

A second order minimality criterion for free discontinuity problems

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Second variation and local minimality

Investigation of **sufficiency minimality conditions** based on the **second variation**, for functionals involving competing terms (bulk energies and surface energies):

- [6, 4]: Mumford-Shah functional
- [1]: diblock copolymers
- [9, 3]: epitaxial growth of elastic films
- [7]: cavities in elastic bodies

Here we develop this approach for a 3-dimensional variational model with a nonlinear elastic energy, arising in the context of epitaxial growth of strained elastic films.

The model

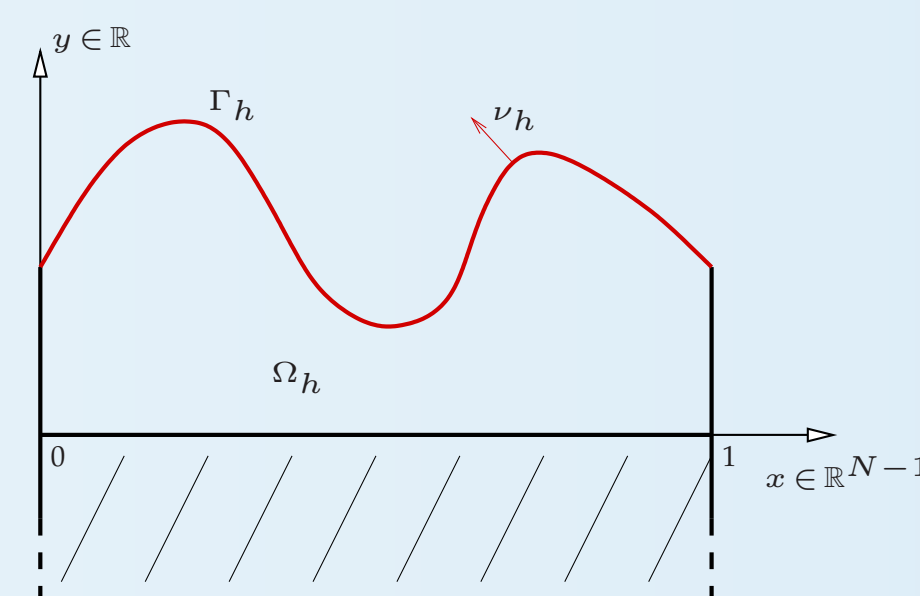
Denote $Q = (0, 1)^{N-1}$, $(x, y) \in \mathbb{R}^{N-1} \times \mathbb{R}$. We prescribe

- $d > 0$ (volume constraint)
- $u_0(x, y) := (A[x] + q(x), 0)$, with $A \in \mathbb{M}_+^{N-1}$ and $q : \mathbb{R}^{N-1} \rightarrow \mathbb{R}^{N-1}$ 1-periodic (mismatch strain at the interface $\{y = 0\}$).

Space of **admissible pairs**: $(h, u) \in X$ if

- $h : \mathbb{R}^{N-1} \rightarrow (0, +\infty)$ Lipschitz, 1-periodic in the coordinate directions,
 - $\Omega_h := \{(x, y) \in \mathbb{R}^N : x \in Q, 0 < y < h(x)\}$ (**reference configuration**),
 - $\Gamma_h := \{(x, h(x)) \in \mathbb{R}^N : x \in Q\}$ (**free profile** of the film),
 - $\Omega_h^\#, \Gamma_h^\#$ periodic extensions,
- $u : \Omega_h \rightarrow \mathbb{R}^N$ (**deformation** of the film),
- $u - Id - u_0 \in \mathcal{V}(\Omega_h)$ (Dirichlet boundary condition + periodicity), where

$$\mathcal{V}(\Omega_h) := \left\{ w \in C^1(\bar{\Omega}_h^\#; \mathbb{R}^N) : w(x, 0) = 0, w(x + e_i, y) = w(x, y) \right\}.$$



Total energy of the system:

$$F(h, u) := \int_{\Omega_h} W(\nabla u) dz + \int_{\Gamma_h} \psi(\nu_h) d\mathcal{H}^{N-1} \quad (h, u) \in X.$$

Assumptions on the **elastic energy density** and **anisotropic surface energy density**:

- $W : \mathbb{M}_+^N \rightarrow [0, +\infty)$ of class C^3 , $W(\xi) \rightarrow +\infty$ as $\det \xi \rightarrow 0^+$,
- $\psi : \mathbb{R}^N \rightarrow [0, +\infty)$ of class C^3 (away from the origin), positively 1-homogeneous, $m|z| \leq \psi(z) \leq M|z|$ for all $z \in \mathbb{R}^N$, and

$$\nabla^2 \psi(v)[w, w] > c|w|^2 \quad \text{for all } v \in S^{N-1} \text{ and } w \perp v.$$

Second variation

Assume that $(h, u) \in X$ satisfies **(H1)**, **(H2)**, **(H4)**.

