Stability and minimality for a nonlocal variational problem

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Diblock Copolymers

The model

Second variation and local minimality

Copolymers

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Copolimer = product arising from the linkage of repeating units of different polymers by covalent chemical bonds

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Diblock Copolymers

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Microphase separation
Formation of nanostructures

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Multiplication of the properties
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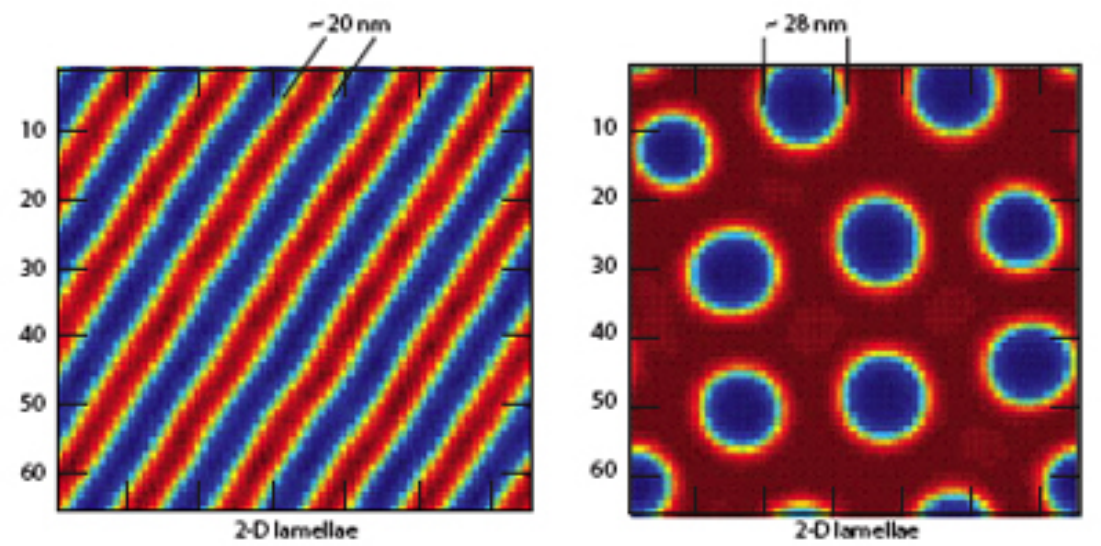
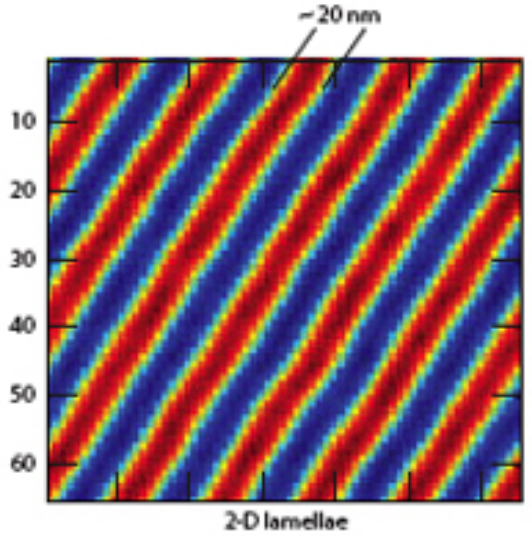
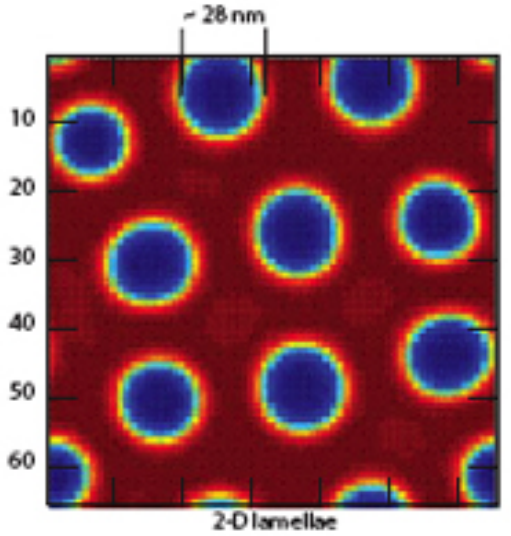
The relative lenghts of each block $\Longrightarrow$ different morphologies



