}(F_2 : A)(t, s')}{1 - s'\kappa(t)} \right) ds'. \end{aligned}$$

We can now finish the proof of Theorem 3.2.

Proof of Theorem 3.2 (ii). Since $\bar{Q}_2$ is a quadratic function on $\mathbb{R}^{2\times 2}$, the limit functional I^0 is $W^{2,2}$-continuous on $\mathcal{A}$. By Proposition 2.3 and a standard argument in Γ-convergence, we therefore only have to construct recovery sequences for $y \in \mathcal{A}_0$.

So suppose $y \in \mathcal{A}_0$ $(\subset W^{2,\infty})$. Let $d \in C_0^\infty(\Omega_1; \mathbb{R}^3)$, $g_1, g_2, \alpha \in C^\infty(\bar{S}; \mathbb{R})$, $g = (g_1, g_2)$, and define

$$y^{(h)}(x', x_3) = y(x') + h\Big[(x_3 - \alpha(x'))b(x') + \nabla' y(x') \cdot g(x')\Big] + h^2 D(x', x_3)$$

for $D(x',x_3) = \int_0^{x_3} d(x',t)dt$. Furthermore, denote $R(x') := (\nabla' y(x'), b(x'))$ and

$$\begin{aligned} R^T \nabla_h y^{(h)} &= R^T \left((\nabla' y, b) + h(\nabla'[(x_3-\alpha)b + \nabla' y \cdot g], D_{,3}) + h^2(\nabla' D, 0) \right) \\ &=: \mathrm{Id} + hA^{(h)} \end{aligned}$$

with $|A^{(h)}| \leq C$ for all $h \leq h_0$. Using that $W_0(x_3, \mathrm{Id}+F) \leq C \operatorname{dist}^2(\mathrm{Id} + F, SO(3))$ in a neighborhood of $SO(3)$ by Assumptions 1.1 (ii) and (iii), we obtain for all $h \leq h_0$

$$\frac{1}{h^2} W_0(x_3, (\mathrm{Id}+hA^{(h)})(\mathrm{Id}+hB^{(h)})) \;\leq\; \frac{C}{h^2}\left(|hA^{(h)}|^2 + |hB^{(h)}|^2\right) \;\leq\; C.$$

Furthermore,

$$\frac{1}{h^2} W_0(x_3, (\mathrm{Id}+hA^{(h)})(\mathrm{Id}+hB^{(h)})) \to \frac{1}{2} Q_3(x_3, R^T(\nabla'[(x_3-\alpha)b + \nabla' y \cdot g], D_{,3}) + B)$$

a.e. So by frame indifference and dominated convergence

$$\begin{aligned} \frac{1}{h^2}\int_{\Omega_1} W\left(x_3, \nabla_h y^{(h)}\right) dx &= \frac{1}{h^2}\int_{\Omega_1} W_0(x_3, R^T \nabla_h y^{(h)}(\mathrm{Id}+hB^{(h)}))dx \\ \to \frac{1}{2}\int_{\Omega_1} & Q_3(x_3, R^T(\nabla'[(x_3-\alpha)b + \nabla' y\cdot g], d) + B)dx. \end{aligned}$$

Now $\nabla'[(x_3-\alpha)b] = (x_3-\alpha)\nabla' b - b\nabla'\alpha$, and therefore

$$R^T \nabla'[(x_3-\alpha)b] = (x_3-\alpha)\begin{pmatrix} \mathrm{II}_{11} & \mathrm{II}_{12} \\ \mathrm{II}_{21} & \mathrm{II}_{22} \\ 0 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ \alpha_{,1} & \alpha_{,2} \end{pmatrix}.$$

