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multi-layers

by

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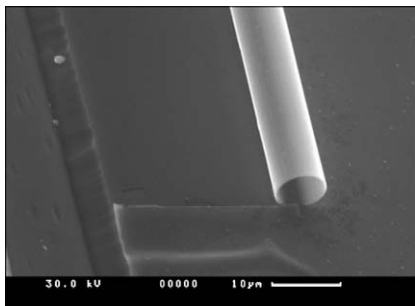
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Abstract

We derive an effective plate theory for internally stressed thin elastic layers as are used e.g. in the fabrication of nano- and microscrolls. The shape of the energy minimizers of the effective energy functional is investigated without a priori assumptions on the geometry. For configurations in two dimensions (corresponding to Euler-Bernoulli theory) we also take into account a non-interpenetration condition for films of small but non-vanishing thickness.

1 Introduction

In the present paper we investigate thin elastic films whose (flat) reference configuration $S \times (-h/2, h/2)$, $h \ll 1$, is stressed due to some small mismatch of equilibria in the x_3 -direction. This mismatch can be caused e.g. by a temperature gradient or is due to differing lattice constants for a film consisting of layers of different materials. If such a 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 of nanotubes (nanoscrolls, nanobelts, etc.) by growing bi-layers of films with mismatching lattice constants and relieving them from the substrate (see e.g. [8, 4]).



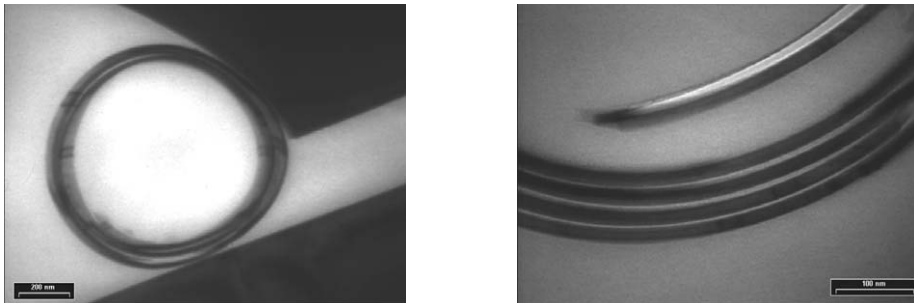
SEM image of a multi-layer tube (courtesy of H. Paetzelt, V. Gottschalch, J. Bauer, H. Herrnberger, G. Wagner, Universität Leipzig, see [4])

In the physics literature so far (mostly linear) three-dimensional elasticity theory is used to describe the energy of such objects (cf. e.g. [5], [9]); and in order to discuss the geometry of energy minimizers, one uses appropriate ansatz functions (cylinders, belts, etc.) and optimizes with respect to certain parameters (e.g. radius, winding direction).

Our aim is first to derive an effective plate theory from three-dimensional nonlinear elasticity theory rigorously as a suitable Γ -limit in the bending energy regime for $h \rightarrow 0$, see section 2. (This is the appropriate energy scale for objects as nanoscrolls etc. mentioned above.) We have not chosen the most general model of a heterogeneous film, so that in fact this derivation is a rather straightforward extension of the results in [2], yet it models thermally stressed films of a single material or stress induced due to mismatching lattice constants of materials with similar elastic constants (as e.g. in [4]) reasonably well. We do not re-derive all the steps needed from [2]; rather we focus on those parts of the derivation that are new. (For more general models, the adaptation of the methods in [2] is not so straightforward, however still possible as will be detailed elsewhere.) The outcome is an integral expression for the energy in terms of the second fundamental form of the film surface similar as in [2]. However, the reference state is not a state of minimal energy any more; the thin film can reduce energy by rolling up.

The following section 3 is devoted to an ansatz free study of minimal energy configurations (for free boundary conditions). An elementary observation shows that indeed one cannot do better than cylinders. Using results of Pakzad (cf. [6]) on the developability of $W^{2,2}$ isometric immersions, it is proved that in fact every minimizer must be a cylinder. We also describe the set of optimal winding directions and radii in detail.

While in the previous section admissible functions were all $W^{2,2}$ isometric immersions, in section 4 we will also take into account a non-interpenetration condition for films of small but non-vanishing thickness. Motivated by the results of section 3, we study Euler-Bernoulli type deformations that can be described by a planar curve of length L , say. We investigate the minimal energy configurations in the most interesting regime $L \sim h^{-1}$ in detail and find non-trivial minimal energy configurations. According to the boundary conditions chosen, they will turn out to be spirals or double spirals.



TEM cross sectional images of a BGaAs 7nm / InGaAs 9 nm two layer system rolled up in $(1, 0, 0)$ direction (courtesy of H. Paetzelt, V. Gottschalch, J. Bauer, H. Herrnberger, G. Wagner, Universität Leipzig, see [4])

2 Bending energy for strained multi-layers

Assume that $\Omega_h = S \times (-h/2, h/2) \subset \mathbb{R}^3$, $S \subset \mathbb{R}^2$ a bounded Lipschitz domain, is the reference configuration of a thin film. If the material is homogeneous, the

elastic energy of a deformation $v : \Omega_h \rightarrow \mathbb{R}^3$ is given by

$$\int_{\Omega_h} W(\nabla v(z)) dz.$$

Here $W : \mathbb{R}^{3 \times 3} \rightarrow \mathbb{R}$ is the stored energy function which shall satisfy the following hypotheses:

- (i) W is continuous, C^2 in a neighborhood of $SO(3)$.
- (ii) W is frame indifferent: $W(F) = W(RF)$ for all $F \in \mathbb{R}^{3 \times 3}$ and all $R \in SO(3)$.
- (iii) $W(F) \geq C \text{dist}^2(F, SO(3))$ for all $F \in \mathbb{R}^{3 \times 3}$, $W(F) = 0$ if $F \in SO(3)$.

For strained thin films we will consider potentials varying in x_3 -direction

$$\int_{\Omega_h} W(x_3, \nabla v(z)) dz.$$

In detail, we are interested in the following two regimes:

$$W(x_3, F) := W_0 \left(\frac{1}{a(x_3)} F \right) \quad (1)$$

for $a : (-\delta, \delta) \rightarrow \mathbb{R}$ differentiable at 0 and

$$W(x_3, F) := W^{(h)}(x_3, F) := W_0 \left(\frac{1}{1 + hf(x_3/h)} F \right) \quad (2)$$

for $f \in L^\infty((-1/2, 1/2); \mathbb{R})$ where W_0 satisfies the above hypotheses (i)-(iii). Here (1) serves as a model of a thermally strained film of a single material whereas (2) describes films consisting of different layers internally stressed due to mismatching energy wells. In order to avoid stretching energies in the reference configurations we assume that $a(0) = 1$ resp. $f \in L^\infty((-1/2, 1/2); \mathbb{R})$ satisfies $\int_{-1/2}^{1/2} f(t) dt = 0$.

To treat both cases simultaneously, we will from on – slightly more general – assume that W is of the form

$$W(x_3, F) := W^{(h)}(x_3, F) := W_0 \left(\frac{1}{1 + hf^{(h)}(x_3/h)} F \right) \quad (3)$$

with $f^{(h)}(t) = f(t) + o(1)$ for $f(t) = a'(0)t$, a as in (1), resp. f as in (2). Changing variables $y(x', x_3) = v^{(h)}(x', hx_3)$, the 3-dimensional energy functional is

$$E^{(h)}(v^{(h)}) = \int_{\Omega_h} W(x_3, \nabla v^{(h)}(x)) dx = h \int_{\Omega_1} W(hx_3, \nabla' y(x), \frac{1}{h} y_{,3}(x)) dx \quad (4)$$

for $y \in W^{1,2}(\Omega_1, \mathbb{R}^3)$.

The following compactness result is proved in [2] in case $W = W_0$.

Theorem 2.1 (Compactness) *Let the energy be of the form (4) with W as in (3). Suppose a sequence $y^{(h)} \subset W^{1,2}(\Omega; \mathbb{R}^3)$ has finite bending energy, i.e.*

$$\limsup_{h \rightarrow \infty} \frac{1}{h^2} \int_{\Omega_1} W \left(hx_3, \nabla' y^{(h)}(x), \frac{1}{h} y_{,3}^{(h)}(x) \right) dx < \infty.$$

Then $\nabla_h y^{(h)} = (\nabla' y^{(h)}, \frac{1}{h} y_{,3}^{(h)})$ is precompact in $L^2(\Omega)$ as $h \rightarrow 0$: there exists a subsequence (not relabeled) such that

$$\nabla_h y^{(h)} \rightarrow (\nabla' y, b) \in L^2(\Omega),$$

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

Proof. This follows directly from the homogeneous case (cf. [2]) since

$$\limsup_{h \rightarrow \infty} \frac{1}{h^2} \int_{\Omega_1} \text{dist}^2 \left(\nabla_h y^{(h)}, SO(3) \right) dx < \infty :$$

By hypothesis (iii) on W_0 , $\text{dist}^2(F, SO(3))$ is bounded by

$$\begin{aligned} & 2 \text{dist}^2 \left(\frac{1}{1 + hf^{(h)}(x_3)} F, SO(3) \right) + 2 \left| F - \frac{1}{1 + hf^{(h)}(x_3)} F \right|^2 \\ & \leq \frac{2}{C} W(hx_3, F) + 2 \left(\frac{1}{1 + hf^{(h)}(x_3)} - 1 \right)^2 |F|^2 \end{aligned}$$

for all $x_3 \in (-1/2, 1/2)$. Noting that $(\frac{1}{1 + hf^{(h)}(x_3)} - 1)^2 = \mathcal{O}(h^2)$ and $|F| \leq C(1 + \text{dist}(F, SO(3)))$ implies

$$\text{dist}^2(F, SO(3)) \leq C' (W(hx_3, F) + h^2).$$

□

The main result of this section is the following derivation of limiting bending energies by Γ -convergence. For a deformation $y \in W^{2,2}(S; \mathbb{R}^3)$ we denote by Π its second fundamental form: $\Pi_{ij} = y_{,i} \cdot b_{,j}$, $b = y_{,1} \wedge y_{,2}$. The set of $W^{2,2}$ -isometric immersions is denoted

$$\mathcal{A} := \{y \in W^{2,2}(S; \mathbb{R}^3) : |y_{,1}| = |y_{,2}| = 1, y_{,1} \cdot y_{,2} = 0\}$$

(viewed as a set of functions in $W^{2,2}(\Omega_1; \mathbb{R}^3)$ independent of x_3 whenever convenient). Depending on Q_3 , the Hessian of W_0 at the identity, we define a relaxed quadratic form on 2×2 -matrices by

$$Q_2(F) = \min_{c \in \mathbb{R}^3} Q_3(\hat{F} + c \otimes e_3)$$

where \hat{F} is the 3×3 -matrix $\sum_{i,j=1}^2 F_{ij} e_i \otimes e_j$.

