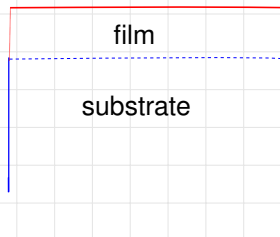


**Motion of elastic thin films by anisotropic
surface diffusion with curvature regularization**
(work in collaboration with I. Fonseca, G. Leoni and M. Morini)

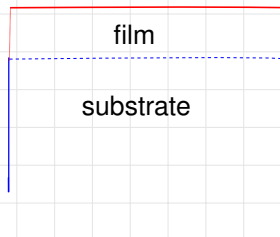
Nicola Fusco

A model for epitaxial growth: Static theory



- ▶ Fonseca, F., Leoni & Morini
(*Arch. Rational Mech. Anal* (2007))
- ▶ F., Morini
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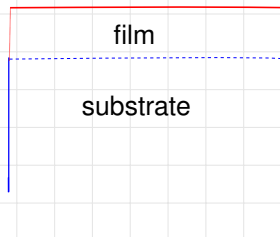
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Deposition of a thin film over a thick substrate

A model for epitaxial growth: Static theory

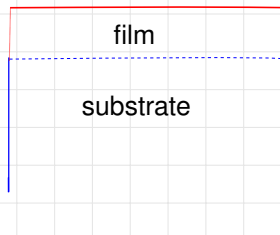


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Deposition of a thin film over a thick substrate

Mismatch strain

A model for epitaxial growth: Static theory



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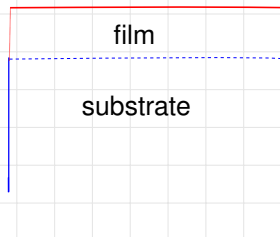
Deposition of a thin film over a thick substrate

Mismatch strain



instability of the flat configuration and island formation

A model for epitaxial growth: Static theory



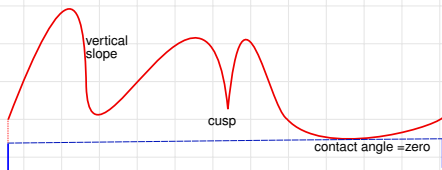
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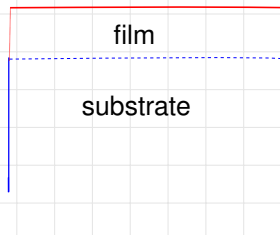
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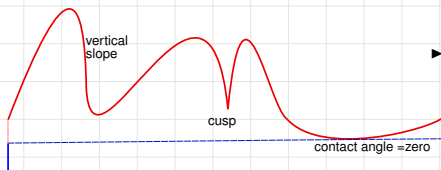
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Deposition of a thin film over a thick substrate

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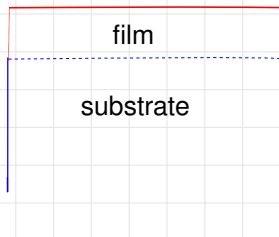


instability of the flat configuration and island formation



- ▶ **Asaro-Tiller-Grinfeld** morphological instability

A model for epitaxial growth: Static theory



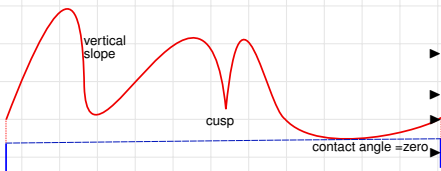
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Deposition of a thin film over a thick substrate

Mismatch strain

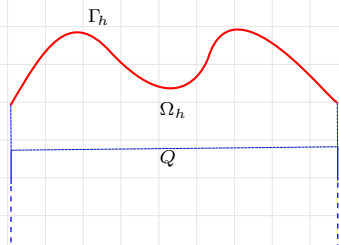


instability of the flat configuration and island formation



- ▶ **Asaro-Tiller-Grinfeld** morphological instability
- ▶ B.Spencer, D.Meiron (*Acta Metal. Mater.*, 1994)
- ▶ B.Spencer, J.Tersoff (*Phy. Rev. Letter*, 1997)
- ▶ **further numerical results:** Chiu, H. Gao, W. Nix