Furthermore, for $i = 1,2$, $\nabla'[g_i y_{,i}] = g_i \nabla' y_{,i} + y_{,i}\nabla' g_i$, and therefore

$$R^T \nabla'[g_i y_{,i}] = -g_i \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ \mathrm{II}_{i1} & \mathrm{II}_{i2} \end{pmatrix} + e_i \nabla' g_i,$$

i.e.,

$$R^T \nabla'[\nabla' y \cdot g] = -\begin{pmatrix} 0 & 0 \\ 0 & 0 \\ g_1 \mathrm{II}_{11} + g_2 \mathrm{II}_{21} & g_1 \mathrm{II}_{12} + g_2 \mathrm{II}_{22} \end{pmatrix} + \begin{pmatrix} g_{1,1} & g_{1,2} \\ g_{2,1} & g_{2,2} \\ 0 & 0 \end{pmatrix}.$$

Since $C_0^\infty(\Omega_1;\mathbb{R}^3)$ is dense in $L^2(\Omega_1;\mathbb{R}^3)$, by a standard diagonalization argument choosing $d = d^{(h)}$ suitably leads to $(y^{(h)})$ such that

$$\begin{aligned} &\frac{1}{h^2}\int_{\Omega_1} W\left(x_3, \nabla_h y^{(h)}\right) dx \\ &\quad \to \frac{1}{2}\int_{\Omega_1} Q_2(x_3, (x_3-\alpha)\mathrm{II} + \nabla'_{\mathrm{sym}} g + \frac{1}{2}(\check{B} + \check{B}^T))dx, \end{aligned}$$

where we have used that Q_3 vanishes on antisymmetric matrices.

To finish the proof by another application of this diagonalization argument, we have to show that

$$A_{\min} = \operatorname*{argmin}_{A\in\mathbb{R}^{2\times 2}_{\rm sym}} \int_{-1/2}^{1/2} Q_2(t, A + t\mathrm{II} + \frac{1}{2}(\check{B} + \check{B}^T))dt \in L^2(S;\mathbb{R}^{2\times 2}_{\rm sym}) \qquad (4)$$

can be approximated in L^2 by smooth functions $A = \nabla'_{\rm sym} g - \alpha\mathrm{II}$ for appropriately chosen g and α.

But this is not hard: First, note that $\mathcal{A}_{\min} \equiv A_0$ on $\{\mathrm{II} = 0\}$ for some constant matrix A_0. Then choose $\tilde{g}$ and $-\alpha$ according to Lemma 3.3 for $A \in C^\infty(\overline{S};\mathbb{R}^{2\times 2}_{\rm sym})$, where A is supported on $\{\mathrm{II} \neq 0\}$ and approximates $x \mapsto A_{\min}(x) - A_0$ in L^2. Setting $g(x) = \tilde{g}(x) + A_0 x$, we obtain

$$\|\nabla_{\rm sym}\, g - \alpha\mathrm{II} - A_{\min}\|_{L^2} = \|\chi_{\{\mathrm{II}\neq 0\}}(A + A_0 - A_{\min})\|^2_{L^2}.$$

Therefore $\nabla_{\rm sym}\, g - \alpha\mathrm{II}$ approximates $A_{\min}$. □

The above theorems imply convergence of (almost) minimizers under appropriate body forces (cf. [7] for the homogeneous counterpart). Suppose $f^{(h)} : \Omega_1 \to \mathbb{R}^3$ is a body force such that $h^{-2} f^{(h)} \to f$ in $L^2(\Omega_1;\mathbb{R}^3)$ with $\int_{\Omega_1} f^{(h)}(x)dx = 0$ for all h. Define the energy functionals under the load $f^{(h)}$ resp. the limiting energy functional by

$$\begin{aligned} J^h(y) &:= \int_{\Omega_1} \Big(W(x_3, \nabla_h y(x)) - y(x)\cdot f^{(h)}(x')\Big)\, dx \quad \text{resp.} \\ J^0(y) &:= \begin{cases} \frac{1}{2}\int_S \left(\bar{Q}_2(\mathrm{II}(x')) - y(x')\cdot \bar{f}(x')\right) dx' & \text{for } y \in \mathcal{A}, \\ \infty & \text{else,} \end{cases} \end{aligned}$$

where $\bar{f} = \int_{-1/2}^{1/2} f(\cdot, t)dt$.

