Analytical validation of the Young-Dupré law for epitaxially-strained thin films

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Joint work with E. Davoli, Vienna

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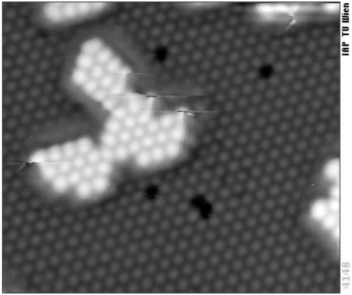
VIENNA SCIENCE
AND TECHNOLOGY FUND

The focus is on:

- deriving reliable variational models for thin films deposited on substrates;
- studying the morphology and the geometry of film profiles.

Plan of the talk:

1. Description of the deposition process;
2. Variational formulation of the model;
3. Existence of minimizers;
4. Properties of minimizers.



STM image of Pt on Pt(111) by PLD, Diebold's lab, TU Wien.

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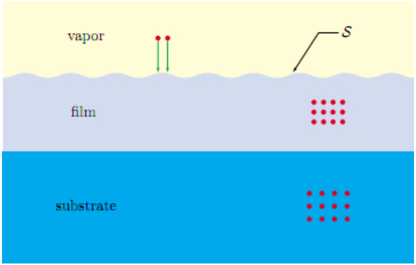
We consider:

- heteroepitaxy (different elasticity properties of the 2 materials);
- the presence of a mismatch between the crystalline lattices;
- the 3 interfaces: film/vapor (free), substrate/vapor and substrate/film;
- both wetting and dewetting regimes.



Epitaxy [Fried-Gurtin, 2004].

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(FM) Frank–van der Merwe;

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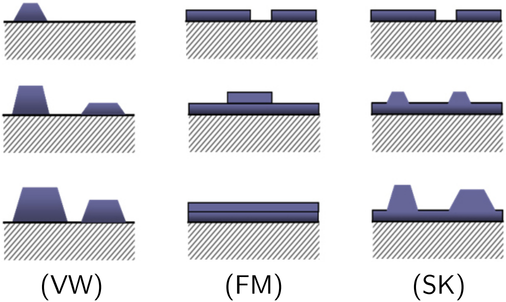

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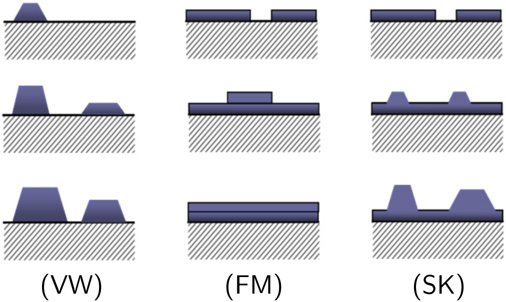

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Variables are:

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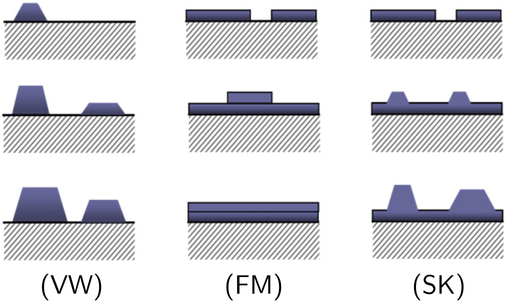

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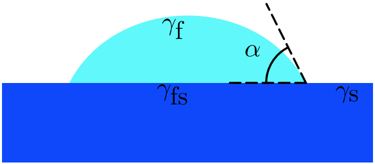
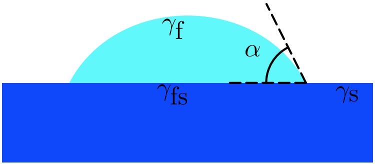
How large is the island angle formed at the substrate?