Static theory: variational formulation



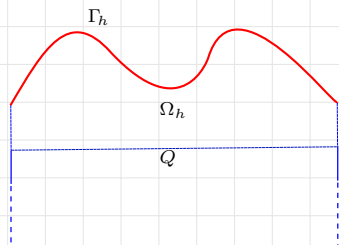
$h : \mathbb{R}^2 \rightarrow [0, \infty)$ Q -periodic, Lipschitz

$\Omega_h = \{(x, y) \in Q \times \mathbb{R} : 0 < y < h(x)\}$

$\Gamma_h = \partial\Omega_h \cap \{y > 0\}$

$Q = [0, 1] \times [0, 1]$

Static theory: variational formulation



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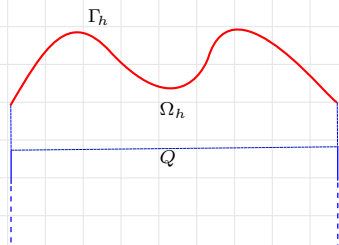
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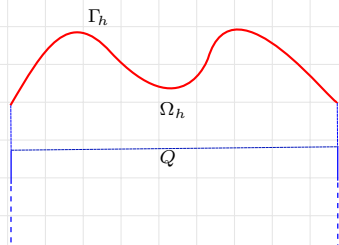
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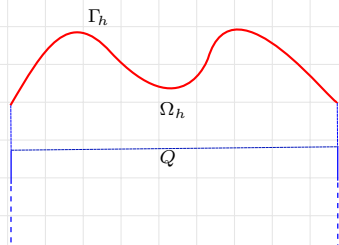
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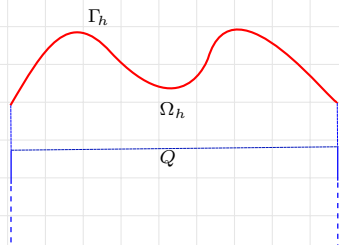
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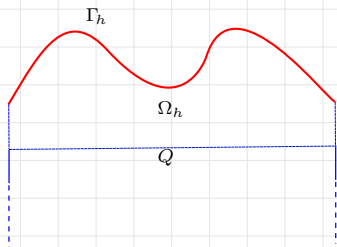
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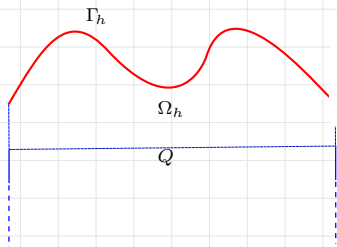
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- ▶ $e_0 > 0$ measure the mismatch between the two lattices

Static theory: variational formulation

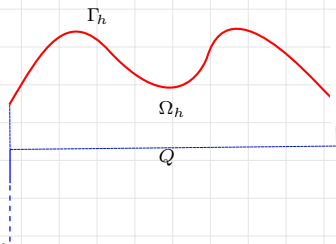


Static theory: variational formulation



$$F(h, u) := \int_{\Omega_h} W(E(u)) \, dx dy + \int_{\Gamma_h} \psi(\nu) \, d\sigma$$

Static theory: variational formulation

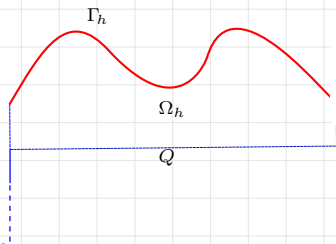


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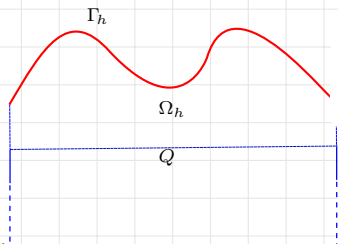


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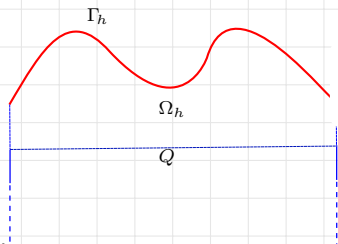