Corollary 3.4 *If $(y^{(h)})$ is a sequence of almost minimizers of J^h, i.e.,*

$$\frac{1}{h^2}\left(J^h(y^{(h)}) - \inf J^h\right) \to 0,$$

then there exists $y \in \mathcal{A}$ such that $y^{(h)} \to y$ in $W^{1,2}$ (for a subsequence) and y minimizes J^0.

Proof. The test function $y(x', x_3) = (x', hx_3)$ shows that $\inf J^h \leq Ch^2$. Using that $\int_{\Omega_1} f^{(h)}(x)dx = 0$, from Poincaré's inequality we deduce

$$\begin{aligned} I^h(y^{(h)}) &\leq J^h(y^{(h)}) + \|f^{(h)}\|_{L^2}\|\nabla y^{(h)}\|_{L^2} \\ &\leq Ch^2 + Ch^2\left(1 + \sqrt{I^h(y^{(h)})}\right) \end{aligned}$$

along almost minimizing sequences. So $I^h(y^{(h)}) \leq Ch^2$. The claim now follows from Theorems 3.1 and 3.2. □

For applications it is useful to give a more explicit formula for $\bar{Q}_2$ in terms of the moments of Q_2. To this end, we view elements of $\mathbb{R}^{2\times 2}_{\rm sym}$ as vectors in $\mathbb{R}^3$ that are referred to by the corresponding bold lowercase letters via

$$\mathbf{f} = (F_{11}, F_{22}, F_{12})^T \quad \text{for } F \in \mathbb{R}^{2\times 2}_{\rm sym}.$$

To the quadratic forms $Q_2(t,\cdot)$ we can then associate symmetric positive definite 3×3-matrices $\mathcal{M}(t)$ in the usual manner.

Define the symmetric 3×3-matrices $\mathcal{M}_1$, $\mathcal{M}_2$, $\mathcal{M}_3$ by

$$\mathcal{M}_1 := \int \mathcal{M}(t), \quad \mathcal{M}_2 := \int t\mathcal{M}(t), \quad \mathcal{M}_3 := \int t^2\mathcal{M}(t),$$

the vectors $\mathbf{b}_1, \mathbf{b}_2 \in \mathbb{R}^3$ and the constant β by

$$\mathbf{b}_1 := \int \mathcal{M}(t)\mathbf{b}(t), \quad \mathbf{b}_2 := \int t\mathcal{M}(t)\mathbf{b}(t), \quad \beta := \int \mathbf{b}^T(t)\mathcal{M}(t)\mathbf{b}(t),$$

where $\mathbf{b}(t)$ represents $\frac{1}{2}(\check{B}(t)^T + \check{B}(t))$. It is not hard to see that

$$\mathcal{M}_0 := \mathcal{M}_3 - \mathcal{M}_2\mathcal{M}_1^{-1}\mathcal{M}_2$$

is a positive definite matrix. We can therefore define

$$\mathbf{f}_0 := \mathcal{M}_0^{-1}(\mathcal{M}_2\mathcal{M}_1^{-1}\mathbf{b}_1 - \mathbf{b}_2) \quad \text{and} \quad \alpha := -\mathbf{f}_0^T\mathcal{M}_0\mathbf{f}_0 + \beta - \mathbf{b}_1^T\mathcal{M}_1^{-1}\mathbf{b}_1.$$

Proposition 3.5 *Denote the quadratic form on $\mathbb{R}^{2\times 2}_{\mathrm{sym}}$ corresponding to $\mathcal{M}_0$ by Q_2^*. As before let $A_{\min}$ denote the minimizer of (4). Then*

$$\bar{Q}_2(F) = Q_2^*(F - F_0) + \alpha,$$

and $A_{\min}(F)$ is given by

$$\mathbf{a}_{\min}(\mathbf{f}) = -\mathcal{M}_1^{-1}(\mathcal{M}_2\mathbf{f} + \mathbf{b}_1).$$

Proof. This is elementary matrix algebra. □

Remarks.

