Stability of equilibrium configurations for elastic films in two and three dimensions

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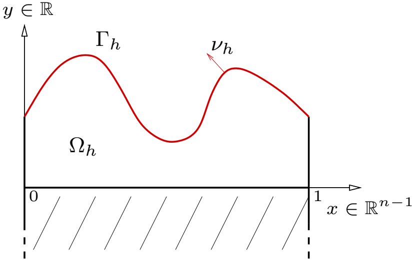
A variational model in epitaxial films theory

(Bonnetier & Chambolle 2002, Fonseca, Fusco, Leoni & Morini 2007, Fusco & Morini 2012)

Class $\mathcal{X}$ of admissible pairs (h,u):

- $h : Q = (0,1)^{n-1} \to (0,+\infty)$ Lipschitz, 1-periodic (free profile)
- $u \in W^{1,\infty}(\Omega_h;\mathbb{R}^n)$, periodic (deformation of the film)
- $u(x,0) = w_0(x,0)$ (typical choice: $w_0(x,y) = (e_0^1 x_1, e_0^2 x_2, 0)$)



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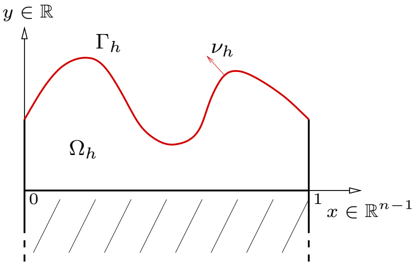

Total energy of the system:

$$F(h, u) := \int_{\Omega_h} W(\nabla u)\, \mathrm{d}z + \int_{\Gamma_h} \psi(\nu_h)\, \mathrm{d}\mathcal{H}^{n-1}$$

- $W : \mathbb{M}^n_+ \to [0, +\infty)$ of class C^3,
- $\psi : \mathbb{R}^n \to [0, +\infty)$ of class C^3, positively 1-homogeneous,

$$D^2\psi(v)[w, w] > c_0 |w|^2 \qquad \text{for all } v \in \mathbb{S}^{n-1}, \text{ for all } w \perp v$$

Critical pair

A pair $(h, u) \in \mathcal{X}$ is a (regular) critical pair for F if

- $h \in C^2(\mathbb{R}^{n-1})$, $u \in C^2(\overline{\Omega}_h^{\#}; \mathbb{R}^n)$,
- u solves
$$\int_{\Omega_h} W_\xi(\nabla u) : \nabla w = 0$$
for every $w \in \mathcal{V}(\Omega_h) := \{w \in W^{1,\infty}_{\#}(\Omega_h; \mathbb{R}^n) : w(x,0) = 0\}$,
or equivalently
$$\begin{cases} \operatorname{div}\left[W_\xi(\nabla u)\right] = 0 & \text{in } \Omega_h^{\#} \\ W_\xi(\nabla u)[\nu_h] = 0 & \text{on } \Gamma_h^{\#} \end{cases}$$
- $W(\nabla u) + H^\psi = \text{const}$ on Γ_h, where $H^\psi = \operatorname{div}(\nabla\psi \circ \nu_h)$

Implicit function theorem

Assume that (h, u) is a critical pair satisfying

$$\int_{\Omega_h} W_{\xi\xi}(\nabla u)\nabla w : \nabla w \geq c_0 \|w\|^2_{H^1(\Omega_h;\mathbb{R}^n)} \qquad \text{for every } w \in \mathcal{V}(\Omega_h)$$

(the elastic second variation is uniformly positive at u).

Then by the Implicit Function Theorem we can prove:

Proposition

There exist a neighbourhood $\mathcal{U}$ of h in $W^{2,p}$ and a map $g \in \mathcal{U} \mapsto u_g \in W^{2,p}(\Omega_g;\mathbb{R}^n)$ such that:

(i) *u_g is a critical point for the elastic energy in Ω_g,*

(ii) *$u_h = u$;*

(iii) *the map $g \mapsto u_g \circ \Phi_g$ is of class C^1 from $W^{2,p}_{\#}(Q)$ to $W^{2,p}(\Omega_h;\mathbb{R}^n)$.*

Moreover, for every $w \in \mathcal{V}(\Omega_g)$ with $0 < \|\nabla w\|_\infty < \delta$

$$\int_{\Omega_g} W(\nabla u_g) < \int_{\Omega_g} W(\nabla u_g + \nabla w)\,.$$

Second variation

Let (h, u) satisfy the previous assumptions.