Theorem 2.2 (Γ -limit) *The functionals $\frac{1}{h^3}E^{(h)}$ Γ -converge to I^0 in $W^{1,2}$ as $h \rightarrow 0$. The two-dimensional limiting energy functional is given by*

$$I^0(y) = \begin{cases} \frac{1}{24} \int_S Q_2(\Pi - a_1 \text{Id}) - a_2 \, dx & \text{for } y \in \mathcal{A}, \\ \infty & \text{else} \end{cases} \quad \text{where}$$

$$a_1 = 12 \int_{-1/2}^{1/2} t f(t) dt \quad \text{and}$$

$$a_2 = \left(6 \left(\int_{-1/2}^{1/2} t f(t) dt \right)^2 - \frac{1}{2} \int_{-1/2}^{1/2} f^2(t) dt \right) Q_2(\text{Id}).$$

If W is as in (1), this reads

$$I^0(y) = \begin{cases} \frac{1}{24} \int_S Q_2(\Pi - a'(0) \text{Id}) dx & \text{for } y \in \mathcal{A}, \\ \infty & \text{else.} \end{cases}$$

Proof. The proof closely follows the proof of theorem 6.1 in [2].

(i) *Lower bound.* For sequences $(y^{(h)})$ with bounded energy converging to y , it is shown in [2] that one can construct a piecewise constant approximation $R^{(h)} : S'_h \subset S \rightarrow \mathbb{R}^{3 \times 3}$ to $\nabla_h y^{(h)}$ such that (for a subsequence)

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

If G' denotes the 2×2 -matrix obtained by omitting the third row and third column, it is further shown that

$$G'(x', x_3) = G'(x', 0) + x_3 \Pi(x'), \quad \Pi = (\nabla' y)^T \nabla' b \quad (5)$$

and

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

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

It remains to estimate the energy in terms of G . This is done in analogy to [2] by a careful Taylor-expansion of W_0 around the identity: $W_0(\text{Id} + A) = \frac{1}{2} Q_3(A) + \eta(A)$ with $\eta(A)/|A|^2 \rightarrow 0$ as $|A| \rightarrow 0$ and set $\omega(t) := \sup_{|A| \leq t} |\eta(A)|$.

Frame indifference leads to

$$\begin{aligned} \frac{1}{h^2} \int_{\Omega} W(hx_3, \nabla_h y^{(h)}) dx &\geq \frac{1}{h^2} \int_{\Omega} \chi_h W_0 \left(\frac{1}{1 + hf^{(h)}(x_3)} (R^{(h)})^T \nabla_h y^{(h)} \right) dx \\ &= \frac{1}{h^2} \int_{\Omega} \chi_h W_0 \left(\text{Id} + hA^{(h)} \right) dx \\ &\geq \int_{\Omega} \frac{1}{2} \chi_h Q_3 \left(A^{(h)} \right) - \frac{1}{h^2} \chi_h \omega \left(|hA^{(h)}| \right) dx \end{aligned}$$

where

$$A^{(h)} = \frac{\frac{1}{1 + hf^{(h)}(x_3)} - 1}{h} \text{Id} + \frac{1}{1 + hf^{(h)}} G^{(h)}, \quad \chi_h A^{(h)} \rightharpoonup -f(x_3) \text{Id} + G \quad \text{in } L^2(\Omega).$$

Using lower semicontinuity of Q_3 , $hA^{(h)} \rightarrow 0$ in L^∞ , and $Q_3(F) \geq Q_2(F')$, as in [2] we find that

$$\liminf_{h \rightarrow 0} \frac{1}{h^2} \int_{\Omega} W(hx_3, \nabla_h y^{(h)}) dx \geq \frac{1}{2} \int_{\Omega} Q_2(G'(x', 0) + x_3 \Pi(x') - f(x_3) \text{Id}') .$$

Because of $\int_{-1/2}^{1/2} x_3 dx_3 = \int_{-1/2}^{1/2} f(x_3) dx_3 = 0$, integrating over x_3 yields

$$\begin{aligned} & \liminf_{h \rightarrow 0} \frac{1}{h^2} \int_{\Omega} W(hx_3, \nabla_h y^{(h)}) dx \\ & \geq \frac{1}{24} \int_S Q_2(\Pi(x)) dx - c_1 \int_S Q_2(\Pi(x), \text{Id}) dx + \frac{c_2}{2} \int_S Q_2(\text{Id}) dx \\ & = \frac{1}{24} \int_S Q_2(\Pi(x) - 12c_1 \text{Id}) dx - \left(6c_1^2 - \frac{1}{2}c_2 \right) Q_2(\text{Id}) dx \end{aligned}$$

where $c_1 = \int_{-1/2}^{1/2} x_3 f(x_3) dx_3$, $c_2 = \int_{-1/2}^{1/2} f^2(x_3) dx_3$.

(ii) *Attainment of the lower bound.* Let $y \in \mathcal{A}$. As in [2] we choose approximations y^λ and b^λ to y and $b = y_{,1} \wedge y_{,2}$ (extended to maps in $W^{2,2}(\mathbb{R}^2, \mathbb{R}^3)$ resp. $W^{1,2}(\mathbb{R}^2, \mathbb{R}^3)$) such that

$$\|\nabla^2 y^\lambda\|_{L^\infty}, \|\nabla b^\lambda\|_{L^\infty} \leq \lambda, \quad |S^\lambda| \leq C \frac{\omega(\lambda)}{\lambda^2}$$

where

$$S^\lambda = \{x \in \mathbb{R}^2 : y(x) \neq y^\lambda(x) \text{ or } b(x) \neq b^\lambda(x)\}, \quad \omega(\lambda) \rightarrow 0 \text{ as } \lambda \rightarrow \infty.$$

Let $\lambda_h = c/h$. More generally than in [2] we define

$$y^{(h)}(x', x_3) = y^{\lambda_h}(x') + hx_3 b^{\lambda_h}(x') + h^2 D(x', x_3)$$

for $D(x', x_3) = \int_0^{x_3} d(x', t) dt$, $d \in C^1(\Omega_1; \mathbb{R}^3)$. (If W is as in (1), we can use trial functions with $d(x', x_3) = x_3 d(x')$ as in [2].) Furthermore denote $R(x') := (\nabla' y(x'), b(x'))$ and

$$\begin{aligned} R^T \left(\nabla' y^{(h)}, \frac{1}{h} y_{,3}^{(h)} \right) &= R^T \left((\nabla' y^{\lambda_h}, b^{\lambda_h}) + h(x_3 \nabla' b^{\lambda_h}, d) + h^2 (\nabla' D, 0) \right) \\ &=: \text{Id} + B^{(h)}. \end{aligned}$$

Similar as above let

$$A^{(h)} = \left(\frac{1}{1 + hf^{(h)}(x_3)} - 1 \right) \text{Id} + \frac{1}{1 + hf^{(h)}(x_3)} B^{(h)}.$$

On the good set $S \setminus S^{\lambda_h}$, we have $R^T(\nabla' y^{\lambda_h}, b^{\lambda_h}) = \text{Id}$ and

$$|B^{(h)}| \leq C(h\lambda_h + h + h^2) \leq C(c + h_0 + h_0^2) \quad \text{for all } h \leq h_0.$$

An analogous estimate holds for $|A^{(h)}|$. Choosing c small enough and using that $W_0(\text{Id} + A) \leq C \text{dist}^2(\text{Id} + A, SO(3))$ in a neighborhood of $SO(3)$ (and letting χ_h denote the characteristic function of $S \setminus S^{\lambda_h}$), we obtain for all $h \leq h_0$

$$\begin{aligned} \frac{1}{h^2} \chi_h W_0(\text{Id} + A^{(h)}) &\leq \frac{C}{h^2} \chi_h |A^{(h)}|^2 \\ &\leq \frac{2C}{h^2} \chi_h \left(3 \left(\frac{1}{1 + hf^{(h)}(x_3)} - 1 \right)^2 + \left| \frac{1}{1 + hf^{(h)}(x_3)} B^{(h)} \right|^2 \right) \\ &\leq C \left(\left(\frac{\frac{1}{1 + hf^{(h)}(x_3)} - 1}{h} \right)^2 + \frac{|(\nabla' b, d)|^2 + h^2 |\nabla' D|^2}{|1 + hf^{(h)}(x_3)|} \right) \\ &\leq C(1 + |(\nabla' b, d)|^2 + h_0^2 |\nabla' D|^2) \in L^1(\Omega). \end{aligned}$$