Lamellae

Spheres





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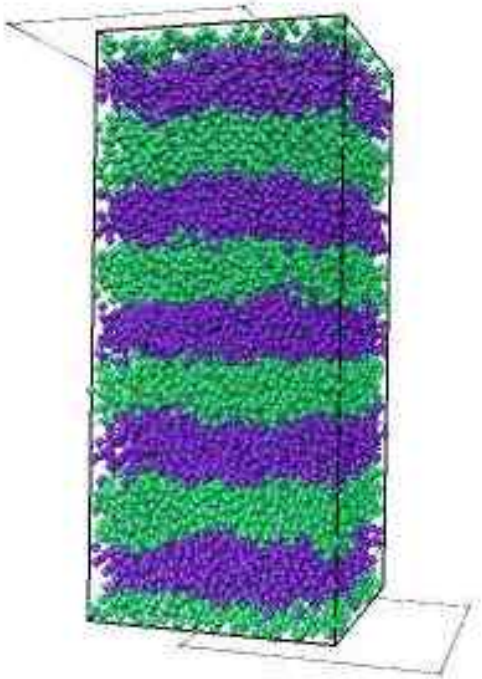

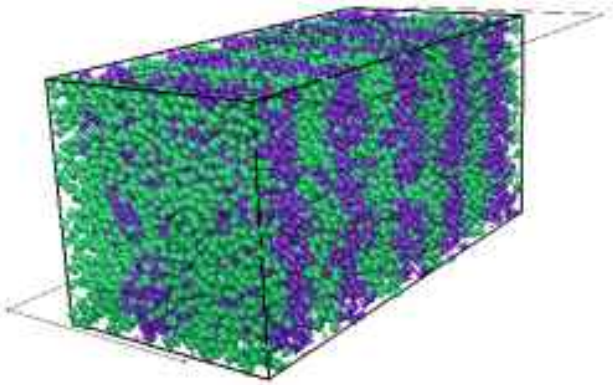

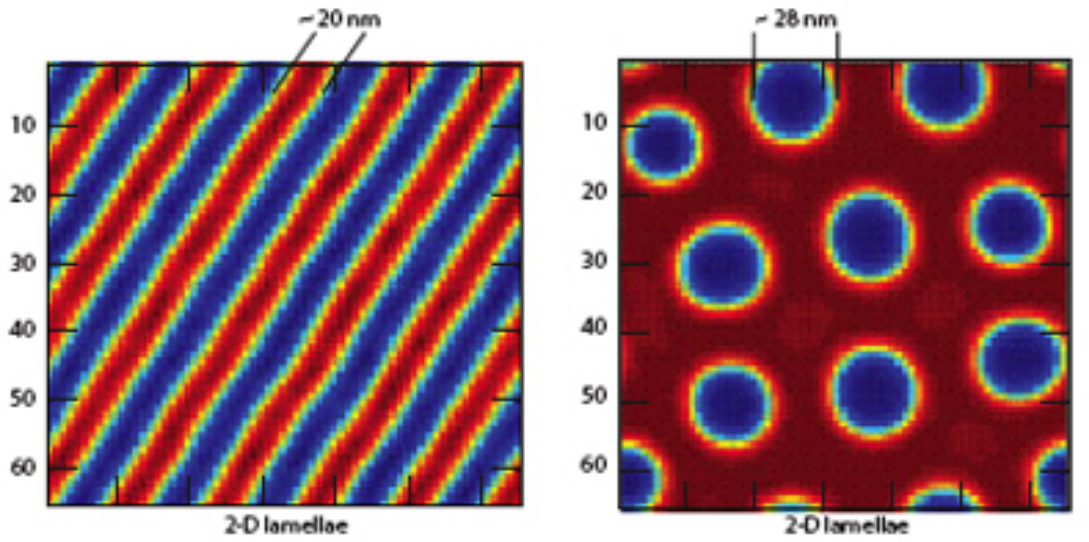

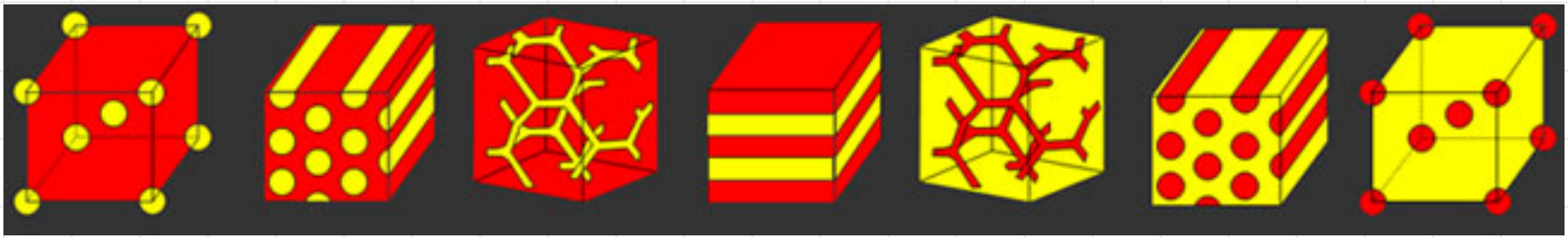

Spheres Cylinders Gyroids Lamellae

A mathematical model (Ohta-Kawasaki, 1986)

Denote by $u : \Omega \to \mathbb{R}$ the function describing the density:

$$\begin{cases} u(x) = 1 & \text{on phase } A \\ u(x) = -1 & \text{on phase } B \end{cases}$$

$$m = \frac{1}{|\Omega|} \int_\Omega u \, dx \qquad \text{fixed}$$