- Fix $\phi \in C^2_\#(Q)$ with $\int_Q \phi = 0$ and set $h_t := h + t\phi$.
- For t small we have $h_t \in \mathcal{U}$ and we can consider a critical point for the elastic energy u_t in Ω_{h_t}, constructed in the previous proposition.
- We define the second variation of F at (h, u) along the direction ϕ to be

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2} F(h_t, u_t)|_{t=0}.$$

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Quadratic form associated with the second variation at a critical pair (h, u):

$$\partial^2 F(h,u)[\varphi] := -\int_{\Omega_h} W_{\xi\xi}(\nabla u)\nabla v_\varphi : \nabla v_\varphi \, \mathrm{d}z + \int_{\Gamma_h} (D^2\psi \circ \nu)[\nabla_{\Gamma_h}\varphi, \nabla_{\Gamma_h}\varphi] \, \mathrm{d}\mathcal{H}^{n-1}$$
$$+ \int_{\Gamma_h} \big(\partial_\nu (W \circ \nabla u) - \mathrm{tr}(\mathbf{B}^\psi \mathbf{B})\big)\varphi^2 \, \mathrm{d}\mathcal{H}^{n-1},$$

defined for $\varphi \in H^1_\#(\Gamma_h)$, $\int_{\Gamma_h} \varphi = 0$.

Local minimality criterion

Theorem (Bonacini, Adv. Calc. Var. 2014)

Let $n = 2, 3$. Assume that $(h, u) \in \mathcal{X}$ is a critical pair, the elastic second variation is uniformly positive:

$$\int_{\Omega_h} W_{\xi\xi}(\nabla u)\nabla w : \nabla w \geq c_0 \|w\|^2_{H^1(\Omega_h;\mathbb{R}^n)} \qquad \text{for every } w \in \mathcal{V}(\Omega_h)\,,$$

and (h, u) is strictly stable ($\partial^2 F(h, u)[\varphi] > 0$ for every $\varphi \neq 0$).
Then (h, u) is a local minimizer for F.

We say that (h, u) is a local minimizer if there exists $\delta > 0$ such that

$$F(h, u) \leq F(g, v)$$

for every $(g, v) \in \mathcal{X}$ with

- $\|g - h\|_\infty < \delta$, $|\Omega_g| = |\Omega_h|$,
- $\|\nabla v - \nabla u\|_{L^\infty(\Omega';\mathbb{M}^n)} < \delta$.

The linearly elastic case

Theorem (Bonacini, Adv. Calc. Var. 2014)

Let $n = 2, 3$, *and assume that the elastic energy density has the form*

$$W(\xi) := \frac{1}{2}\mathbb{C}\left(\frac{\xi+\xi^T}{2}\right) : \left(\frac{\xi+\xi^T}{2}\right), \qquad \xi \in \mathbb{M}^n,$$

for some constant fourth-order tensor $\mathbb{C}$ *such that*

$$\mathbb{C}\xi : \xi \geq c_0|\xi|^2 \quad \textit{for every } \xi \in \mathbb{M}^n_{\mathrm{sym}}, \quad c_0 > 0.$$

If (h, u) *is a strictly stable critical pair, then* (h, u) *is an isolated local minimizer for* F *in the following sense: for every* $M > \|\nabla u\|_\infty$ *there exists* $\delta = \delta(M) > 0$ *such that*

$$F(h, u) < F(g, v)$$

for every $(g, v) \in \mathcal{X}$ *with* $0 < \|g - h\|_\infty < \delta$, $|\Omega_g| = |\Omega_h|$, *and* $v \in \mathrm{Lip}_M(\Omega_g; \mathbb{R}^n)$.

Comments on the proof

Two steps strategy (Fusco & Morini 2012. Acerbi, Fusco & Morini 2013)

- Local $W^{2,p}$-minimality
  - minimality with respect to competitors (g, v) with $\|g - h\|_{W^{2,p}}$ sufficiently small
  - holds in dimensions $n = 2, 3$
  - requires to control the trace of the gradient of $W(\nabla u)$ on Γ_h in a proper Sobolev space of negative fractional order
  - careful new estimates for the elliptic system associated with the first variation of the elastic energy

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- Local $W^{2,p}$-minimality implies local minimality (as before)
  - contradiction argument
  - the L^∞-bound on the deformation gradient allows to regard the elastic energy as a volume perturbation of the surface energy
  - appeal to the regularity theory for *quasi-minimizers of the area functional*

Application: stability of the flat configuration

Asaro-Grinfeld-Tiller instability: instability of the flat layer above a critical value of the thickness of the film

Flat configuration with volume $d > 0$:

- Reference configuration: $\Omega_d = Q \times (0, d)$ (profile $h(x) \equiv d$)
- Affine critical point for the elastic energy: $v_0(z) = M[z]$, $M \in \mathbb{M}^n_+$

Theorem

There exists $d_0 > 0$ such that for every $d < d_0$

$$\partial^2 F(d, v_0)[\varphi] > 0 \qquad \textit{for every } \varphi \neq 0.$$

- The result is proved by Fusco & Morini (2012) in two dimension and linearized elasticity (here the local minimality threshold of the flat configuration is determined analytically)

The crystalline case

- For crystalline anisotropies, *the AGT instability is suppressed*

Assume that $\psi_c : \mathbb{R}^n \to [0, +\infty)$ satisfies:

- ψ_c is convex and positively 1-homogeneous,
- the associated Wulff shape W_{ψ_c} contains a neighbourhood of the origin,
- ∂W_{ψ_c} contains a horizontal facet:

$$\left\{(x, y) \in \mathbb{R}^{n-1} \times \mathbb{R} : |x| < a,\ y = b\right\} \subset \partial W_{\psi_c}\,.$$

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Theorem

For every $d > 0$ the flat configuration (d, v_0) is a local minimizer for the functional corresponding to the surface energy density ψ_c.