Furthermore,

$$\frac{1}{h^2} \chi_h W_0(\text{Id} + A^{(h)}) \rightarrow \frac{1}{2} Q_3(-f(x_3) + R^T(x_3 \nabla' b, d)) dx$$

in measure. So, by dominated convergence,

$$\begin{aligned} \frac{1}{h^2} \int_{\Omega} \chi_h W \left(x_3, \nabla' y^{(h)}, \frac{1}{h} y_{,3}^{(h)} \right) dx &= \frac{1}{h^2} \int_{\Omega} \chi_h W_0(\text{Id} + A^{(h)}) dx \\ &\rightarrow \frac{1}{2} \int_{\Omega} Q_3(-f(x_3) + R^T(x_3 \nabla' b, d)) dx. \end{aligned}$$

On the bad set S^{λ_h} , as shown in [2], $\text{dist}(\text{Id} + B^{(h)}, SO(3)) \leq C$, thus also $\text{dist}(\text{Id} + A^{(h)}, SO(3)) \leq C$. So

$$\frac{1}{h^2} \int_{\Omega} (1 - \chi_h) W \left(x_3, \nabla' y^{(h)}, \frac{1}{h} y_{,3}^{(h)} \right) dx \leq C \frac{|S^{\lambda_h}|}{h^2} \rightarrow 0 \quad (h \rightarrow 0).$$

Together with our previous estimate we find

$$\frac{1}{h^2} \int_{\Omega} W \left(x_3, \nabla' y^{(h)}, \frac{1}{h} y_{,3}^{(h)} \right) dx \rightarrow \int_{\Omega} Q_3(-f(x_3) + R^T(x_3 \nabla' b, d)) dx.$$

To finish the proof as in [2], it suffices to note that

$$d_{\min}(x', x_3) := \text{argmin} Q_3(-f(x_3) + R^T(x_3 \nabla' b, d)) \in L^2$$

and

$$Q_3(-f(x_3) + R^T(x_3 \nabla' b, d_{\min})) = Q_2(-f(x_3) + x_3 \Pi) :$$

(ii) then follows by a standard approximation procedure. \square

Remarks.

- (i) By standard arguments in Γ -convergence the above results imply convergence of (almost) minimizers. Note also that appropriate body forces and boundary conditions can be included in the above analysis.

- (ii) Due to the assumptions made on W_0 , Q_3 is positive semidefinite and positive definite when restricted to symmetric matrices. It is not hard to see that this implies that Q_2 is positive definite on symmetric 2×2 -matrices.
- (iii) Consider deformations of Euler-Bernoulli type. Suppose $S = (0, L) \times (0, w)$ and we are only considering deformations y in the $x_1 - x_3$ plane, i.e. $y(x_1, x_2, \cdot) = (f_1(x_1), x_2, f_2(x_1))$. The class of isometric deformations can then be described by the curve $\gamma \in W^{2,2}((0, L); \mathbb{R}^2)$, $\gamma(t) = (f_1(t), f_2(t))$, where $|\frac{d\gamma}{dt}| \equiv 1$. The second fundamental form is given by $\text{II}_{ij} = -\kappa$ for $i = j = 1$ and $\text{II}_{ij} = 0$ else. Here κ is the curvature of the curve γ . This leads to a limiting energy

$$E(\gamma) = \alpha_1 \int_0^L (\kappa(t) - \alpha_2)^2 + \alpha_3 dt \quad (6)$$

for constants $\alpha_1 > 0, \alpha_2, \alpha_3 \in \mathbb{R}$.

3 Minimal energy configurations in 3D

As seen in the previous section, thin strained multi-layers deformed by $y : S \subset \mathbb{R}^2 \rightarrow \mathbb{R}^3$ have bending energy

$$E(y) = \begin{cases} \int_S Q(\text{II} - c_0 \text{Id}) + c'_0 dx & \text{for } y \in \mathcal{A} \\ \infty & \text{else} \end{cases} \quad (7)$$

for some Q , positive definite on symmetric matrices, $c_0, c'_0 \in \mathbb{R}$. In the following we will address the question what one can say about the set of energy minimizers of (7)

$$\mathcal{M} = \{u \in W^{2,2}(S; \mathbb{R}^3) : E(u) = \min_{y \in W^{2,2}(S; \mathbb{R}^3)} E(y)\}.$$

Note that energy minimizers in general will be non-unique. For isotropic material, e.g., every winding direction will be equally well suited to reduce energy.

We will, slightly more general, only assume that Q is any positive semidefinite quadratic form on symmetric 2×2 -matrices. We start with the following observation.

Lemma 3.1 *Let $\mathcal{N} := \text{argmin}\{Q(F - c_0 \text{Id}) : F \text{ singular and symmetric}\}$. Then $u \in \mathcal{M}$ if and only if $\text{II} \in \mathcal{N}$ a.e. In particular, \mathcal{M} contains cylinders.*

Proof. Any u of finite energy is an $W^{2,2}$ -isometry, so $\det(\text{II}) = 0$ (see [6]). Since the set of symmetric singular 2×2 -matrices is $\mathbb{R} \cdot \{n \otimes n : n \in \mathbb{R}^2, |n| = 1\}$ which is just the set of (constant) fundamental forms of cylinders, we can – and therefore have to – minimize E in (7) by minimizing the integrand pointwise subject to II being singular and symmetric. Choosing u to be a cylinder with $\text{II} \equiv F_0 \in \mathcal{N}$ constant, u lies in \mathcal{M} . \square

In the following we will identify a symmetric matrix $F = (F_{ij})$ with the vector $(F_{11}, F_{22}, F_{12})^T \in \mathbb{R}^3$. Accordingly, Q will be viewed as a positive semidefinite quadratic form on \mathbb{R}^3 with $\text{rank}(Q)$ denoting the rank of the corresponding

symmetric 3×3 -matrix. The cone of singular symmetric matrices is denoted $\mathcal{C} := \{m \in \mathbb{R}^3 : m_1 m_2 - m_3^2 = 0\}$, and we set $c = (c_0, c_0, 0)^T$ for c_0 is as in (7). (Note that c lies on the symmetry axis of \mathcal{C} .)

As noted, $u \in \mathcal{M}$ iff $\mathbb{I} \in \mathcal{N}$ a.e. It is therefore interesting to examine \mathcal{N} in more detail. Depending on the rank of Q , \mathcal{N} is the intersection of \mathcal{C} with an ellipsoid centered at c and touching \mathcal{C} from inside, with a straight line through c , or with a plane containing c .

In fact it is elementary to see that, if $\text{rank}(Q) = 2$, \mathcal{N} consists of at most two points, in case $\text{rank}(Q) = 1$ and $c_0 Q(\text{Id}) \neq 0$, \mathcal{N} is a non-degenerate conic, and, for $\text{rank}(Q) = 1$ and $c_0 Q(\text{Id}) = 0$, $\mathcal{N} = \mathbb{R}N^{(1)} \cup \mathbb{R}N^{(2)}$ where $N_{ij}^{(1)} \geq 0$ and $N_{11}^{(2)} = N_{22}^{(1)}$, $N_{22}^{(2)} = N_{11}^{(1)}$, $N_{12}^{(2)} = -N_{12}^{(1)}$. Except for this last case, any two elements of \mathcal{N} are linearly independent.

Claim. If $\text{rank}(Q) = 3$, then $\#\mathcal{N} = 1$, $\#\mathcal{N} = 2$, or \mathcal{N} is a circle. In every case, if $F^{(1)}, F^{(2)} \in \mathcal{N}$, then $\text{trace}(F^{(1)}) = \text{trace}(F^{(2)})$.

Proof. The proof is completely elementary; we indicate the main steps. If $\min\{Q(m - c) : m \in \mathcal{C}\} = q_0$, then $\mathcal{N} = \mathcal{C} \cap \mathcal{E}$ for $\mathcal{E} = \{Q(m - c) = q_0\}$, an ellipsoid touching \mathcal{C} from inside. If $\#\mathcal{N} \geq 2$, choose $a, b \in \mathcal{N}$, $a \neq b$, and consider a plane \mathcal{P} through a, b, c . On \mathcal{P} choose a coordinate system (x, y) with origin at c such that the y -axis lies in $\mathbb{R}(1, 1, 0)^T + \mathbb{R}(0, 0, 1)^T$, i.e. is an axis of symmetry of the conic $\mathcal{C} \cap \mathcal{P}$. In these coordinates let $a = (a_1, a_2)$, $b = (b_1, b_2)$. Since the ellipse $\mathcal{E} \cap \mathcal{P}$ touches $\mathcal{C} \cap \mathcal{P}$ from inside, a_2 and b_2 have the same sign, say $a_2, b_2 < 0$. Now suppose $a_2 \neq b_2$.

In case $\mathcal{C} \cap \mathcal{P}$ is not compact, after a suitable linear transformation we obtain either a circle touching a hyperbola or parabola from inside at two points where the center of the circle does not lie on the axis of symmetry of the hyperbola resp. parabola, or a circle touching a hyperbola or parabola from inside at four points where the center of the circle lies on the axis of symmetry of the hyperbola resp. parabola.

In case $\mathcal{C} \cap \mathcal{P}$ is compact, after a suitable linear transformation we obtain either an ellipse touching a circle from inside at two points where the center of the circle does not lie on an axis of symmetry of the ellipse, or an ellipse touching a circle from inside at four points where the center of the circle lies on an axis of symmetry of the ellipse.