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$$\begin{aligned} \mathcal{E}_\varepsilon(u) &= \varepsilon\int_\Omega |\nabla u|^2 dx + \frac{1}{\varepsilon}\int_\Omega (1-u^2)^2 dx \\ &+ \gamma_0 \int_\Omega \int_\Omega G(x,y)(u-m)(u-m)\,dx\,dy \end{aligned}$$

$G(x,y)$ is the Green function for the Laplacian

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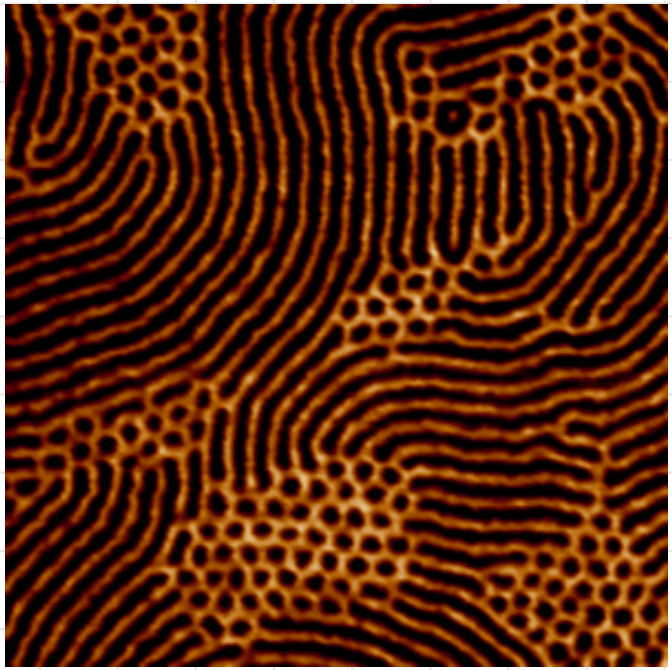

(A non homogeneous distribution at the moment of solidification
$\Rightarrow$ Different nano structures)