- α is the contact angle formed by island profiles with the substrates;
- γ_s := substrate/vapor surface tension;

† Study of contact angles of nanoclusters on zirconia through STM images, Courtesy of U. Diebold lab, TU Wien



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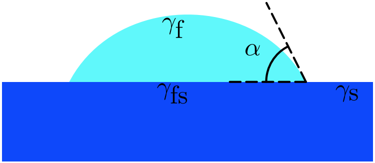

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$$\cos\alpha = \frac{\gamma_s - \gamma_{fs}}{\gamma_f},$$

with $\alpha = 0$ if $\gamma_s - \gamma_{fs} \geq \gamma_f$ (see [Young, 1805] and [A. Dupré-P. Dupré, 1869]).

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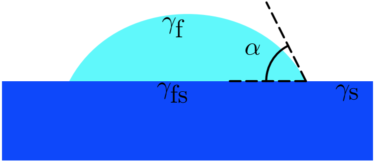

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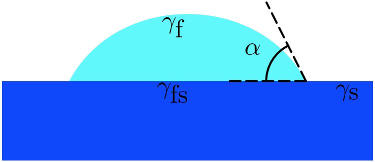

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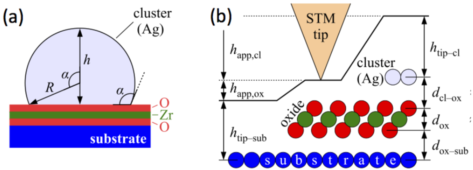

Clusters on zirconia†. Courtesy of Diebold's lab.

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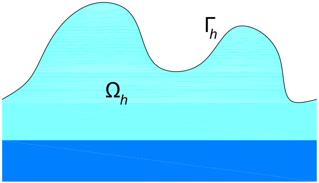

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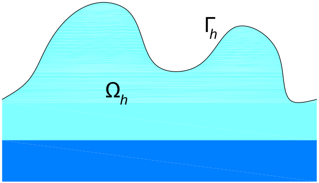

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$h : (0, \ell) \to [0, \infty)$ profile function,

$\Gamma_h := \{(x, h(x)) : 0 < x < \ell\}$,

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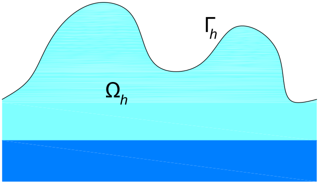

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Theory of small deformations:

- $u : \Omega_h \to \mathbb{R}^2$ being the planar displacement;
- $\boldsymbol{E}u := \frac{1}{2}(\nabla u + (\nabla u)^T)$ represents the strain;
- Energy minimum occurs at the mismatch strain $\boldsymbol{E}_0$ defined by

$$\boldsymbol{E}_0(y) := \begin{cases} e_0 \mathbf{e_1} \otimes \mathbf{e_1} & \text{if } y \geq 0, \\ 0 & \text{otherwise,} \end{cases}$$

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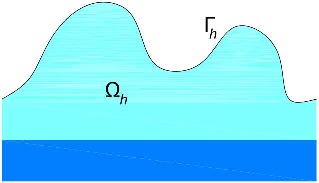

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Regular configurations:

$$X_{\rm Lip} := \{(u, h) \ : \ u \in H^1_{\rm loc}(\Omega_h; \mathbb{R}^2),\ h \in W^{1,\infty}(0, \ell),\ |\Omega_h \cap \{y > 0\}| = V\}$$

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where

- the elastic energy density is defined by $W_0(y, \boldsymbol{A}) := \frac{1}{2}\mathbb{C}_0(y)\boldsymbol{A} : \boldsymbol{A}$ for

$$\mathbb{C}_0(y) := \begin{cases} \mathbb{C}_f & \text{if } y > 0, \\ \mathbb{C}_s & \text{if } y \leq 0 \end{cases}$$

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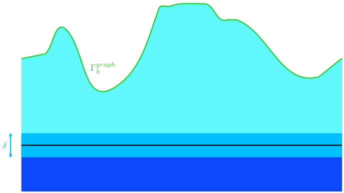
- the interface energy was neglected in [Spencer, 1999].