In all cases all the normals of the touching points to the corresponding circle intersect at the circle centers. This yields a contradiction when viewed as normals to the corresponding hyperbola resp. parabola resp. ellipse. The claim now easily follows. \square

Also note that in case \mathcal{N} is a circle, Q is of the form

$$Q(m_1, m_2, m_3) = \alpha \left(\frac{m_1 + m_2}{2} \right)^2 + \beta \left(\frac{m_1 - m_2}{2} \right)^2 + \beta m_3^2$$

for some $\alpha > 0, \beta \geq 0$, hence Q is isotropic:

$$Q(\mathbb{I}) = \frac{\beta}{2} |\mathbb{I}|^2 + \frac{\alpha - \beta}{4} (\text{trace}(\mathbb{I}))^2 = \frac{\alpha + \beta}{4} |\mathbb{I}|^2$$

where the last equality followed from $\det(\text{II}) = 0$. Furthermore, if Q describes a material with cubic symmetry, then $Q(R^T M R) = Q(M)$ for all symmetric M and $R = e_2 \otimes e_1 - e_1 \otimes e_2 \in \mathbb{R}^{2 \times 2}$. Straight forward calculations for $Q(m_1, m_2, m_3) = \sum_{1 \leq i, j \leq 3} q_{ij} m_i m_j$ with $q_{ij} = q_{ji}$ lead to

$$(q_{ij})_{ij} = \begin{pmatrix} q_{11} & q_{12} & q_{13} \\ q_{12} & q_{11} & -q_{13} \\ q_{13} & -q_{13} & q_{33} \end{pmatrix}.$$

Then $\mathbb{R}c$ is a principal axis for every ellipsoid $\{Q(m_1, m_2, m_3) = \text{const.}\}$. So if Q is not isotropic, i.e. $q_{13} \neq 0$ or $q_{11} - q_{12} - q_{33}/2 \neq 0$, $\mathcal{N} = \{n^{(1)} \otimes n^{(1)}, n^{(2)} \otimes n^{(2)}\}$ with $|n^{(1)}| = |n^{(2)}|$ and $n^{(1)} \perp n^{(2)}$ as expected.

The following theorem gives a complete description of the minimizers of E .

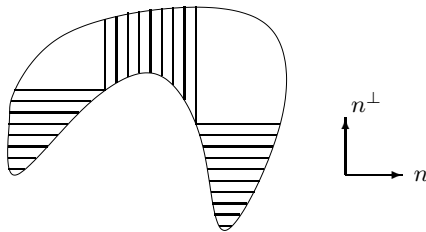
Theorem 3.2 *Suppose $u \in \mathcal{M}$.*

- *If rank $Q = 2$ or 3 or if rank $Q = 1$ and $c_0 Q(\text{Id}) \neq 0$, then u is a cylinder.*
- *If rank $Q = 1$ and $c_0 Q(\text{Id}) = 0$, then there exists a unique normal vector $n \in \mathbb{R}^2$ with $n_1 > 0, n_2 \geq 0$ such that u is locally of Euler-Bernoulli type w.r.t. n or $n^\perp = (-n_2, n_1)^T$.*

Here we say that a deformation $y : S \rightarrow \mathbb{R}^3$ is of *Euler-Bernoulli type* (w.r.t. $n \in \mathbb{R}^2$) if there is a plane $\mathcal{P} \in \mathbb{R}^3$ with normal ν and a function $f : \mathbb{R} \supset I \rightarrow \mathcal{P}$ such that

$$u(x) = f(x \cdot n) + (x \cdot n^\perp) \nu.$$

In the last case we obtain a decomposition of S (as in the following picture) into stripes parallel to n^\perp resp. n on which u is of Euler-Bernoulli type w.r.t. n resp. n^\perp and a rest where $\text{II} = 0$, i.e. u is rigid. These stripes can meet only at the boundary ∂S .



Lemma 3.3 *Let $n \in \mathbb{R}^2$. Suppose $y \in \mathcal{A}$ with $\text{II}(x) = \mu(x)n \otimes n$. Then y is locally of Euler-Bernoulli type w.r.t. n .*

Proof. Elementary calculations using $\nabla y \in O(2; 3)$ a.e. show that $\nabla_{n^\perp} u(x) =: \nu$ is constant. Applying $\nabla y \in O(2; 3)$ again, the claim follows. \square

Proof of theorem 3.2. In [6] it is shown that (locally on convex subdomains) $u \in \mathcal{A}$ implies that u is a developable ruled surface. Moreover, there exists $f_u \in W^{1,2}(S, \mathbb{R}^2)$ such that $\nabla f_u = \text{II}$ and the connected components of the pre-images of f_u are the segments (neighborhoods) on which u is affine. We may choose coordinates (s, t) such that

$$u(\gamma(t) + s\nu(t)) = \tilde{\gamma}(t) + s\nu(t)$$

where, in the regions where f_u is not constant, $\gamma \in W^{2,\infty}$ (parameterized by arclength) is orthogonal to the inverse images of f_u , and $\nu = (\gamma')^\perp$. By κ we denote the curvature of γ , i.e. $\gamma'' = \kappa\nu$.

As in [6] note that $\Gamma(t) = f_u(\gamma(t) + s\nu(t))$ is independent of s . Since both rows of ∇f_u are parallel to γ' and $d\Gamma/dt = \nabla f_u(\gamma(t) + s\nu(t))(\gamma'(t) + s\nu'(t)) = \nabla f_u(\gamma(t) + s\nu(t))(1 - s\kappa)\gamma'(t)$, we can write

$$\nabla f_u(\gamma(t) + s\nu(t)) = \mu(s, t)(\nu(t))^\perp \otimes (\nu(t))^\perp = \frac{\mu(t)}{1 - s\kappa}(\nu(t))^\perp \otimes (\nu(t))^\perp.$$

In case $\text{rank}(Q) = 1$ and $c_0Q(\text{Id}) = 0$, since ν is continuous, it follows from $\text{II} \in \mathcal{N}$ that ν is locally constant, and hence u is locally of Euler-Bernoulli type by lemma 3.3.

In the remaining cases, the elements of \mathcal{N} are pairwise linearly independent, whence in fact $\kappa = 0$ a.e. But then $\nu' = 0$, i.e. $\nu(t) \equiv \nu(t_0)$ and $\text{II} = \mu(t_0)(\nu(t_0))^\perp \otimes (\nu(t_0))^\perp$. Now II being constant on every convex subdomain, it must be constant on S . \square

In case II is smooth we give a self contained proof of the above result not using developability. Note that this is in fact sufficient for the case $\text{rank}(Q) = 3$ interesting for elasticity: by the reasoning above, there is a constant r_0 such that for all $\text{II} \in \mathcal{N}$, $\text{II}_{11} + \text{II}_{22} = r_0$. Also in [6] (cf. lemma 2.6) it is proved that the Codazzi-Mainardi-equations $\text{II}_{11,2} = \text{II}_{12,1}$ and $\text{II}_{12,2} = \text{II}_{22,1}$ hold in distributions. But then locally there exists $f \in W^{1,2}$ such that $\nabla f = \text{II}$. It follows

$$0 = \text{div cof } \nabla f = \text{div} \begin{pmatrix} \text{II}_{22} & -\text{II}_{21} \\ -\text{II}_{12} & \text{II}_{11} \end{pmatrix} = \text{div} \begin{pmatrix} -\text{II}_{11} & -\text{II}_{12} \\ -\text{II}_{21} & -\text{II}_{22} \end{pmatrix},$$

i.e. $\Delta f = \text{div } \nabla f = 0$. But then f and hence II is smooth and we can proceed as follows.

Write $\text{II}(x) = \pm n(x) \otimes n(x)$, $n \in \mathbb{R}^2$. Up to a discrete exceptional set we can solve locally in matrix space, w.l.o.g. for n_2 : $n_2 = f(n_1)$, f analytic. Inserting this into the Codazzi-Mainardi-equations $(n_1^2)_{,2} = (n_1 n_2)_{,1}$ and $(n_2^2)_{,1} = (n_1 n_2)_{,2}$ leads to

$$\begin{aligned} 2n_1 n_{1,2} &= (f(n_1) + n_1 f'(n_1))n_{1,1} \\ 2f(n_1) f'(n_1) n_{1,1} &= (f(n_1) + n_1 f'(n_1))n_{1,2}, \end{aligned}$$

a linear system for ∇n_1 which has non-trivial solutions if and only if

$$0 = \det \begin{pmatrix} (f(n_1) + n_1 f'(n_1)) & -2n_1 \\ -2f(n_1) f'(n_1) & (f(n_1) + n_1 f'(n_1)) \end{pmatrix} = (f(n_1) - n_1 f'(n_1))^2.$$

Now if $\nabla n_1 \neq 0$ on some open set (and hence the image of n_1 not discrete), we have

$$f(t) - t f'(t) = 0 \quad \Rightarrow \quad f(t) = Ct.$$

Hence $n(x) = \mu(x) (1, C)^T =: \mu(x) n_0$. As before this implies that u is locally of Euler-Bernoulli type resp. a cylinder due to the structure of \mathcal{N} . \square

4 Minimal energy configurations in 2D

In this section we consider thin strained multi-layers of Euler Bernoulli type. As noted at the end of section 2, these objects are described by a planar curve γ tracing the position of the middle fiber of a two-dimensional section. In this setting, the determination of energy minimizers of the two-dimensional energy functional (7), (6) becomes trivial. However, considering films of finite thickness $h > 0$, in the regime $L \sim 1/h$, a non-intersection will lead to non-trivial geometric behavior globally.