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$$\int_\Omega G(x,y)(u-m)(u-m)\,dx\,dy = \int_\Omega |\nabla(\Delta^{-1}(u-m))|^2 dx$$

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If we take the limit as $\varepsilon \to 0$ of the diffuse energy (Ren-Wei, 2003) the functionals $\mathcal{E}_\varepsilon$ Γ-converge in L^1 to

$$\mathcal{E}(u) = \frac{1}{2}|Du|(\Omega) + \gamma \int_\Omega |\nabla(\Delta^{-1}(u-m))|^2\,dx$$

where $\gamma = 3\gamma_0/16 \geq 0$ (Modica-Mortola),

$u \in BV(\Omega;\{-1,1\})$, i.e. $u = \chi_E - \chi_{\Omega\setminus E}$, $|Du|(\Omega) = 2P(E;\Omega)$

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Geometric formulation of the energy

$$E \mapsto J(E) = P(E;\Omega) + \gamma \int_\Omega |\nabla(\Delta^{-1}(u_E - m_E))|^2 \, dx$$

where $u_E = \chi_E - \chi_{\Omega\setminus E}$, $m_E = |E| - |\Omega \setminus E|$

. . . in the end we will come back to the diffuse energy

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Choksi-Sternberg, 2007: calculated J'' at critical points

Ren-Wei, 2002–2008: critical spheres, cylinders and lamellae with $J'' > 0$ minimize the energy with respect to some special variations

Cicalese-Spadaro, 2013: global minimality of a single droplet with a very small mass

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$$\begin{cases} -\Delta v_E = u_E - m & \text{in } \mathbb{T}^n \\ \int_{\mathbb{T}^n} v_E = 0 \end{cases}$$

$$m = 2|E| - 1 \Rightarrow |E| = \frac{m+1}{2}$$

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E.L. equation for C^2 minimizers of $J(E)$ with a volume constraint

$$(E.L.) \qquad H_{\partial E}(x) + \gamma v_E(x) = \lambda \qquad \text{on } \partial E$$

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Any C^2 solution E of (E.L.) will be called a regular critical point
(Spheres, cylinders, gyroids, lamellae are always r.c.p. if $\gamma = 0$)

Local Minimizers

Distance between (equivalence classes) of sets:

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Natural definition: $E \subset \mathbb{T}^n$ is a (strict) local minimizers if $\exists \delta > 0$ s.t.

$$J(F) > J(E)$$

whenever $F \subset \mathbb{T}^n$ with $0 < d(E,F) < \delta$, and $|F| = |E|$

Easy fact:

$$\left| \int_{\mathbb{T}^n} |\nabla v_E|^2 \, dx - \int_{\mathbb{T}^n} |\nabla v_F|^2 \, dx \right| \leq c|E \Delta F|$$

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E is a minimizer with volume constraint $\longleftrightarrow$

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Consequence: Regularity of local minimizers

In fact the local minimizers of

$$J(E) = P_{\mathbb{T}^n}(E) + \gamma \int_{\mathbb{T}^n} |\nabla v_E|^2 \, dx$$

are ω-almost minimizers of the perimeter:

$$P_{\mathbb{T}^n}(E) \leq P_{\mathbb{T}^n}(F) + \omega r^n$$

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Theorem (Julin-Pisante)

If $E \subset \mathbb{T}^n$ is a local minimizer of J, then $\partial E \setminus \Sigma$ is C^∞, for any $\alpha < 1$, and Σ is a closed set such that $\dim_{\mathcal{H}}(\Sigma) \leq n - 8$

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Let $E \in C^2$, and fix a C^2 vector field $X : \mathbb{T}^n \mapsto \mathbb{T}^n$. Then, let us consider

$\Phi : \mathbb{T}^n \times (-1, 1) \mapsto \mathbb{T}^n$ the associated flow

$$\frac{\partial \Phi}{\partial t} = X(\Phi), \qquad \Phi(x, 0) = x$$

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$$\frac{d^2}{dt^2} J(E_t)\Big|_{t=0}$$