The Transition-Layer Model

$$\mathcal{F}_\delta(h,u) := \int_{\Omega_h} W_\delta(y, \boldsymbol{E}u(x,y) - \boldsymbol{E}_\delta(y))\,\mathrm{d}x\,\mathrm{d}y + \int_{\Gamma_h} \varphi_\delta(y)\,\mathrm{d}\mathcal{H}^1$$



for a (small) $\delta > 0$ and W_δ defined by

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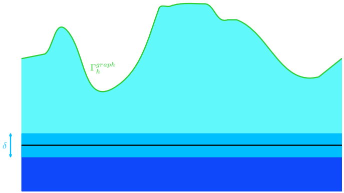

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$$\boldsymbol{E}_\delta(y) := \frac{1}{2}e_0\left(1 + f\left(\frac{y}{\delta}\right)\right)\mathbf{e_1} \otimes \mathbf{e_1},$$

$$\varphi_\delta(y) := \gamma_f\, f\left(\frac{y}{\delta}\right) + (\gamma_s - \gamma_{fs})\left(1 - f\left(\frac{y}{\delta}\right)\right),$$

with f some increasing function such that $\int_{-\infty}^0 (1 + (f(y))^2)\,dy < +\infty$,

$$f(0) = 0, \qquad \text{and} \qquad \lim_{s\to\pm\infty} f(s) = \pm 1.$$

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$$u_n + v_n \rightharpoonup u$$

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We say that $(h_n, u_n) \to (h, u)$ in X where

$$X := \{(u, h) \ : \ u \in H^1_{\mathrm{loc}}(\Omega_h; \mathbb{R}^2),\ h \in BV(0, \ell),\ h \text{ is l.s.c.},\ |\Omega_h \cap \{y > 0\}| = V\}.$$

Since h is l.s.c. and BV for every x there exist $h(x\pm)$ and
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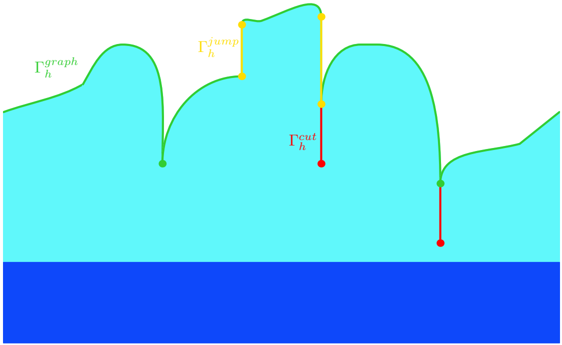

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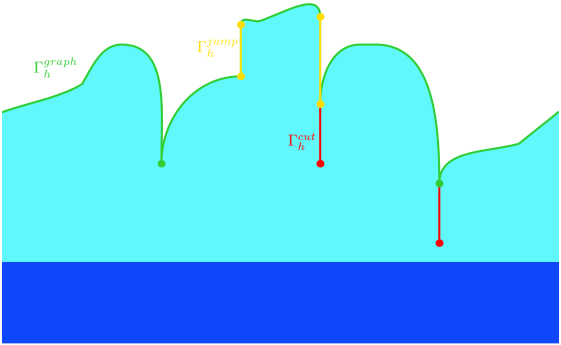

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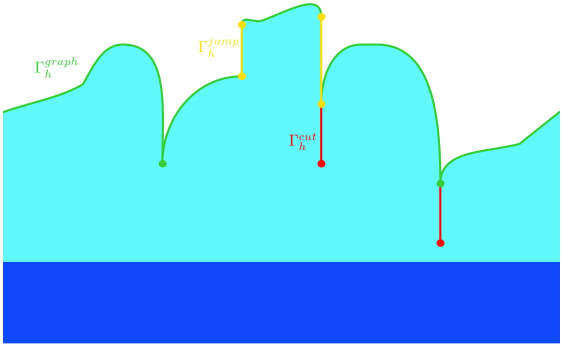

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$\Gamma_h^{graph} := \{(x, h^-(x)) : h^-(x) = h^+(x)\}$ continuous parts of Γ_h,

$\Gamma_h^{jump} := \{(x, y) : h^-(x) \leq y \leq h^+(x)\}$ jump parts of Γ_h,

and $\Gamma_h^{cut} := \{(x, y) : h(x) \leq y < h^-(x)\}$ cut parts of Γ_h.