Consider a curve $\gamma \subset \mathbb{R}^2$ of length $|\gamma| = L$. Let t be arclength, $\gamma : [0, L] \rightarrow \mathbb{R}^2$, $e_1 = d\gamma/dt$, $e_2 = e_1^\perp$. The film of thickness h associated to γ is

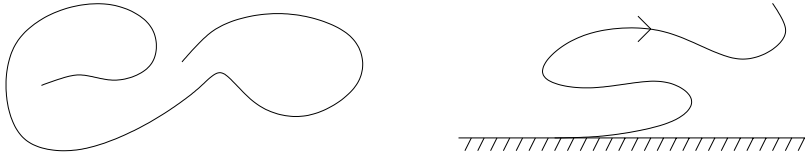
$$\{\gamma(t) + se_2(t) : 0 \leq t \leq L, -h/2 < s < h/2\}.$$

Note that – to first order in h – this is a reasonable model for a film of thickness $0 < h \ll 1$ motivated by the shape of our test functions in the proof of theorem 2.2. We will impose the following non-intersection condition:

$$\gamma(t_1) + s_1 e_2(t_1) = \gamma(t_2) + s_2 e_2(t_2) \implies t_1 = t_2 \text{ and } s_1 = s_2. \quad (8)$$

Seeking for energy minimizers among such curves, we will speak of curves with two free ends.

It will be interesting to also consider curves γ in the upper half plane where one end is attached to the x_1 -axis (curves with one free end).



More precisely, in the second case we demand that $\gamma : [0, L] \rightarrow \mathbb{R} \times [-h/2, \infty)$, $\gamma(0) = (0, -h/2)$ and $((-\infty, 0] \times \{-h/2\}) \cup \gamma$ satisfies the non-intersection condition (8).

According to (6), we define the energy of γ by

$$E(\gamma) = \int_0^L (\kappa(t) - \kappa_0)^2$$

where $\kappa(t)$ denotes the curvature of γ at t , and $\kappa_0 \geq 0$ is a fixed constant. By definition, κ satisfies

$$\frac{d^2\gamma}{dt^2} = \frac{de_1}{dt} = \kappa(t)e_2.$$

The corresponding admissible classes of curves are

$$\mathcal{A}_1 := \{\gamma \in W^{2,2}(0, L; \mathbb{R}^2) : |\gamma'| \equiv 1 \text{ and (8) holds}\},$$

respectively

$$\mathcal{A}_2 := \{\gamma \in W^{2,2}(0, L; \mathbb{R}^2) : |\gamma'| \equiv 1, \gamma(0) = (0, -h/2) \text{ and (8) holds for } ((-\infty, 0] \times \{-h/2\}) \cup \gamma\}.$$

Since the non-intersection condition (8) implies $|\kappa(t)| \leq 2/h$, in fact, for fixed L and h , the elements of \mathcal{A}_i , $i = 1, 2$, are uniformly bounded in $W^{2,\infty}$.

Using the direct method of the calculus of variations, it is easy to show existence of minimizers.

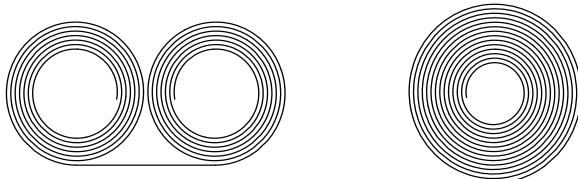
Proposition 4.1 (*Existence of minimizers*) *There exist $u_i \in \mathcal{A}_i$, $i = 1, 2$, such that $E(u_i) = \min_{u \in \mathcal{A}_i} E(u)$.*

Proof. For a minimizing sequence $\gamma^{(n)}$ we may assume that $\gamma^{(n)}(0) = (0, -h/2)$, $e_1^{(n)}(0) = (1, 0)$ for all n , and $\gamma^{(n)} \xrightarrow{*} \gamma$ in $W^{2,\infty}$. Then $\gamma^{(n)} \rightarrow \gamma$ in $W^{1,\infty}$ and, by lower semicontinuity, $E(\gamma) = \inf_{u \in \mathcal{A}_i} E(u)$. It only remains to check that γ (resp. $((-\infty, 0] \times \{-h/2\}) \cup \gamma$) satisfies our non-intersection condition. Suppose not, i.e. $\gamma(t_1) + s_1 e_2(t_1) = p = \gamma(t_2) + s_2 e_2(t_2)$ for some $t_1, t_2 \in (0, L)$, $s_1, s_2 \in (-h/2, h/2)$ with $(t_1, s_1) \neq (t_2, s_2)$. Choosing n large enough we find neighborhoods U_i of t_i and V_i of s_i with $U_1 \cap U_2 = \emptyset$ or $V_1 \cap V_2 = \emptyset$ such that

$$p \in \{\gamma^{(n)}(t) + s e_2^{(n)}(t) : t \in U_i, s \in V_i\}, \quad i = 1, 2,$$

which contradicts our non-intersection assumption on $\gamma^{(n)}$. \square

As energy minimizers for the curve with only one free end we expect a spiral deformation. A moments thought shows that, in case the curve has two free ends, we can do better by joining two spirals by a straight line the energy of which is negligible for large L .



In the following we will determine the minimal mean energy $\frac{1}{L}E(\gamma)$ up to $\mathcal{O}(h)$ in the limit $L \rightarrow \infty$, $h \rightarrow 0$. The result turns out to depend only on $a := Lh$. The proof will also show that minimizing configurations (to leading order) are in fact of the shape described above.

Upper Bounds

To obtain upper bounds for the energy minimizers, we consider a specific example. Let (in polar coordinates)

$$\gamma(t) = (r(t), \varphi(t)) = (r_0 + h\varphi(t)/2\pi, \varphi(t))$$

where $\varphi(0) = 0$ and $\varphi' = 1/\sqrt{(h/2\pi)^2 + r^2} > 0$, so t is arclength. Up to an error of order $\mathcal{O}(1)$, this is the sum of the energies of nested circles with distances h , the smallest of radius r_0 , the largest of radius R_0 where $\pi R_0^2 - \pi r_0^2 = Lh = a$. Up to $\mathcal{O}(1)$, this energy is

$$\frac{1}{h} \int_{r_0}^{R_0} 2\pi r \left(\frac{1}{r} - \kappa_0 \right)^2 dr.$$

Now minimizing this energy expression with respect to $\pi R_0^2 - \pi r_0^2 = a$ for fixed a , yields r_0 and R_0 uniquely in terms of a and κ_0 by

$$\pi R_0^2 - \pi r_0^2 = a \quad \text{and} \quad 1/r_0 - \kappa_0 = \kappa_0 - 1/R_0. \quad (9)$$

Setting

$$E_2(a) = \frac{2\pi}{a} \left[\log(r) - 2\kappa_0 r + \kappa_0^2 r^2 / 2 \right]_{r_0}^{R_0} \quad (10)$$

for r_0, R_0 as in (9), we see that the energy of γ satisfies

$$\frac{1}{L} E(\gamma) = E_2(a) + \mathcal{O}(h). \quad (11)$$

In case the film has two free ends we get an upper bound on the minimal energy by considering a bi-spiral γ whose energy $E(\gamma)$ is, up to $\mathcal{O}(1)$, the energy of two (equal) single spirals:

$$\frac{1}{L} E(\gamma) = E_1(a) + \mathcal{O}(h), \quad E_1(a) = 2E_2(a/2). \quad (12)$$

In theorem 4.4 we will see that indeed

$$\min_{\gamma \in \mathcal{A}_i} \frac{1}{L} E(\gamma) = E_i(a) + \mathcal{O}(h), \quad i = 1, 2, \quad a = Lh.$$

Spirals as minimizers

Consider the case of curves in \mathcal{A}_2 with one fixed end first.

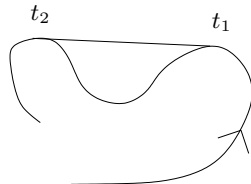
Proposition 4.2 *Let $\gamma \in \mathcal{A}_2$. If $\kappa(t) < 0$ for some t , then there exists another curve in \mathcal{A}_2 having less energy than γ .*

The idea of the proof is to show that the contact set of γ with its convex envelope connected.

Proof. Let $\text{co}(\gamma)$ be the convex hull of γ . Clearly $\gamma(0) \in \partial \text{co}(\gamma)$ and $e_2(0)$ points inward $\text{co}(\gamma)$. Let t_1 be the last time such that $\gamma(t) \in \partial \text{co}(\gamma|_{[t,L]})$ for all $t \leq t_1$. There exists $t_2 > t_1$ such that $\gamma(t_2) \in \partial \text{co}(\gamma|_{[t_1,L]})$ and $\gamma \cap (\gamma(t_1), \gamma(t_2)) = \emptyset$. We obtain three cases:

$$e_1(t_2) = e_1(t_1) \quad \text{or} \quad e_1(t_2) = -e_1(t_1) \quad \text{or} \quad e_1(t_2) \neq \pm e_1(t_1).$$

Case 1: Replace $\gamma|_{[t_1,t_2]}$ by a straight line connecting $\gamma(t_1)$ and $\gamma(t_2)$.



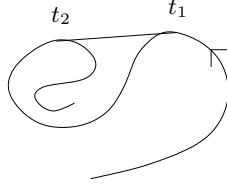
Since by strict convexity of the energy functional

$$E(\gamma|_{[t_1,t_2]}) \geq \kappa_0^2(t_2 - t_1),$$

this yields an amount of energy larger than $\kappa_0^2(t_2 - t_1 - |[\gamma(t_1), \gamma(t_2)]|)$, while it makes the film $t_2 - t_1 - |[\gamma(t_1), \gamma(t_2)]|$ shorter. Note that this procedure does not enlarge the convex hull of $\gamma|_{[t_1, L]}$, so the new configuration is admissible. Now add the segment $[(-t_2 + t_1 + |[\gamma(t_1), \gamma(t_2)]|, -h/2), (0, -h/2)]$ to this new configuration and shift to the right.