Given $\varphi \in C_{per}^2(\Gamma_h)$ with $\int_{\Gamma_h} \varphi d\mathcal{H}^{N-1} = 0$, we set

$$h_t := h + t\phi, \quad \phi(x) := \varphi(x, h(x))\sqrt{1 + |\nabla h(x)|^2}.$$

Thank to **(H4)** and to the Implicit Function Theorem, if t is sufficiently small we can consider a deformation u_t satisfying **(H2)** in Ω_{h_t} (and the Dirichlet condition).

Then the function $\dot{u} = \frac{\partial u_t}{\partial t} \big|_{t=0}$ belongs to $\mathcal{V}(\Omega_h)$ and satisfies the equation

$$\int_{\Omega_h} W_{\xi\xi}(\nabla u) \nabla \dot{u} : \nabla w dz = \int_{\Gamma_h} \operatorname{div}_{\Gamma_h}(\varphi W_{\xi}(\nabla u)) \cdot w d\mathcal{H}^{N-1} \quad \text{for all } w \in \mathcal{V}(\Omega_h),$$

and the **second variation of F at (h, u) along the direction φ** is given by

$$\begin{aligned} \frac{d^2}{dt^2} F(h_t, u_t) \big|_{t=0} &= - \int_{\Omega_h} W_{\xi\xi}(\nabla u) \nabla \dot{u} : \nabla \dot{u} dz + \int_{\Gamma_h} (\nabla^2 \psi \circ \nu_h) [\nabla_{\Gamma_h} \varphi, \nabla_{\Gamma_h} \varphi] d\mathcal{H}^{N-1} \\ &\quad + \int_{\Gamma_h} (\partial_{\nu_h}(W \circ \nabla u) - \operatorname{trace}(\mathbf{B}^\psi \mathbf{B})) \varphi^2 d\mathcal{H}^{N-1} \\ &\quad - \int_{\Gamma_h} (W \circ \nabla u + H^\psi) \operatorname{div}_{\Gamma_h} \left[\left(\frac{(\nabla h, |\nabla h|^2)}{\sqrt{1 + |\nabla h|^2}} \circ \pi \right) \varphi^2 \right] d\mathcal{H}^{N-1}, \end{aligned}$$

where $\mathbf{B} = D\nu_h$, $\mathbf{B}^\psi = D(\nabla \psi \circ \nu_h)$.

Previous related results

- In [5, 8] a two-dimensional variational model for epitaxial growth of strained elastic films, in the framework of linearized elasticity, is introduced by relaxation methods
- In [8] regularity properties of minimizers are studied
- In [9] the local and global minimality of the flat configuration is discussed by means of a second variation approach to local minimality

Local minimizers

An admissible pair (h, u) is a **local minimizer** if $F(h, u) < +\infty$ and there exists $\delta > 0$ such that

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

for all $(g, v) \in X$ such that

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

Here $\Phi_g : \bar{\Omega}_h \rightarrow \bar{\Omega}_g$ is a change of variables such that

$$\|\Phi_g - Id\|_\infty \leq \|g - h\|_\infty.$$

Critical pairs

An admissible pair $(h, u) \in X$ is a **regular critical pair** if:

- (H1)** $h \in C^2$, $u \in C^2$, $\det \nabla u > 0$ in $\bar{\Omega}_h$
- (H2)** u is a critical point for the elastic energy in Ω_h , that is,

$$\begin{cases} \operatorname{div} [W_\xi(\nabla u)] = 0 & \text{in } \Omega_h \\ W_\xi(\nabla u)[\nu_h] = 0 & \text{on } \Gamma_h \end{cases} \quad (1)$$

- (H3)** $W(\nabla u) + H^\psi = \text{const}$ on Γ_h , with $H^\psi := \operatorname{div}_{\Gamma_h}(\nabla \psi \circ \nu_h)$