Theorem 1 (Acerbi-F.-Morini 2013)

If E and X are as above, then

$$\frac{d^2}{dt^2} J(E_t)\Big|_{t=0} = \int_{\partial E} \Big(|D_\tau (X\cdot\nu)|^2 - |B_{\partial E}|^2 (X\cdot\nu)^2 \Big)\, d\mathcal{H}^{n-1}$$
$$+ 8\gamma \int_{\partial E}\int_{\partial E} G(x,y)\big(X\cdot\nu\big)(x)\big(X\cdot\nu\big)(y) d\mathcal{H}^{n-1}(x) d\mathcal{H}^{n-1}(y)$$
$$+ 4\gamma \int_{\partial E} \partial_\nu v_E (X\cdot\nu)^2 d\mathcal{H}^{n-1}$$
$$- \int_{\partial E} (4\gamma v_E + H_{\partial E}) \mathrm{div}_\tau \big(X_\tau (X\cdot\nu)\big)\, d\mathcal{H}^{n-1}$$
$$+ \int_{\partial E} (4\gamma v_E + H_{\partial E})(\mathrm{div} X)(X\cdot\nu)\, d\mathcal{H}^{n-1}$$

$|B_{\partial E}|^2 =$ sum of the squares of principal curvatures

Some simplifications:

If Φ is volume preserving, i.e., $|E_t| = |E|$,

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Therefore the second variation reduces to (Choksi-Sternberg, 2007)

$$\frac{d^2}{dt^2} J(E_t)\Big|_{t=0} = \int_{\partial E} \Big(|D_\tau (X \cdot \nu)|^2 - |B_{\partial E}|^2 (X \cdot \nu)^2 \Big)\, d\mathcal{H}^{n-1}$$
$$+ 8\gamma \int_{\partial E} \int_{\partial E} G(x,y) \big(X \cdot \nu\big)(x) \big(X \cdot \nu\big)(y) d\mathcal{H}^{n-1}(x)\, d\mathcal{H}^{n-1}(y)$$
$$+ 4\gamma \int_{\partial E} \partial_\nu v_E (X \cdot \nu)^2\, d\mathcal{H}^{n-1}$$

Since the second variation depends only on $X \cdot \nu$,

it is natural to define for a C^2 critical point E

$$\partial^2 J(E)[\varphi] = \int_{\partial E} \left(|D_\tau \varphi|^2 - |B_{\partial E}|^2 \varphi^2 \right) d\mathcal{H}^{n-1}$$
$$+ 8\gamma \int_{\partial E} \int_{\partial E} G(x,y)\varphi(x)\varphi(y) d\mathcal{H}^{n-1}(x)\, d\mathcal{H}^{n-1}(y)$$
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Remark: $\int_{\partial E} X \cdot \nu \, d\mathcal{H}^{n-1} = \frac{d|E_t|}{dt}_{|t=0} = 0$ (if the associated flow is volume preserving)

then we shall assume $\int_{\partial E} \varphi = 0$

Translation invariance

Infinitesimal volume preserving deformations $\Rightarrow$

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$\Longrightarrow \quad J''(E)[\tau \cdot \nu_E(x)] = 0 \quad$ for all $\tau \quad \Longrightarrow \quad J''(E)[\nu_i] = 0 \quad \forall i$

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Let us define $T = \text{span}\{\nu_1, \dots \nu_n\}$ and let us decompose

$$\widetilde{H}^1 = T \oplus T^\perp \qquad \text{where}$$

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$$T^\perp = \{\varphi \in H^1(\partial E) : \int \varphi = \int \varphi \nu_i = 0\}$$

$J''(E) > 0$ then means $J''(E)[\varphi] > 0 \quad \forall \varphi \in T^\perp \setminus \{0\}$

A preliminary quantitative estimate:

Theorem 2 ($W^{2,p}$ local minimality – Acerbi-F.-Morini 2013)
Let E be a C^2 critical point s.t.