(i) Perturbing the reference configuration slightly by $\Omega_h \to (\mathrm{Id} + hB_0)\Omega_h$ where B_0 is a constant 3×3-matrix, we can minimize over in-plane deformations and assume that

$$\mathbf{b}_1 = \int \mathcal{M}(t)\mathbf{b}(t) = 0.$$

(ii) For stress free layers, i.e., $B \equiv 0$, we obviously obtain $F_0 = 0$, $\alpha = 0$ and $\mathbf{a}_{\min} = -\mathcal{M}_1^{-1}\mathcal{M}_2\mathbf{f}$.

(iii) If $Q_2(t,\cdot)$ does not depend on t, then $Q_2^* = \frac{1}{12}Q_2$ and $F_0 = -12\int tB(t)$. If in addition $B \equiv 0$, this leads to the formula

$$\bar{Q}_2(F) = \frac{1}{12}Q_2(F),$$

i.e., we recover Kirchhoff's plate theory for homogeneous materials as derived in [6].

4 Low energy sequences and energy minimizers

The main task of this section is to investigate the convergence of the rescaled nonlinear strain

$$\frac{1}{h}\left(\left((\nabla_h y^{(h)})^T\nabla_h y^{(h)}\right)^{1/2} - \mathrm{Id}\right)$$

on low energy sequences. In contrast to the homogeneous case, the limiting strain will in general not be linear in x_3 any more.

Recall that for $F \in \mathbb{R}^{2\times 2}$, $\hat{F}$ is the 3×3-matrix $\hat{F} = \sum_{i,j=1}^{2} F_{ij} e_i \otimes e_j$. The last column of the matrix $\frac{1}{2}(B+B^T)$ will be denoted $b^s_{\cdot 3}$.

Theorem 4.1 *Assume $\nabla_h y^{(h)}$ converges to $(\nabla' y, b)$ in $L^2(\Omega_1)$ and has limiting bending energy $h^{-2} I^h(\nabla_h y^{(h)}) = I^0(y) < \infty$. Then $y \in \mathcal{A}$ and*

$$\begin{aligned}
&\frac{1}{h}\left(\left((\nabla_h y^{(h)})^T\nabla_h y^{(h)}\right)^{1/2} - \mathrm{Id}\right)\\
&\quad \to x_3\hat{\mathrm{II}} + \hat{A}_{\min} + \frac{(c_{\min} + b^s_{\cdot 3})\otimes e_3 + e_3 \otimes (c_{\min} + b^s_{\cdot 3})}{2}
\end{aligned}$$

in $L^2(\Omega_1)$. As before, $A_{\min}$ is given uniquely by (4), and and $c_{\min}$ is the unique minimizer in $\mathbb{R}^3$ of

$$\min_c Q_3\left(\hat{A}_{\min} + x_3\hat{\mathrm{II}} + B + \frac{c\otimes e_3 + e_3\otimes c}{2}\right)$$

depending on $A_{\min}$ and II.

Proof. Inspect the proof of the lower bound in Theorem 3.2 (i): On low energy sequences, all the inequalities in

$$\begin{aligned}
I^0(y) &= \limsup_{h\to\infty} \frac{1}{h^2}\int_{\Omega_1} W(x_3, \nabla_h y^{(h)})\\
&\geq \limsup_{h\to\infty} \frac{1}{h^2}\int_{\Omega_1} \chi_h W_0(x_3, \nabla_h y^{(h)}(\mathrm{Id} + hB^{(h)}))\\
&\geq \limsup_{h\to\infty} \frac{1}{2}\int_{\Omega_1} Q_3(x_3, \chi_h A^{(h)})\\
&\geq \frac{1}{2}\int_{\Omega_1} Q_3(x_3, G(x) + B(x_3))\\
&\geq \frac{1}{2}\int_{\Omega_1} Q_2(x_3, \check{G}(x',0) + x_3\mathrm{II}(x') + \frac{1}{2}(\check{B}(x_3) + \check{B}^T(x_3)))\\
&\geq \frac{1}{2}\int_{\Omega_1} Q_2(x_3, A_{\min}(x') + x_3\mathrm{II}(x') + \frac{1}{2}(\check{B}(x_3) + \check{B}^T(x_3)))
\end{aligned} \tag{5}$$