Case 3: If $e_1(t_2) \neq \pm e_1(t_1)$, then $t_2 = L$, and we replace γ by $\gamma|_{[0, t_1]} \cup [(-t_2 + t_1, -h/2), (0, -h/2)]$ and shift to the right. As in case 1, one sees that this lowers energy noting that $\int_{t_1}^{t_2} \kappa(t) dt < 0$.

Case 2:



γ on $[t_1, t_2]$ together with the line segment $[\gamma(t_2), \gamma(t_1)]$ forms a closed curve such that $\gamma(t)$ lies in its interior Ω for $t > t_2$ and in its exterior $\bar{\Omega}^c$ for $t < t_1$.

For $s \geq t_2$ we define g_s to be the shortest curve in $\bar{\Omega}$ that connects $\gamma(t_1)$ to $\gamma(s)$. (Note that g_s is unique since Ω is simply connected. Furthermore, $g_s \setminus \gamma$ consists of intervals where g_s is a straight line, and – as does $\gamma - g_s$ lies in $W^{2, \infty}$.) By $I \subset [t_2, L]$ we denote the set of those s for which $g_s \cap \gamma|_{[t_2, L]} = \{\gamma(s)\}$. Let $t^{(s)}$ be arclength of g_s , $e_1^{(s)} = dg_s/dt^{(s)}$, and $\kappa^{(s)}$ the curvature of g_s .

Claim. Suppose $s \in I$. If $\gamma|_{[t_1, t_2]} \cap g_s \neq \emptyset$, say $\gamma(t) = g_s(t^{(s)})$, then $e_1(t) = e_1^{(s)}(t^{(s)})$. Furthermore, $\kappa^{(s)} \geq 0$ a.e.

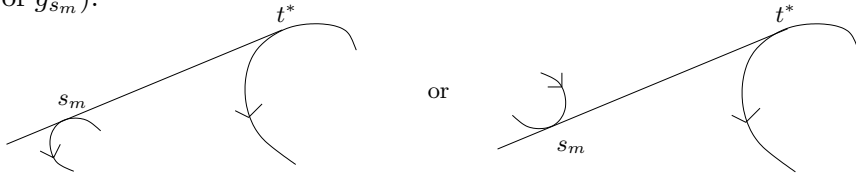
Proof of the claim.

for small $t^{(s)} > 0$ with $g_s(t^{(s)}) \in \gamma([t_1, t_2])$, $(e_1^{(s)})^\perp$ points outside Ω .

Assuming one of the statements of the claim is not satisfied, there are points $g_s(t^{(s)})$ on $\gamma|_{[t_1, t_2]}$ such that $(e_1^{(s)}(t^{(s)}))^\perp$ points inside Ω . Choose $t_2^{(s)}$ minimal with this property, and suppose $t_1^{(s)} < t_2^{(s)}$ is maximal with $g_s(t_1^{(s)}) \in \gamma|_{[t_1, t_2]}$, $(e_1^{(s)}(t_1^{(s)}))^\perp$ pointing outside Ω (recall (8)). But then the union of $g_s([t_1^{(s)}, t_2^{(s)}])$ and $\gamma([\gamma^{-1}(g_2(t_1^{(s)})), \gamma^{-1}(g_2(t_2^{(s)}))])$ is the graph of a closed curve with $\gamma(s)$ lying in its interior and $\gamma(t_2)$ in the exterior. This contradicts the fact that this curve does not intersect $\gamma|_{[t_2, L]}$ due to $s \in I$. \square

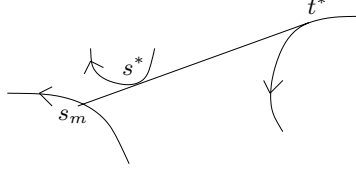
Define $s_m := \sup I$ ($> t_2$), $t^* = \max\{t \in [t_1, t_2] : \gamma(t) \in g_{s_m}\}$. Our aim is, as in case 1, to connect some $\gamma(t)$, $t \in [t_1, t_2]$, to some $\gamma(s)$, $s \in [t_2, L]$, by a straight line.

Suppose first $s_m < L$. If $s_m \in I$, set $s^* = s_m$. Then $e_1(s^*) = e_1(t^*)$ and, in a neighborhood of s^* , γ lies on one side of its tangent at s^* (which contains the last part of g_{s_m}).



If $s_m \notin I$, then g_{s_m} intersects $\gamma|_{[t_2, L]}$ before s_m and we choose s^* such that $s^* \in I$ and $\gamma(s^*) \in g_{s_m}$. Note that there is a sequence $s^{(n)} \in I$, $s^{(n)} \rightarrow s_m$, such

that $g_{s^{(n)}}$ converges to g_{s_m} uniformly, in particular, $e_1(s^*)$ is parallel to $e_1(t^*)$ and γ lies on one side of g_{s_m} in a neighborhood of s^* .



Indeed we must have $e_1(s^*) = e_1(t^*)$, for else consider the closed curve $\gamma|_{[s^*, s_m]} \cup [\gamma(s_m), \gamma(s^*)]$. For ε small enough, this curve would have to be intersected by $\gamma|_{[t_2, s^* - \varepsilon]}$ which is not possible.

Now we have to take care of our non-intersection condition (8). Let $B = B_1 \cup B_2$ where

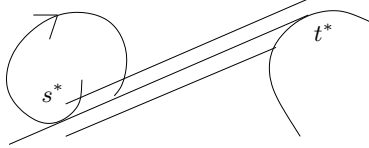
$$\begin{aligned} B_1 &= \{\tau\gamma(t^*) + (1 - \tau)\gamma(s^*) + \sigma e_2(t^*) : 0 < \tau < 1, 0 \leq \sigma < h\}, \\ B_2 &= \{\tau\gamma(t^*) + (1 - \tau)\gamma(s^*) + \sigma e_2(t^*) : 0 < \tau < 1, -h < \sigma < 0\}. \end{aligned}$$

First note that $\gamma|_{[t_1, t^*]}$ does not intersect B : enlarge g_{s_m} after s_m straightly until it hits $\gamma|_{[t_1, t_2]}$ at $\gamma(t')$. Then note that $\gamma|_{[t_1, t^*]}$ does not enter $\{\gamma(t) + \sigma e_2(t) : t^* < t \leq t', 0 \leq \sigma < h\}$ nor $[\gamma(t^*), \gamma(t')]$, hence $\gamma|_{[t_1, t^*]} \cap B_1 = \emptyset$.

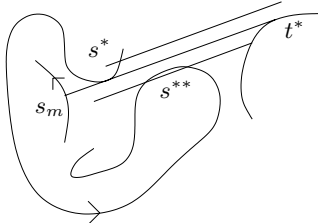
To see that $\gamma|_{[t_1, t^*]}$ does not intersect B_2 , note $(\gamma(t^*), \gamma(s^*))$ lies in the interior of $g_{s_m}|_{[0, g_{s_m}^{-1}(\gamma(t^*))]} \cup \gamma|_{[t^*, t_2]} \cup [\gamma(t_2), \gamma(t_1)]$. If $\gamma|_{[t_1, t^*]}$ intersected B_2 , then also $g_{s_m}|_{[0, g_{s_m}^{-1}(\gamma(t^*))]}$ would have to intersect B_2 . But this is impossible since $\kappa^{(s_m)} \geq 0$ a.e. due to our claim above.

If also $\gamma|_{(s^*, L]}$ does not intersect B , then replacing $\gamma|_{[t^*, s^*]}$ by the straight line $[\gamma(t^*), \gamma(s^*)]$ leads to a configuration satisfying (8).

Suppose now $\gamma|_{(s^*, L]}$ intersects B . This intersection can not take place on the same side of g_{s_m} as γ lies in a neighborhood of s^* since then $s^* - \varepsilon$ could not be connected to t_2 .



For $s_m = s^*$ the intersection can not take place on the other side of g_{s_m} either, due to maximality of s_m , and we are done. Now consider the remaining case. Note that if $\gamma(s) \in B$, $s > s^*$, then $s \leq s_m$ since $\gamma(s)$ lies in the interior of $\gamma|_{[s^*, s_m]} \cup [\gamma(s_m), \gamma(s^*)]$ for $s > s_m$ and $\langle e_1(s), e_1(t^*) \rangle > 0$ (else t_2 can not be connected to s_m).



Let $s^{**} \in (s^*, s_m]$ be such that $\gamma(s^{**}) \in B$ is closest to $[\gamma(t^*), \gamma(s^*)]$. Now shift $\gamma|_{[s^{**}, L]}$ (by an amount $< h$) perpendicular to $\gamma(s^*) - \gamma(t^*)$ such that

$\gamma(s^{**})$ lies on (the old) g_{s_m} and connect $\gamma(t^*)$ to $\gamma(s^{**})$. This does not violate our non-intersection condition since $\gamma|_{[t^*, s^{**}]}$ is removed.

As in the previous cases we add a suitable line segment $[(-l, -h/2), (0, -h/2)]$ so that our new configuration has length L and shift to the right. As before this lowers energy: note that $\int_{t^*}^{s^*} \kappa(t)dt$ and $\int_{t^*}^{s^{**}} \kappa(t)dt$ are equal to 0 or -2π .