In addition to these conditions, we will also assume that the second variation of the elastic energy is uniformly positive:

- (H4)** for every $w \in \mathcal{V}(\Omega_h)$

$$\int_{\Omega_h} W_{\xi\xi}(\nabla u) \nabla w : \nabla w dz \geq c_0 \|w\|_{H^1(\Omega_h; \mathbb{R}^N)}^2$$

Main result

Introduce the subspace of $H^1(\Gamma_h)$

$$\tilde{H}_\#^1(\Gamma_h) := \left\{ \vartheta \in H_{loc}^1(\Gamma_h^\#) : \vartheta(x + e_i, h(x + e_i)) = \vartheta(x, h(x)), \int_{\Gamma_h} \vartheta d\mathcal{H}^{N-1} = 0 \right\}.$$

Note that the last integral in the expression of the second variation vanishes at a regular critical pair, due to **(H3)**.

We define the quadratic form $\partial^2 F(h, u) : \tilde{H}_\#^1(\Gamma_h) \rightarrow \mathbb{R}$

$$\begin{aligned} \partial^2 F(h, u)[\varphi] &:= - \int_{\Omega_h} W_{\xi\xi}(\nabla u) \nabla v_\varphi : \nabla v_\varphi dz + \int_{\Gamma_h} (\nabla^2 \psi \circ \nu_h) [\nabla_{\Gamma_h} \varphi, \nabla_{\Gamma_h} \varphi] d\mathcal{H}^{N-1} \\ &\quad + \int_{\Gamma_h} (\partial_{\nu_h}(W \circ \nabla u) - \operatorname{trace}(\mathbf{B}^\psi \mathbf{B})) \varphi^2 d\mathcal{H}^{N-1}, \end{aligned}$$

where $v_\varphi \in \tilde{\mathcal{V}}(\Omega_h)$ is the unique solution to

$$\int_{\Omega_h} W_{\xi\xi}(\nabla u) \nabla v_\varphi : \nabla w = \int_{\Gamma_h} \operatorname{div}_{\Gamma_h}(\varphi W_\xi(\nabla u)) \cdot w d\mathcal{H}^{N-1} \quad \text{for every } w \in \tilde{\mathcal{V}}(\Omega_h).$$

Theorem. Let $N = 2, 3$. Assume that $(h, u) \in X$ is a regular critical pair satisfying (H4) and

$$\partial^2 F(h, u)[\varphi] > 0 \quad \text{for every } \varphi \in \tilde{H}_\#^1(\Gamma_h) \setminus \{0\}. \quad (2)$$

Then (h, u) is a local minimizer for the functional F .

Two main steps in the proof

1. $W^{2,p}$ -local minimality ($N = 2, 3$)

- Minimality w.r.t. $W^{2,p}$ -perturbations of the profile
- Estimate carefully all the terms appearing in the expression of the second variation
- Work in fractional Sobolev spaces

2. $W^{2,p}$ -local minimality $\implies L^\infty$ -local minimality ($N \geq 2$)

- Contradiction argument: $F(h_n, u_n) < F(h, u)$, $h_n \rightarrow h$
- Consider solutions to penalization/obstacle problems
- Use the regularity theory for quasi-minimizers of the area functional to deduce $C^{1,\alpha}$ convergence
- Use Euler-Lagrange equations to deduce $W^{2,p}$ -convergence

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Application: stability of flat morphologies

Flat configuration with volume d :

$$(d, v_0), \quad v_0(z) = M[z], \quad M \in \mathbb{M}_+^N$$

satisfying **(H2)**, **(H4)** in $\Omega_d = Q \times (0, d)$.

Then:

- there exists $d_0 > 0$ such that condition (2) is satisfied at the flat configuration for every $d < d_0$;
- for large values of d , the flat configuration is no longer a local minimizer;
- **crystalline case**: assume $\psi : \mathbb{R}^N \rightarrow [0, +\infty)$ Lipschitz, convex, positively 1-homogeneous, such that the associated Wulff shape

$$W_\psi := \{z \in \mathbb{R}^N : z \cdot \nu \leq \psi(\nu) \text{ for every } \nu \in S^{N-1}\}$$

has a flat horizontal facet intersecting the y -axis. Then for every $d > 0$ the flat configuration is a local minimizer for the associated functional (if $N = 2, 3$).