are in fact equalities. So first from the last inequality we deduce

$$\frac{(\check{G}(x',0))^T + \check{G}(x',0)}{2} = A_{\min}(x') \quad \text{a.e.}$$

and then, from the last but one,

$$\begin{aligned}
&\frac{(G+B)^T+(G+B)}{2} \\
&\quad = x_3\hat{\mathrm{I\!I}}(x') + \hat{A}_{\min}(x') + \frac{1}{2}(\check{B}+\check{B}^T)\hat{} + \frac{\tilde{c}_{\min}(x)\otimes e_3 + e_3\otimes \tilde{c}_{\min}(x)}{2} \\
&\quad = x_3\hat{\mathrm{I\!I}}(x') + \hat{A}_{\min}(x') + \frac{1}{2}(B+B^T) + \frac{c_{\min}(x)\otimes e_3 + e_3\otimes c_{\min}(x)}{2}, \quad (6)
\end{aligned}$$

where $\tilde{c}_{\min} \in \mathbb{R}^3$ is the unique minimizer of

$$\min_c Q_3\left(\hat{A}_{\min} + x_3\hat{\mathrm{I\!I}} + (\check{B})\hat{} + \frac{c\otimes e_3 + e_3\otimes c}{2}\right).$$

In fact, by Assumption 1.1, the mappings $Q_3(t,\cdot)$ are uniformly strictly convex on symmetric matrices uniformly in t: there exists $\gamma > 0$ such that for all $F_0, F \in \mathbb{R}^{3\times 3}_{\mathrm{sym}}$ and a.e. $t \in (-1/2, 1/2)$,

$$D^2Q_3(t,F_0)(F,F) = 2Q_3(t,F) \geq \gamma |F|^2.$$

By a standard argument (see, e.g., [4], page 21) we therefore deduce from the third (in-)equality above and $\chi_h A^{(h)} \rightharpoonup G + B$

$$\chi_h \frac{(A^{(h)})^T + A^{(h)}}{2} \to \frac{(G+B)^T + (G+B)}{2} \qquad (7)$$

strongly in L^2.

Now, since on $\{\chi = 1\}$

$$A^{(h)} = \frac{1}{h}(R^{(h)})^T \nabla_h y^{(h)}(\mathrm{Id} + hB^{(h)}) - \frac{1}{h}\mathrm{Id}$$

with $hA^{(h)} \leq \sqrt{h} + Ch$, $|hB^{(h)}| \leq Ch$ and thus

$$(R^{(h)})^T\nabla_h y^{(h)} = (\mathrm{Id} + hA^{(h)})(\mathrm{Id} + hB^{(h)})^{-1} = \mathrm{Id} + hA^{(h)} - hB^{(h)} + \mathcal{O}(h^{3/2}),$$

we obtain

$$\begin{aligned}
(\nabla_h y^{(h)})^T\nabla_h y^{(h)} &= ((R^{(h)})^T\nabla_h y^{(h)})^T R^{(h)}\nabla_h y^{(h)} \\
&= \mathrm{Id} + (hA^{(h)} - hB^{(h)})^T + hA^{(h)} - hB^{(h)} \\
&\quad + h^2(A^{(h)})^T A^{(h)} + \mathcal{O}(h^{3/2})
\end{aligned}$$

and

$$\begin{aligned}
&\left|\left((\nabla_h y^{(h)})^T\nabla_h y^{(h)}\right)^{1/2} - \left(\mathrm{Id} + \frac{h}{2}\left((A^{(h)} - B^{(h)})^T + A^{(h)} - B^{(h)}\right)\right)\right| \\
&\quad \leq C\left(|hA^{(h)}|^2 + h^{3/2}\right).
\end{aligned}$$

Multiplying by $\frac{1}{h}\chi_h$ yields

$$\begin{aligned}
&\left\|\chi_h\left(\frac{\left((\nabla_h y^{(h)})^T\nabla_h y^{(h)}\right)^{1/2} - \mathrm{Id}}{h} - \frac{(A^{(h)} - B^{(h)})^T + A^{(h)} - B^{(h)}}{2}\right)\right\|_{L^2} \\
&\quad \leq C\|A^{(h)}\|_{L^2}\|\chi_h hA^{(h)}\|_{L^\infty} + C\sqrt{h}.
\end{aligned}$$