Now if $s_m = L$ we proceed as above replacing $\gamma|_{[t^*, s_m]}$ by $[\gamma(t^*), \gamma(s_m)]$, adding a suitable segment and shifting. Note that here $\int_{t^*}^{s^*} \kappa(t)dt \leq 0$. \square

Minimal Energy Estimates for Spirals

We consider the subclass of spirals of \mathcal{A}_2 : $\mathcal{A}_2^{\text{sp}} = \{\gamma \in \mathcal{A}_2 : \kappa(t) \geq 0 \text{ a.e.}\}$.

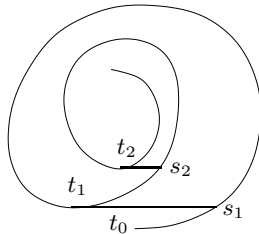
Lemma 4.3 *Define $E_2(a)$ as in (10). There exists a constant C depending on h and L only through $a = hL$ such that for each $\gamma \in \mathcal{A}_2^{\text{sp}}$,*

$$\frac{1}{L}E(\gamma) \geq E_2(a) - Ch.$$

Proof. Choose $t_0 = 0 < t_1 < t_2, \dots, t_N \leq L$ such that $\int_{t_{n-1}}^{t_n} \kappa(t)dt = 2\pi$ and $\int_{t_N}^L \kappa(t)dt < 2\pi$. By convexity,

$$\begin{aligned} E(\gamma) &= \int_0^L (\kappa(t) - \kappa_0)^2 dt \\ &\geq \sum_{n=1}^N \int_{t_{n-1}}^{t_n} (\kappa(t) - \kappa_0)^2 dt \\ &\geq \sum_{n=1}^N (t_n - t_{n-1}) \left(\frac{2\pi}{t_n - t_{n-1}} - \kappa_0 \right)^2. \end{aligned} \quad (13)$$

Now consider the following closed curves: For $n = 1, \dots, N$ choose s_n maximal such that $\gamma(s_n)$ lies on the half line starting at $\gamma(t_n)$ with direction $e_1(t_n)$. Define γ^n to be the closed curve $[\gamma(t_n), \gamma(s_n)] \cup \gamma|_{[s_n, t_n]}$.



Recall the definition of r_0 and R_0 from (9) and assume first that $r_0/6 \leq |\gamma^n| \leq 8\pi R_0$ for all n . (Then also $L - t_N$ is bounded.) Also suppose that $|\gamma(t_1) - \gamma(t_0)| \leq 4\pi R_0$.

Since γ^n are nested closed and convex curves with mutual distance $\geq h$, we deduce from lemma A.1 that

$$|\gamma^{n+1}| \geq |\gamma^n| + 2\pi h.$$

Also note that there exists C independent of N such that

$$\left| \sum_{k=1}^n |\gamma^k| - \sum_{k=1}^n (t_k - t_{k-1}) \right| \leq C \quad \forall n \in \{1, \dots, N\}. \quad (14)$$

(To see this, note that, in components $\gamma = (\gamma_1, \gamma_2)$,

$$\sum_{k=1}^n (t_k - t_{k-1}) - |\gamma^k| = \sum_{k=1}^n (s_k - t_{k-1}) - (\gamma_1(s_k) - \gamma_1(t_k))$$

with $\gamma_1(s_k) - \gamma_1(t_{k-1}) \leq s_k - t_{k-1} \leq \gamma_1(s_k) - \gamma_1(t_{k-1}) + \gamma_2(s_k) - \gamma_2(t_{k-1})$, i.e.

$$s_k - t_{k-1} - (\gamma_1(s_k) - \gamma_1(t_k)) \begin{cases} \geq \gamma_1(t_k) - \gamma_1(t_{k-1}) \\ \leq \gamma_1(t_k) - \gamma_1(t_{k-1}) + \gamma_2(t_k) - \gamma_2(t_{k-1}). \end{cases}$$

Summing over k we get lower and upper bounds by evaluating telescoping sums which are bounded, since the spiral occupies a bounded region.)

By the lemma A.4 below, we may therefore replace $t_n - t_{n-1}$ in (13) by $|\gamma^n|$ and obtain

$$E(\gamma) \geq \sum_{n=1}^N |\gamma^n| \left(\frac{2\pi}{|\gamma^n|} - \kappa_0 \right)^2 + \mathcal{O}(1).$$

Now this is exactly the energy of N nested circles (annuli) of length $|\gamma^n|$. Since for two such annuli of different size enlarging the smaller one and shortening the bigger one by the same amount yields energy, we may assume that the annuli touch (i.e. have distances h). Since, by (14), $\sum_{k=1}^N |\gamma^k| = t_N + \mathcal{O}(1) = L + \mathcal{O}(1)$, the previous calculation of the upper bound (cf. (11)) applies to this configuration and we find that

$$\frac{1}{L} E(\gamma) \geq E_2(a) - Ch.$$

Now if $\gamma^n \geq 8\pi R_0$ for $n \leq N_1$, $\gamma^n \leq r_0/6$ for $n \geq N_2$ and $r_0/6 \leq |\gamma^n| \leq 8\pi R_0$ else, we apply the above reasoning to $\gamma|_{[t_{N_1}, t_{N_2}]}$ replacing the middle part of γ by nested circles of optimal energy leading to inner and outer radii $\bar{r}_0 \geq r_0$ and $\bar{R}_0 \leq R_0$, resp.

Consider $\gamma|_{[t_{N_2}, L]}$. If $L - t_{N_2} \leq r_0$, this part is negligible. If not, we proceed as follows: Since $\gamma|_{[t_{N_2}, L]}$ is contained in the domain bounded by γ^{N_2} of diameter $\leq r_0/12$, by lemma A.2 we have $\int_{t_{N_2}}^L \kappa(t) dt \geq \lfloor (L - t_{N_2}) / (r_0/3) \rfloor \geq 2(L - t_{N_2}) / r_0$. By convexity we may lower energy replacing $\gamma|_{[t_{N_2}, L]}$ by a curve of constant curvature $2/r_0$. The energy can be reduced further by replacing this part by nested touching annuli whose biggest radius is $\bar{r}_0 - h$. (Note that curvature is reduced pointwise, since $(L - t_{N_2})h \leq 2\pi r_0^2/36 < \pi r_0^2(1 - 1/4)$.)

For the first part of the curve observe that since $\gamma|_{[0, t_{N_1}]}$ lies outside the domain Ω bounded by γ^{N_1} , which has diameter $\geq 8\pi R_0$, $t_n - t_{n-1} \geq 4\pi R_0$ for $n \leq N_1$. (Apply lemma A.3 with $p = \gamma(t_{n-1})$ and $q = \gamma(t_n)$.) As in (13) replacing this part of the curve by annuli of circumference $t_n - t_{n-1}$ yields energy. Similar as in the case just treated we may lower the energy even further replacing these by nested annuli whose smallest radius is $\bar{R}_0 + h$.

If $|\gamma(t_1) - \gamma(t_0)| \geq 4\pi R_0$, we apply the above procedure to $\gamma|_{[t_1, L]}$. Noting that $t_1 - t_0 \geq 4\pi R_0$, we can then replace $\gamma|_{[t_0, t_1]}$ by a circle of radius $2R_0$. Continue as in the previous case. \square

We summarize the above results in the following

Theorem 4.4 *Let $a = Lh$, E_1 , E_2 as in (12), resp. (10). Then*

(i)

$$\inf_{\gamma \in \mathcal{A}_2} \frac{1}{L} E(\gamma) = \min_{\gamma \in \mathcal{A}_2} \frac{1}{L} E(\gamma) = \min_{\gamma \in \mathcal{A}_2^{\text{sp}}} \frac{1}{L} E(\gamma) = E_2(a) + \mathcal{O}(h),$$

(ii)

$$\inf_{\gamma \in \mathcal{A}_1} \frac{1}{L} E(\gamma) = \min_{\gamma \in \mathcal{A}_1} \frac{1}{L} E(\gamma) = E_1(a) + \mathcal{O}(h).$$

Proof. It only remains to prove $\frac{1}{L} E(\gamma) \geq E_1(a) - Ch$ for $\gamma \in \mathcal{A}_1$. Let $\text{co}(\gamma)$ be the convex hull of γ . If there exists $t_0 \in [0, L]$ with $\gamma(t_0) \in \partial \text{co}(\gamma)$ such that $e_2(t_0)$ is not an outward normal of $\text{co}(\gamma)$, we consider $\gamma|_{[0, t_0]}$ and $\gamma|_{[t_0, L]}$ separately. This reduces (up to $\mathcal{O}(h)$) to the spiral case (i) already treated. For $a_1 = t_0 h$, $a_2 = (L - t_0)h$ we see that

$$\frac{1}{L} E(\gamma) \geq \frac{1}{L} (t_0 E_2(a_1) + (L - t_0) E_2(a_2)) - Ch \geq 2E_2(a/2) - Ch.$$

If such a t_0 does not exist, we see as in the proof proposition 4.2 (cf. ‘case 1’) that $\{t : \gamma(t) \in \partial \text{co}(\gamma)\}$ is an interval $[t_1, t_2]$, say, and $\int_{t_1}^{t_2} \kappa(t) dt = -2\pi$. Now let t'_1 (resp. t'_2) be the largest (resp. smallest) time such that $\partial \text{co}(\gamma|_{[0, t'_1]}) \cap \gamma|_{[0, t'_1]}$ (resp. $\partial \text{co}(\gamma|_{[t'_2, L]}) \cap \gamma|_{[t'_2, L]}$) contains a point $\gamma(t)$ with $e_2(t)$ not an outward normal. Choose $t''_1 \in [0, t'_1]$ maximal with this property ($t''_2 \in [t'_2, L]$ minimal). Now treat $\gamma|_{[0, t''_1]}$ and $\gamma|_{[t''_2, L]}$ as in the spiral case. Observe that $\int_{t''_1}^{t'_1} \kappa, \int_{t'_2}^{t''_2} \leq \pi$, so replacing $[t''_1, t''_2]$ by a straight line yields energy. Now add this straight line to one of the two spirals to obtain two spirals with lower energy. As above it follows that $\frac{1}{L} E(\gamma) \geq 2E_2(a/2) - Ch$. \square

Remark. The proof shows that the minimal energy configurations are (up to $\mathcal{O}(h)$) indeed of the form depicted on page 13.