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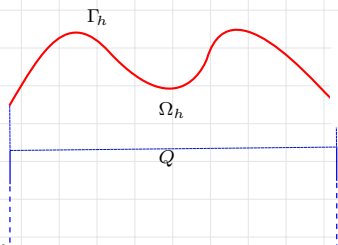
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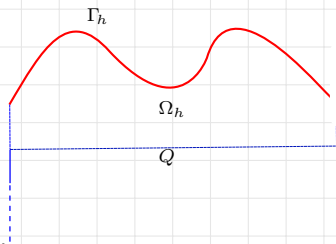
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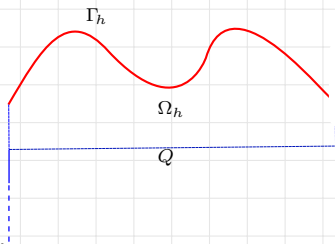
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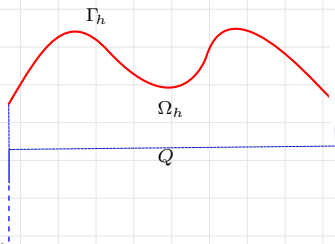
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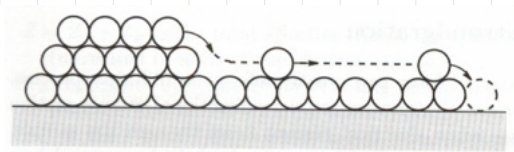
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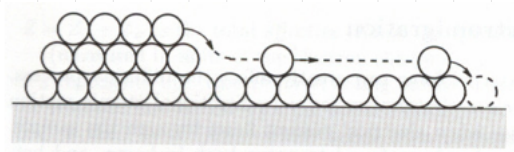
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- ▶ Bonacini (2013): the case of anisotropic surface energies in 2D and 3D.

Morphology evolution: surface diffusion

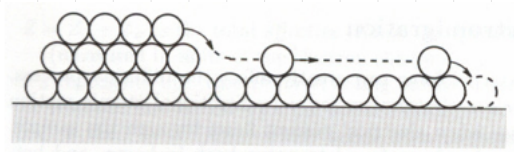


Morphology evolution: surface diffusion



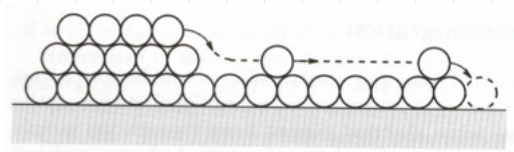
Einstein-Nernst law:

Morphology evolution: surface diffusion



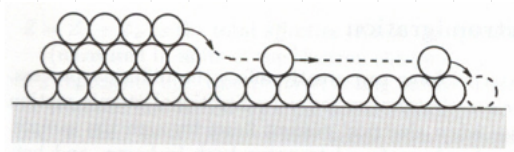
Einstein-Nernst law: **surface flux of atoms**

Morphology evolution: surface diffusion



Einstein-Nernst law: **surface flux of atoms** $\propto \nabla_{\Gamma} \mu$

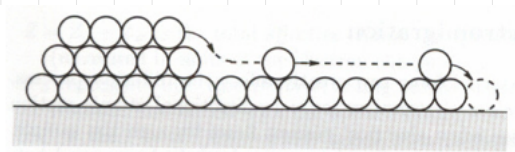
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μ = chemical potential

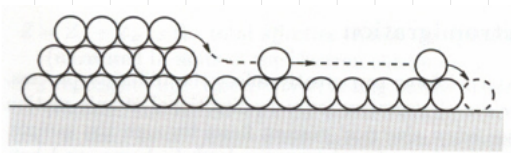
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Morphology evolution: surface diffusion

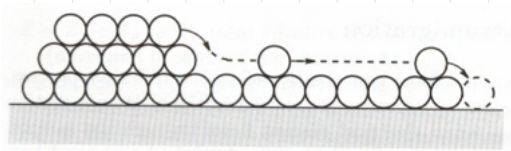


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$$V = \Delta_{\Gamma} \left(\text{div}_{\Gamma} D\psi(\nu) + W(E(u)) \right)$$

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$$V = \Delta_\Gamma \left[\operatorname{div}_\Gamma(D\psi(\nu)) + W(E(u)) \right. \\ \left. - \varepsilon \left(\Delta_\Gamma(|H|^{p-2}H) - |H|^{p-2}H \left(\kappa_1^2 + \kappa_2^2 - \frac{1}{p}H^2 \right) \right) \right]$$