Since $A^{(h)} \rightharpoonup G+B$ in L^2 and $\|\chi_h h A^{(h)}\|_{L^\infty} \leq 2\sqrt{h}$, we have from (7)

$$\chi_h \frac{\left((\nabla_h y^{(h)})^T \nabla_h y^{(h)}\right)^{1/2} - \mathrm{Id}}{h} \to \frac{(G+B)^T + G + B}{2} - \frac{B^T + B}{2}$$

in L^2.

To remove χ_h, we estimate, using that $|\sqrt{F^TF} - \mathrm{Id}| \leq \mathrm{dist}(F, SO(3)) \leq C(\sqrt{W(x_3, F)} + h)$ for $F \in \mathbb{R}^{3\times 3}$,

$$\begin{aligned}
&\limsup_{h\to\infty} \int_{\Omega_1} (1-\chi_h) \left| \frac{\left((\nabla_h y^{(h)})^T \nabla_h y^{(h)}\right)^{1/2} - \mathrm{Id}}{h} \right|^2 \\
&\leq \limsup_{h\to\infty} \frac{C}{h^2} \int_{\Omega_1} (1-\chi_h) \left(W(x_3, \nabla_h y^{(h)}) + h^2 \right) \\
&= \limsup_{h\to\infty} \frac{C}{h^2} \int_{\Omega_1} (1-\chi_h) W(x_3, \nabla_h y^{(h)}) \\
&= 0
\end{aligned}$$

since the first inequality in (5) is an equality. This finishes the proof by (6). □

For applications it is particularly interesting to investigate the minimizers of the limiting energy functional I^0 under free boundary conditions. The following proposition was proved in [19] under slightly different conditions. We include the short proof for the convenience of the reader.

Proposition 4.2 *The minimizers of I^0 are cylinders, i.e., their second fundamental form is constant.*

Proof. Minimizers satisfy $\mathrm{II} \in \mathcal{N}$ a.e., where $\mathcal{N}$ is the set of minimizers $F \in \mathbb{R}^{2\times 2}_{\mathrm{sym}}$ of $Q_2^*(F - F_0)$ subject to $\det(F) = 0$. If for $F \in \mathcal{N}$, $Q_2^*(F - F_0) = c$, then $\mathcal{N}$, viewed as a subset of $\mathbb{R}^3$, is the intersection of the cone $\{\mathbf{f} : \mathbf{f}_1 \mathbf{f}_2 - \mathbf{f}_3^2 = 0\}$ with the ellipsoid $\{(\mathbf{f} - \mathbf{f}_0)^T \mathcal{M}_0 (\mathbf{f} - \mathbf{f}_0) = c\}$. It is easily seen that, since $\mathcal{M}_0$ is positive definite, any two elements of $\mathcal{N}$ are linearly independent, in particular $0 \notin \mathcal{N}$. As

$$\mathrm{II}(\Phi_\gamma(t,s)) = \frac{\lambda(t)}{1 - s\kappa(t)} \mu(t) \otimes \mu(t)$$

on covered domains, this implies that $\kappa \equiv 0$, and therefore also $\mu \equiv$ const. and $\lambda \equiv$ const. in a neighborhood of any point $x \in S$. □

Remarks.

(i) This is essentially the same reasoning as in [19]. There it is also shown that minimizers need not be unique. However, under the more restrictive assumptions in [19], F_0 turns out to be a multiple of the identity matrix which implies that the optimal radius of energy minimizing cylinders is uniquely determined (see [19] for details). This is no longer true under our general assumptions here. Generically, however, minimizers are unique up to rotations.

(ii) A similar argument shows that for fixed winding direction ($\mu \equiv \mu_0$, $\kappa \equiv 0$) the optimal radius λ^{-1} of a cylinder is unique.