We now consider a sharp-interface model $\mathcal{F}$ defined by

$$\mathcal{F}(u,h) := \int_{\Omega_h} W_0(y, \boldsymbol{E}u(x,y) - \boldsymbol{E}_0(y))\, dx\, dy + \int_{\widetilde{\Gamma}_h} \varphi(y)\, d\mathcal{H}^1 + 2\gamma_{\mathrm{f}} \mathcal{H}^1(\Gamma_h^{cut})$$

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Notice that:

- $\mathcal{F}$ was introduced for the case $\mathbb{C}_{\mathrm{f}} = \mathbb{C}_{\mathrm{s}}$ and $\gamma_{\mathrm{fs}} = 0$ in [Bonnetier-Chambolle, 2002] and [Fonseca-Fusco-Leoni-Morini, 2007];
- Cuts are counted twice as they are approximated by shrinking valleys;
- If $\gamma_{\mathrm{f}} \leq \gamma_{\mathrm{s}} - \gamma_{\mathrm{fs}}$, then $\varphi \equiv \gamma_f$.

Model Derivation [Davoli-P., 2017]

The energy $\mathcal{F}$ satisfies the following assertions:

1. $\mathcal{F}_\delta \xrightarrow{\Gamma} \mathcal{F}$ *in* X *as* $\delta \to 0^+$;
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$$\mathcal{F}(u,h) := \inf \Big\{ \liminf_{n\to+\infty} \mathcal{F}_0(u_n,h_n) : \, (u_n,h_n) \in X_{\mathrm{Lip}}, \\ (u_n,h_n) \to (u,h) \text{ in } X, \text{ and } |\Omega^+_{h_n}| = |\Omega^+_h| \Big\}.$$

Remark on the proof:

- For the Γ-convergence we extend the argument in [Fonseca-Fusco-Leoni-Morini, 2007] based on the integral formula for the relaxation $\bar{\mathcal{F}}_\delta$ of the $\mathcal{F}_\delta$ in X, i.e.,

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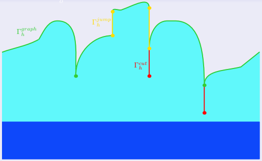
- Extra care is needed for the relaxation of the sharp-interface model for $\gamma_{\mathrm{s}} - \gamma_{\mathrm{fs}} < \gamma_{\mathrm{f}}$ in the construction of a recovery sequence that matches the volume constraint.

Proposition ([Fonseca-Fusco-Leoni-Morini, 2007], [Davoli-P., 2017])



If $(h, u) \in X$ is a minimum configuration for $\mathcal{F}$, then

- *Cusps points and vertical cuts are at most finite;*
- $\Gamma_h^{reg} := \Gamma_h \setminus (\Gamma_h^{cut} \cup \Gamma_h^{cusp})$, *where*

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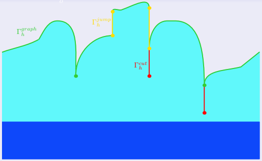

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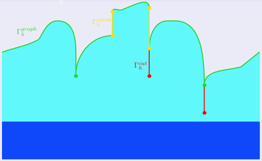

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2. Internal-Ball condition ([Chambolle, Larsen; 2003]): There exists $\rho > 0$ such that for every $z \in \overline{\Gamma}_h$ a ball B_ρ with radius ρ can be chosen so that

$$B_\rho \subset \Omega_h \qquad \text{and} \qquad \partial B_\rho \cap \overline{\Gamma}_h = \{z\}$$

   (established by a comparison argument and the isoperimetric inequality).