Highly anisotropic surface energies in 2D

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Regularized energy:

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Highly anisotropic surface energies in 2D

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↓

$$V = \left(\operatorname{div}_\sigma D\psi(\nu) + W(E(u)) - \varepsilon \left(k_{\sigma\sigma} + \frac{1}{2} k^3 \right) \right)_{\sigma\sigma}$$

- ▶ Fonseca, F., Leoni, and Morini (ARMA 2012): evolution of films in two-dimensions

Highly anisotropic surface energies in 2D

Regularized energy:

$$F(h, u) := \int_{\Omega_h} W(E(u)) \, dx dy + \int_{\Gamma_h} \left(\psi(\nu) + \frac{\varepsilon}{2} k^2 \right) d\mathcal{H}^1$$

↓

$$V = \left(\operatorname{div}_\sigma D\psi(\nu) + W(E(u)) - \varepsilon(k_{\sigma\sigma} + \frac{1}{2}k^3) \right)_{\sigma\sigma}$$

- ▶ Fonseca, F., Leoni, and Morini (ARMA 2012): evolution of films in two-dimensions
- ▶ Fonseca, F., Leoni, and Morini (2014): evolution of films in three-dimensions

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Given W , we wish to find $h: \mathbb{R}^2 \times [0, T_0] \rightarrow (0, +\infty)$ s.t.

$$\left\{ \begin{array}{l} \frac{1}{J} \frac{\partial h}{\partial t} = \Delta_{\Gamma} \left[\operatorname{div}_{\Gamma}(D\psi(\nu)) + W(E(u)) \right. \\ \quad \left. - \varepsilon \left(\Delta_{\Gamma}(|H|^{p-2}H) - |H|^{p-2}H \left(\kappa_1^2 + \kappa_2^2 - \frac{1}{p}H^2 \right) \right) \right], \quad \text{in } \mathbb{R}^2 \times (0, T_0), \\ \operatorname{div} \mathbb{C}E(u) = 0 \quad \text{in } \Omega_h, \\ \mathbb{C}E(u)[\nu] = 0 \quad \text{on } \Gamma_h, \quad u(x, 0, t) = e_0(x, 0), \\ h(\cdot, t) \text{ and } Du(\cdot, t) \quad \text{are } Q\text{-periodic,} \\ h(\cdot, 0) = h_0, \end{array} \right.$$

Here $J := \sqrt{1 + |Dh|^2}$.

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- ▶ no analytical results for the sharp interface evolution with elasticity

The gradient flow structure

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- ▶ First observed by **Cahn & Taylor (1994)** in the context of **surface diffusion**

The minimizing movements scheme in our case

- ▶ Given $T > 0$, $N \in \mathbb{N}$, we set $\tau := \frac{T}{N}$. For $i = 1, \dots, N$ we define **inductively** (h_i, u_i) as the solution of the **incremental** minimum problem

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The discrete Euler-Lagrange equation

- ▶ The Euler-Lagrange equation of the **incremental problem** is

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which is a **discrete version** of the continuous evolution law.

Estimates

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Higher regularity (difficult!)

Set $\tilde{H}_N(\cdot, t) = H_i$, for $(i-1)\Delta T \leq t < i\Delta T$, the sum of the principal curvatures of $h_i(\cdot)$, then we have

$$(*) \quad \int_0^{T_0} \int_Q |D^2(|\tilde{H}_N|^{p-2} \tilde{H}_N)|^2 dx dt \leq C$$

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$$\begin{aligned} & \varepsilon \int_Q |H_i|^{p-2} H_i \left[\Delta \varphi - \frac{D^2 \varphi [DH_i, DH_i]}{J_i^2} \right. \\ & \quad \left. - \frac{\Delta H_i DH_i \cdot D\varphi}{J_i^2} - 2 \frac{D^2 H_i [DH_i, D\varphi]}{J_i^2} + 3 \frac{D^2 H_i [DH_i, DH_i] DH_i \cdot D\varphi}{J_i^4} \right] dx \\ & - \frac{\varepsilon}{p} \int_Q |H_i|^p \frac{DH_i \cdot D\varphi}{J_i} - \int_Q D\psi(-DH_i, 1) \cdot (-D\varphi, 0) dx \\ & - \int_Q W(E(u_i(x, H_i(x)))) \varphi dx + \frac{1}{\tau} \int_Q v_{h_i} \varphi dx = 0, \end{aligned}$$