5 An application to nanoscrolls

Propositions 3.5 and 4.2 induce an algorithm to determine optimal shapes of thin stressed multilayers: One only has to minimize $Q_2^*(\cdot - F_0)$ with respect to the constant second fundamental form $\lambda n \otimes n$, $|n| = 1$. To deduce the optimal radius for fixed winding direction n simply amounts to solving a linear equation. Then, in order to optimize with respect to the direction n, one needs to solve an algebraic equation. For general energy functions the calculations quickly become very messy, so we confine ourselves to a specific example to illustrate our results.

Consider the BGaAs/InGaAs bilayer discussed in [17], where the thickness of the BGaAs layer is approximately 0.8 times the thickness of the InGaAs layer. The linearized energy within the layers is of the form

$$\begin{aligned} Q_3(F) &= C_{11}\left(F_{11}^2 + F_{22}^2 + F_{33}^2\right) + C_{44}\left(F_{12}^2 + F_{23}^2 + F_{31}^2\right) \\ &\quad + 2C_{12}\left(F_{11}F_{22} + F_{22}F_{33} + F_{33}F_{11}\right), \end{aligned}$$

and therefore Q_2 is given by

$$Q_2(F) = \left(C_{11} - \frac{C_{12}^2}{C_{11}}\right)\left(F_{11}^2 + F_{22}^2\right) + C_{44}F_{12}^2 + 2\left(C_{12} - \frac{C_{12}^2}{C_{11}}\right)F_{11}F_{22}.$$

For InGaAs, resp., BGaAs, we have (in GPa)

$$\begin{aligned} C_{11}^{\mathrm{InGaAs}} &= 105.8, & & & C_{11}^{\mathrm{BGaAs}} &= 123.0, \\ C_{12}^{\mathrm{InGaAs}} &= 50.4, & &\text{resp.,} & C_{12}^{\mathrm{BGaAs}} &= 54.0, \\ C_{44}^{\mathrm{InGaAs}} &= 52.2, & & & C_{44}^{\mathrm{BGaAs}} &= 59.6 \end{aligned}$$

(see, e.g., [17]). So $Q_2(t, \cdot)$ is represented by the 3×3-matrix

$$\mathcal{M}(t) = \begin{pmatrix} 81.8 & 26.4 & 0 \\ 26.4 & 78.2 & 0 \\ 0 & 0 & 52.2 \end{pmatrix}, \quad \text{resp.,} \quad \begin{pmatrix} 99.3 & 30.3 & 0 \\ 30.3 & 99.3 & 0 \\ 0 & 0 & 59.6 \end{pmatrix},$$

for $-1/2 < t < 1/18$ resp., $1/18 < t < 1/2$, whence

$$Q_2^*(F) \approx 7.5\left(F_{11}^2 + F_{22}^2\right) + 4.6F_{12}^2 + 4.7F_{11}F_{22}.$$

The lattice constants are 0.58031nm for InGaAs resp. 0.56313nm for BGaAs. Since the film is grown epitaxially, the flat reference configuration is under stress. The misfit being of the order $\sim 1\%$, our theory applies to films whose aspect ratio is of the order $\sim 1\%$. To calculate the optimal radius, w.l.o.g. we let $h = 1/100$ and $B(t) \approx 1.50 \cdot \mathrm{Id}$ resp. $1.51 \cdot \mathrm{Id}$ for $-1/2 < t < 1/18$ resp. $1/18 < t < 1/2$ (so that $\mathbf{b}_1 = 0$, $\mathbf{b}_2 \approx (43.44, 43.44, 0)^T$).

Assuming the film rolls up in $(1,0,0)$-direction, i.e., $\mathrm{II} = \mathrm{diag}(\kappa, 0)$, F_0 turns out to be $-4.49 \cdot \mathrm{Id}$. Now minimizing the energy with respect to κ yields an energetically optimal cylinder with BGaAs in its interior of radius $R = 1/|\kappa| \approx 0.17$. Since the aspect ratio is $h = 0.01$, assuming that the film is of microscopic thickness d (in nanometers), we obtain

$$R_{\mathrm{opt}}(d) \approx 17d \text{ nm}.$$

for the optimal radius in $(1,0,0)$-direction. This is in good agreement with the measurements in [17].

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