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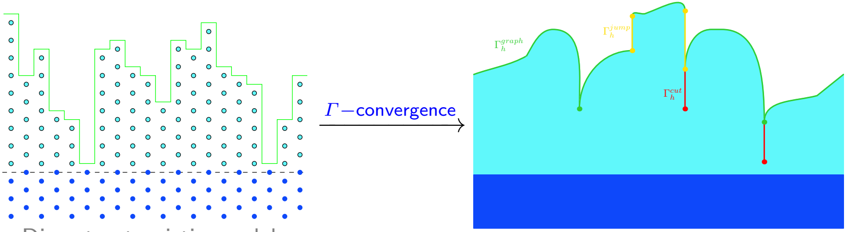

Discrete atomistic models

Functional $\mathcal{F}$

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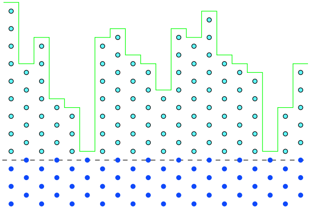
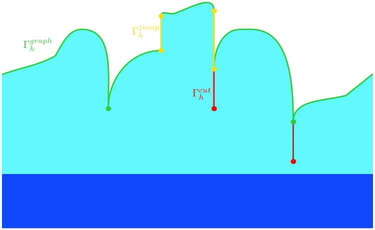


Discrete atomistic models

Γ−convergence



Functional $\mathcal{F}$

What about the contact angles of minimal profiles of $\mathcal{F}$?

4. Properties of Minimizers

$$\mathcal{F}(u,h) := \int_{\Omega_h} W_0(y, \boldsymbol{E}u(x,y) - \boldsymbol{E}_0(y))\, dx\, dy + \int_{\widetilde{\Gamma}_h} \varphi(y)\, d\mathcal{H}^1 \; + \; 2\gamma_{\mathrm{f}} \mathcal{H}^1(\Gamma_h^{cut})$$

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Evolution: surface diffusion [Fonseca-Fusco-Leoni-Morini, 2011, 2014], evaporation-condensation [P., 2012], vicinal surfaces [Dal Maso-Fonseca-Leoni, 2014] and [Fonseca-Leoni-Lu, 2015], [Lu, 2018],. . .

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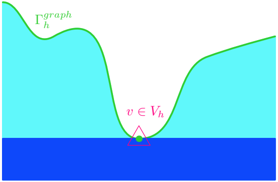
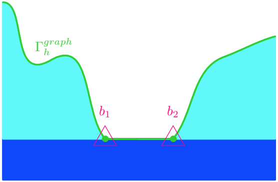
Two types of h-zeros in Z_h have nontrivial contact angles:



v is a valley.



b_1 and b_2 are island borders.

Contact-angle conditions [Davoli-P., 2017]

The following assertions hold for every μ-local minimizer $(u, h) \in X$ of $\mathcal{F}$:

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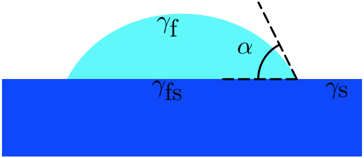
- (YD) is the Young-Dupré law;



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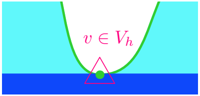

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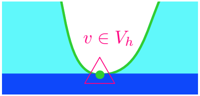
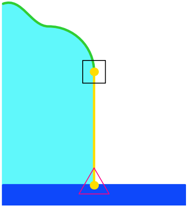


- Jumps at island borders are allowed only if $\min\{\gamma_f, \gamma_s - \gamma_{fs}\}/\gamma_f = 0$, i.e., the YD angle is $90°$;



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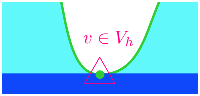

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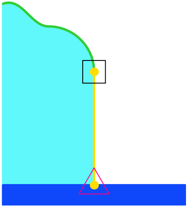
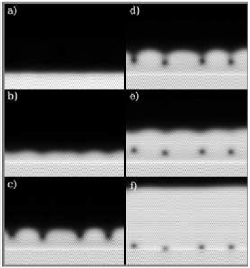
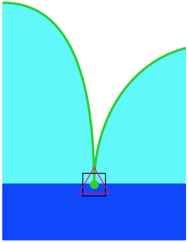
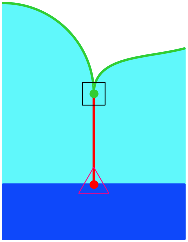


- Cusps (left) and cuts (right) may represents dislocations at the film/substrate interface observed by experiments.