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Lemma

Let $p > 2$, $u \in L^{\frac{p}{p-1}}(Q)$ such that

$$\int_Q u A D^2 \varphi dx + \int_Q b \cdot D\varphi + \int_Q c \varphi dx = 0 \quad \forall \varphi \in C^\infty(Q) \text{ with } \int_Q \varphi dx = 0,$$

where $A \in W^{1,p}(Q; \mathbb{M}_{sym}^{2 \times 2})$, $b \in L^1(Q; \mathbb{R}^2)$, and $c \in L^1(Q)$. Then $u \in L^q(Q)$ for all $q \in (1, 2)$. Moreover, if $b, u \operatorname{div} A \in L^r(Q; \mathbb{R}^2)$ and $c \in L^r(Q)$ for some $r > 1$, then $u \in W^{1,r}(Q)$.

Local in time existence of weak solutions

$$\frac{1}{J_{i-1}} \frac{h_i - h_{i-1}}{\tau} = \Delta_{\Gamma_{h_{i-1}}} \left[\operatorname{div}_{\Gamma_{h_i}} (D\psi(\nu)) + W(E(u_i)) \right. \\ \left. - \varepsilon \left(\Delta_{\Gamma_{h_i}} (|H_i|^{p-2} H_i) - |H_i|^{p-2} H_i \left((\kappa_1^i)^2 + (\kappa_2^i)^2 - \frac{1}{p} H_i^2 \right) \right) \right]$$

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► h is a **weak solution** in the following sense:

Theorem (Local existence)

$h \in L^\infty(0, T_0; W_{\#}^{2,p}(Q)) \cap H^1(0, T_0; H_{\#}^{-1}(Q))$ is a weak solution in $[0, T_0]$ in the following sense:

(i) $\operatorname{div}_{\Gamma}(D\psi(\nu)) + W(E(u)) - \varepsilon \left(\Delta_{\Gamma}(|H|^{p-2} H) - \frac{1}{p}|H|^p H + |H|^{p-2} H (\kappa_1^2 + \kappa_2^2 - \frac{1}{p} H^2) \right) \in L^2(0, T_0; H_{\#}^1(Q)),$

(ii) for a.e. $t \in (0, T_0)$

$$\frac{1}{J} \frac{\partial h}{\partial t} = \Delta_{\Gamma} \left[\operatorname{div}_{\Gamma}(D\psi(\nu)) + W(E(u)) \right. \\ \left. - \varepsilon \left(\Delta_{\Gamma}(|H|^{p-2} H) - |H|^{p-2} H (\kappa_1^2 + \kappa_2^2 - \frac{1}{p} H^2) \right) \right] \quad \text{in } H_{\#}^{-1}(Q).$$

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In two dimensions:

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- The proof is based on the following estimate.

Proposition

Let $h \in H^5$, $h \geq c_0 > 0$, and let u be corresponding elastic equilibrium. Then, there exists a constant C depending only on $\|h\|_{H^2}$, c_0 , and $\|E(u)\|_{L^\infty(\Omega_h)}$ s.t.

$$\int_{\Gamma_h} |DE(u)|^2 d\mathcal{H}^1 \leq C \int_0^b (1 + |h^{(iv)}|^2) dx$$

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$$\int_{\Gamma_h} |D^2E(u)|^2 d\mathcal{H}^1 + \int_{\Gamma_h} |D_\sigma(E(u))|^4 d\mathcal{H}^1 \leq C \int_0^b (1 + |h^{(v)}|^2) dx.$$

Second variation approach

Let

$$G(h, u) = \int_{\Omega_h} W(E(u)) \, dx dy + \mathcal{H}^1(\Gamma_h)$$

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Theorem (F.-Morini, 2012)

Let (h, u) be a *critical configuration*, $h \in C^2$, $h > 0$ s.t.

$$\partial^2 G(h, u)[\varphi] > 0 \quad \forall \varphi \neq 0.$$

Then, there exists $\delta > 0$ s.t.