Appendix: Analytical Lemmas

In this appendix we prove more or less elementary facts for curves resp. domains in \mathbb{R}^2 and a lemma on convex functions on the line that where needed in section 4.

Lemma A.1 *Suppose $\Omega_1, \Omega_2 \subset \mathbb{R}^2$ are convex domains with $\Omega_1 \subset \Omega_2$ and $\text{dist}(\partial \Omega_1, \partial \Omega_2) \geq h$. Then*

$$|\partial \Omega_2| \geq |\partial \Omega_1| + 2\pi h,$$

and equality holds iff $\Omega_2 = \Omega_1^h := \{x \in \mathbb{R}^2 : \text{dist}(x, \partial \Omega_1) < h\}$.

Proof. Suppose first $\partial\Omega_1$ is C^2 , parameterized by $[t_1, t_2] \ni t \mapsto \gamma(t)$, where t is arclength oriented such that $e_2 = e_1^\perp$ is the inner normal to $\partial\Omega_1$, $e_1 = d\gamma/dt$, and $\kappa \geq 0$. Then $\partial\Omega_2$ can be parameterized by $\tilde{\gamma}(t) = \gamma(t) - f(t)e_2(t)$, $f \in W^{1,\infty}$ and $f \geq h$.

Since $de_2/dt = de_1^\perp/dt = \kappa e_2^\perp = -\kappa e_1$, we can calculate:

$$\begin{aligned} |\partial\Omega_2| &= \int_{t_1}^{t_2} \left| \frac{d}{dt} \tilde{\gamma} \right| dt = \int_{t_1}^{t_2} \left| \frac{d\gamma}{dt} - \frac{df}{dt} e_2 - f \frac{de_2}{dt} \right| dt \\ &= \int_{t_1}^{t_2} \left| e_1 - \frac{df}{dt} e_2 + f \kappa e_1 \right| dt \geq \int_{t_1}^{t_2} |1 + \kappa f| dt \\ &= \int_{t_1}^{t_2} (1 + \kappa f) dt \geq t_2 - t_1 + h \int_{t_1}^{t_2} \kappa dt \\ &= |\partial\Omega_1| + 2\pi h \end{aligned}$$

with equality everywhere iff $f \equiv h$, i.e. $\Omega_2 = \Omega_1^h$. For general Ω_1 approximate by an interior convex domain having smooth boundary.

(Alternatively assume that Ω_1 has polygonal boundary (else approximate). Projecting (i.e. contracting) Ω_2 onto $\overline{\Omega_1^h}$ yields $|\partial\Omega_2| \geq |\partial\Omega_1^h| = |\partial\Omega_1| + 2\pi h$ with equality iff $\Omega_2 = \Omega_1^h$. This argument also shows that we do not have to require that Ω_2 be convex.) \square

Lemma A.2 *Suppose $\Omega \subset \mathbb{R}^2$ is a domain of diameter d , $\gamma : [0, l] \rightarrow \Omega$ a curve (parameterized by arclength) in Ω . Then*

$$\int_0^l |\kappa(t)| dt \geq \frac{1}{2} \left\lfloor \frac{l}{2d} \right\rfloor.$$

Proof. W.l.o.g. $l > 2d$. Since for $0 \leq t_1 < t_2 \leq l$

$$d \geq |\gamma(t_2) - \gamma(t_1)| = \left| \int_{t_1}^{t_2} \left(\frac{d\gamma}{dt}(t_1) + \int_{t_1}^t \frac{d^2\gamma}{dt^2}(s) ds \right) dt \right|,$$

we have

$$\begin{aligned} \left| (t_2 - t_1) \frac{d\gamma}{dt}(t_1) \right| &\leq d + \int_{t_1}^{t_2} \int_{t_1}^{t_2} \left| \frac{d^2\gamma}{dt^2}(s) \right| ds dt \\ &= d + (t_2 - t_1) \int_{t_1}^{t_2} |\kappa(t)| dt. \end{aligned}$$

Therefore $\int_{t_1}^{t_2} |\kappa(t)| dt \geq 1 - d/(t_2 - t_1)$. In particular, if $t_2 - t_1 = 2d$, then $\int_{t_1}^{t_2} |\kappa(t)| dt \geq 1/2$. Cutting γ into $\lfloor l/2d \rfloor$ pieces of length $2d$, we thus find that

$$\int_0^l |\kappa(t)| dt \geq \frac{1}{2} \left\lfloor \frac{l}{2d} \right\rfloor.$$

\square

Lemma A.3 Suppose $\Omega \subset \mathbb{R}^2$ is a convex domain, $p, q \in \mathbb{R}^2$ separated (not necessarily strictly) from Ω by some hyper-plane. Then any domain Ω' (with sufficiently smooth boundary) containing Ω, p, q satisfies

$$|\partial\Omega'| \geq |p - q| + \frac{1}{2}|\partial\Omega|.$$

Proof. W.l.o.g. assume that Ω' is the convex hull of Ω, p and q . Reducing $|\partial\Omega'| - |p - q|$ we may also assume that p and q lie on the separating hyper-plane, even that the image of the orthogonal projection of Ω to this line is $[p, q]^\circ$. But then $|p - q| \leq |\partial\Omega|/2$, so the claim follows from $|\partial\Omega'| \geq |\partial\Omega|$, because of $\Omega' \supset \Omega$ (cf. lemma A.1).

Lemma A.4 Let $I \subset \mathbb{R}$ be an interval and $f : I \rightarrow \mathbb{R}$ be convex. Let $x_1, \dots, x_N, y_1, \dots, y_N \in I$ such that $y_1 \leq y_2, \dots, y_N$. Assume that there is c such that $|\sum_{k=1}^n x_k - \sum_{k=1}^n y_k| \leq c$ for all $n \in \{1, \dots, N\}$. Then there exists $C > 0$ only depending on $c, f'(y_1)$ and $f'(y_N)$ such that

$$\sum_{k=1}^N f(x_k) \geq \sum_{k=1}^N f(y_k) - C.$$

Proof. Let $a_n := f'(y_n) - f'(y_{n-1})$ if $n \geq 2$, $a_1 := f'(y_1)$, $b_n := x_n - y_n$, and set $A_n = a_1 + \dots + a_n$, $B_n = b_1 + \dots + b_n$. By convexity and partial summation,

$$\begin{aligned} \sum_{n=1}^N f(x_n) - \sum_{n=1}^N f(y_n) &\geq \sum_{n=1}^N f'(y_n)(x_n - y_n) = \sum_{n=1}^N A_n b_n \\ &= A_N B_N - \sum_{n=2}^N a_n B_{n-1} \\ &= f'(y_N) \sum_{n=1}^N (x_n - y_n) - \sum_{n=2}^N a_n B_{n-1} \\ &\geq C(f'(y_N), c) - \max_{1 \leq n \leq N-1} |B_n| \sum_{n=2}^N a_n \\ &\geq C(f'(y_N), f'(y_1), c). \end{aligned}$$

(Note that by convexity and (y_n) being increasing, $a_n \geq 0$ for $n \geq 2$.) □

Of course this lemma also applies to $y_1 \geq y_2, \dots, y_N$. Just note that

$$\left| \sum_{k=n}^N x_k - y_k \right| = \left| \sum_{k=1}^N x_k - y_k - \sum_{k=1}^{n-1} x_k - y_k \right| \leq 2c.$$

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REFERENCES

- [1] G. FRIESECKE, R. D. JAMES, S. MÜLLER. *Rigorous derivation of nonlinear plate theory and geometric rigidity*. C. R. Acad. Sci. Paris **334** (2002), 173-178.
- [2] G. FRIESECKE, R. D. JAMES, S. MÜLLER. *A theorem on geometric rigidity and the derivation of nonlinear plate theory from three-dimensional elasticity*. Comm. Pure Appl. Math. **55** (2002), 1461-1506.
- [3] G. FRIESECKE, R. D. JAMES, S. MÜLLER. *A hierarchy of plate models derived from nonlinear elasticity by Gamma-convergence*. Max-Planck Institut für Mathematik in den Naturwissenschaften, Leipzig, preprint 7/2005.
- [4] H. PAETZELT, V. GOTTSCHALCH, J. BAUER, H. HERRNBERGER, G. WAGNER. *Fabrication of A(III)-B(II) nano- and microtubes using MOVPE grown materials*. Submitted.
- [5] M. GRUNDMANN. *Nanoscroll formation from strained layer heterostructures*. Appl. Phys. Lett. **83** (2003), 2444-2446.
- [6] M. R. PAKZAD. *On the Sobolev space of isometric immersions*. J. Differ. Geom. **66** (2004), 47-69.
- [7] B. SCHMIDT. *PhD thesis*. In preparation.
- [8] O. G. SCHMIDT, K. EBERL. *Thin solid films roll up into nanotubes*. Nature **410** (2001), 168.
- [9] J. C. TSUI, T. W. CLYNE. *An analytical model for predicting residual stress in progressively deposited coatings I*. Thin Solid Films **306** (1997), 23-33.