Courtesy of [Elder et al., 2007].





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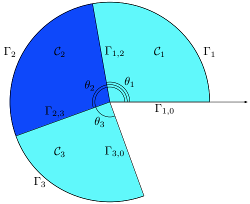
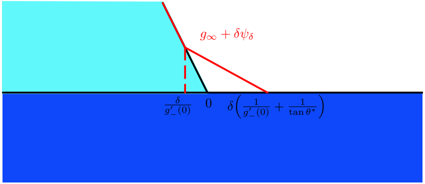
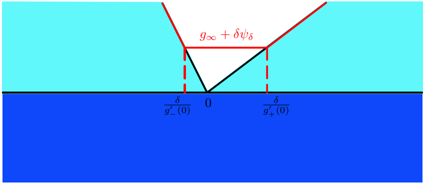
Decay obtained by contradiction and a blow-up argument in order to reduce to a transmission-problem on cones (see [Nicaise-Sändig, 1999]).



- By a suitable choice of ψ_μ depending on the point z_0 we compare with the optimal angle (red profile):



Island borders, red profile with YD angle.



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Therefore, $S_n := S_n(h + \mu\psi_n) - S_n(h) \to S(\arccos\sigma, \alpha)$ and

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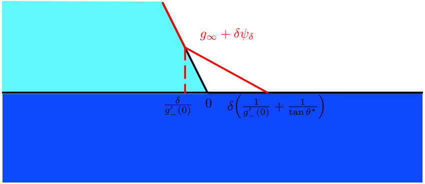

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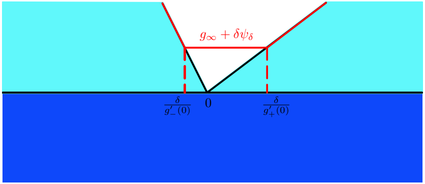

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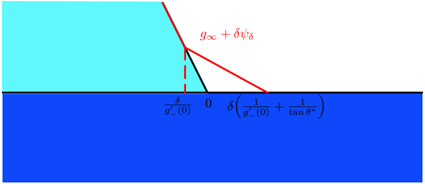

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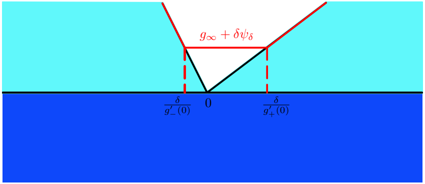

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Remark

(*i*) Equilibrium contact angles are not impacted by elastic field and depend only on surface tensions;

(*ii*) If $\gamma_{\mathrm{f}} \le \gamma_{\mathrm{s}} - \gamma_{\mathrm{fs}}$, then there is a wetting layer (FM and SK modes are preferable to VW);

(*iii*) VW occurs if and only if $\gamma_{\mathrm{f}} > \gamma_{\mathrm{s}} - \gamma_{\mathrm{fs}}$.

Further regularity [Davoli-P., 2017]

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Finally, we also have that the Euler-Lagrange equation

$$k_{\varphi,A_h} = \tau_{A_h}\left(W_0(\cdot, \boldsymbol{E}u(\cdot) - \boldsymbol{E}_0)\right) + \lambda_0 \quad \text{on } A_h,$$

holds for μ-local minimizer $(u,h) \in X$, where:

- k_{φ,A_h} is the anisotropic curvature of A_h;
- $\tau_{A_h}(\cdot)$ is the trace operator on A_h;
- λ_0 is a suitable Lagrange multiplier.

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THANK YOU FOR YOUR ATTENTION!