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

for all admissible (g, v) , with $|\Omega_g| = |\Omega_h|$ and $0 < \|g - h\|_{L^\infty} < \delta$.

Local minimality of the 2D flat configuration

- ▶ the flat configuration in the $[0, b]$

$$\left(\frac{d}{b}, u_0\right) \quad u_0(x, y) = e_0\left(x, -\frac{\lambda y}{2\mu + \lambda}\right)$$

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- if $b > \frac{\pi}{4} \frac{2\mu + \lambda}{e_0^2 \mu (\mu + \lambda)}$, the flat configuration is an isolated local minimizer for $0 < d < d_{loc}(b)$, where $d_{loc}(b)$ is the unique solution to

$$K\left(\frac{2\pi d_{loc}(b)}{b^2}\right) = \frac{\pi}{4} \frac{2\mu + \lambda}{e_0^2 \mu (\mu + \lambda)} \frac{1}{b}, \quad K \text{ explicit}$$

while for $d > d_{loc}(b)$ the flat configuration is *never* an isolated local minimizer

Local minimality of the 3D flat configuration: anisotropic case

Let

$$G(h, u) = \int_{\Omega_h} W(E(u)) \, dx dy + \int_{\Gamma_h} \psi(\nu) d\mathcal{H}^2$$

and as before

$$F(h, u) = G(h, u) + \frac{\varepsilon}{p} \int_{\Gamma_h} |H|^p \, d\mathcal{H}^2.$$

Theorem (Bonacini, 2013)

Assume that $D^2\psi(e_3) > 0$ on $(e_3)^\perp$ and $\partial^2 G(d, u_0) > 0$. Then there exists $\varepsilon > 0$ s.t.

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$$\implies F(d, u_d) = G(d, u_d) < G(h, u_h) \leq F(h, u_h)$$

Global in time existence and asymptotic stability

Consider the regularized surface diffusion equation

$$\frac{1}{J} \frac{\partial h}{\partial t} = \Delta_{\Gamma} \left[\operatorname{div}_{\Gamma}(D\psi(\nu)) + W(E(u)) \right. \\ \left. - \varepsilon \left(\Delta_{\Gamma}(|H|^{p-2}H) - |H|^{p-2}H \left(\kappa_1^2 + \kappa_2^2 - \frac{1}{p}H^2 \right) \right) \right]$$

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The main result is

Theorem (Fonseca-F.-Leoni-Morini)

Assume that $D^2\psi(e_3) > 0$ on e_3^{\perp} and $\partial^2 G(d, u_0) > 0$. There exists $\varepsilon > 0$ s.t.

if $\|h_0 - d\|_{W^{2,p}} \leq \varepsilon$, then:

- (i) any *variational solution* h exists for all times;
- (ii) $h(\cdot, t) \rightarrow d$ in $W^{2,p}$ as $t \rightarrow +\infty$.

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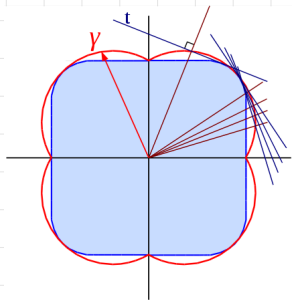
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Liapunov stability in the highly non-convex case

Consider the Wulff shape

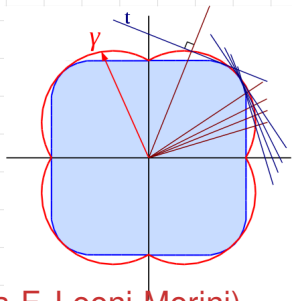
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Theorem (Fonseca-F.-Leoni-Morini)

Assume that W_ψ contains a **horizontal facet**. Then **for every $d > 0$** the flat configuration (d, u_d) is **Liapunov stable**, that is, **for every $\sigma > 0$** there exists **$\delta(\sigma) > 0$** s.t.

$$\int_Q h_0 = d, \quad \|h_0 - d\|_{W^{2,p}} \leq \delta(\sigma) \quad \implies \quad \|h(t) - d\|_{W^{2,p}} \leq \sigma \text{ for all } t > 0.$$

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THANK YOU FOR YOUR ATTENTION!