The crystalline case: sketch of the proof

- Let $\psi_C(x,y) := a|x| + b|y|$ the anisotropy whose Wulff shape is the cylinder $C := \{(x,y) : |x| < a,\ |y| < b\}$, and let F_C be the associated functional.
- We have $\psi_C \leq \psi_c$, $\psi_C(0,1) = \psi_c(0,1) = b$.
- For $\varepsilon > 0$, let F_ε be the functional associated with the "regular" anisotropy $\psi_\varepsilon(x,y) := a\sqrt{\varepsilon^2 y^2 + |x|^2} + (b - a\varepsilon)|y|$.
Notice that $\psi_\varepsilon \nearrow \psi_C$ as $\varepsilon \to 0^+$.
- We have, for $\varepsilon < \varepsilon_0$,

$$\begin{aligned}\partial^2 F_\varepsilon(d, v_0)[\varphi] &= -\int_{Q\times(0,d)} W_{\xi\xi}(\nabla v_0)\nabla v_\varphi : \nabla v_\varphi \,\mathrm{d}z + \frac{a}{\varepsilon}\int_Q |\nabla\varphi|^2 \,\mathrm{d}\mathcal{H}^{N-1} \\ &\geq C\|\varphi\|^2_{H^1(Q)}\,.\end{aligned}$$

Then for every competitor (g, v) sufficiently close to (d, v_0)

$$\begin{aligned}F_c(d, v_0) = \int_{Q\times(0,d)} W(\nabla v_0)\,\mathrm{d}z + \psi_c(0,1) = F_C(d, v_0) \\ = F_{\varepsilon_0}(d, v_0) \leq F_{\varepsilon_0}(g, v) \leq F_C(g, v) \leq F_c(g, v)\,.\end{aligned}$$

Application: Liapunov stability of the flat configuration

(Fonseca, Fusco, Leoni & Morini 2014)

- Evolution of anisotropic epitaxially strained films via surface diffusion with curvature regularization, in three dimension
- Linear elastic energy density $W : \mathbb{M}^{3\times 3}_{\mathrm{sym}} \to [0, +\infty)$, $W(A) := \frac{1}{2}\mathbb{C}A : A$, with $\mathbb{C}$ positive definite fourth order tensor.

Evolution equation: find $h(\cdot, t)$ solution to

$$\frac{1}{J}\frac{\partial h}{\partial t} = \Delta_{\Gamma_{h(\cdot,t)}}\left[H^{\psi} + W(E(u)) - \varepsilon\left(\Delta_{\Gamma_{h(\cdot,t)}}(|H|^{p-2}H) - \frac{1}{p}|H|^{p}H + |H|^{p-2}H|B|^{2}\right)\right]$$

with $J = \sqrt{1 + |\nabla h|^2}$, $u(\cdot, t)$ elastic equilibrium in $\Omega_{h(\cdot,t)}$.

- Short time existence of a variational solution of the geometric evolution equation starting from an initial datum $h_0 \in W^{2,p}_{\#}(Q)$

Application: Liapunov stability of the flat configuration

Theorem (Liapunov stability)

Assume that

- *the flat configuration satisfies* $\partial^2 F(d, v_0)[\varphi] > 0$ *for every* φ, ***or***
- ψ_c *is a crystalline anisotropy.*

Then the flat configuration (d, v_0) *is Liapunov stable: for every* $\sigma > 0$ *there exists* $\delta(\sigma) > 0$ *such that if* $\|h_0 - d\|_{W^{2,p}} < \delta(\sigma)$ *then every variational solution with initial datum* h_0 *exists for all times and* $\|h(\cdot, t) - d\|_{W^{2,p}} < \sigma$ *for every* $t > 0$.

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Theorem (Asymptotic stability)

Assume that $\partial^2 F(d, v_0)[\varphi] > 0$ *for every* $\varphi \neq 0$.
Then the flat configuration (d, v_0) *is asymptotically stable: there exists* $\delta > 0$ *such that if* $\|h_0 - d\|_{W^{2,p}} < \delta(\sigma)$, *then every variational solution with initial datum* h_0 *exists for all times and* $\|h(\cdot, t) - d\|_{W^{2,p}} \to 0$.

Thank you for your attention!