$$\partial^2 J(E)[\varphi] > 0 \qquad \forall \varphi \in T^{\perp}(\partial E) \setminus \{0\}\,,$$

and let $p > \max\{2, n-1\}$. There exist $\delta > 0$ and $C_0 > 0$ s.t. if $F \subset \mathbb{T}^n$,

$$d(E,F) < \delta \qquad |F| = |E|$$

and

$$\partial F = \{x + \psi(x)\nu(x) : x \in \partial E\}, \text{ with } \|\psi\|_{W^{2,p}(\partial E)} < \delta,$$

then

$$(Q) \qquad J(F) \geq J(E) + C_0[d(E,F)]^2$$

Key points of the proof:

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Construction of a suitable volume preserving flow:

For any $\varepsilon > 0$ there exist $\delta, C > 0$ and a neighborhood U of ∂E s.t., given F, with $|F| = |E|$ and

$$\partial F = \{x + \psi(x)\nu(x) : x \in \partial E\}, \text{ with } \|\psi\|_{W^{2,p}(\partial E)} < \delta,$$

we may construct a vector field $X \in C^2(U)$, with $\operatorname{div} X = 0$, s.t.

$$\|X - \psi\nu\|_{L^2(\partial E)} \leq \varepsilon \|\psi\|_{L^2(\partial E)}$$

and the associated flow

$$\Phi(x, 0) = x, \quad \frac{\partial \Phi}{\partial t} = X(\Phi)$$

satisfies

$$\|\Phi(\cdot, t) - \mathrm{Id}\|_{W^{2,p}} \leq C\|\psi\|_{W^{2,p}}, \qquad |E_t| \equiv |E|, \qquad E_1 = F$$

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(Partial) removal of the translational component:

For any $\varepsilon > 0$, there exist $\delta, C > 0$ s.t. if

$$\partial F = \{x + \psi(x)\nu(x) : x \in \partial E\}, \text{ with } \|\psi\|_{W^{2,p}(\partial E)} < \delta,$$

there exist $\sigma \in \mathbb{R}^n$, $\varphi \in W^{2,p}(\partial E)$ s.t. $|\sigma| + \|\varphi\|_{2,p} \leq C\|\psi\|_{2,p}$, and

$$\partial F - \sigma = \{x + \varphi(x)\nu(x) : x \in \partial E\}, \quad \left|\int_{\partial E} \varphi \nu^E\right| \leq C\delta\|\varphi\|_2$$

From $W^{2,p}$ to L^1 local minimality

Theorem 3 (L^1 local minimality – Acerbi-F.-Morini 2013)

Let $E \subset \mathbb{T}^n$ be a C^2 local minimizer of J with respect to $W^{2,p}$-variations.
There exists $\delta > 0$ s.t. for all $F \subset \mathbb{T}^n$ with $|F| = |E|$ and $d(E,F) < \delta$

$$J(F) \geq J(E) + \frac{C_0}{4} d(E,F)^2 \, .$$

(C_0 is the constant of the $W^{2,p}$ theorem)

Consequences: the Ohta-Kawasaki energy

Proposition

If E is a regular critical point of J with $J''(E) > 0$, then there exists a family $\{u_\varepsilon\}_{\varepsilon<\varepsilon_0}$ of strict local minimizers of the diffused energy $\mathcal{E}_\varepsilon$ with $\int_{\mathbb{T}^n} u_\varepsilon \, dx = \int_{\mathbb{T}^n} u_E \, dx$, s.t.

$$u_\varepsilon \to u_E \qquad \text{in} \quad L^1(\mathbb{T}^n)$$

as $\varepsilon \to 0$.

Consequences: $\gamma = 0 \implies$ quantitative isop. ineq.

Corollary

Let $E \subset \mathbb{T}^n$ be smooth open set with constant mean curvature. If

$$\int_{\partial E} \left(|D_\tau \varphi|^2 - |B_{\partial E}|^2 \varphi^2 \right) d\mathcal{H}^{n-1} > 0 \qquad \forall\, \varphi \in T^\perp(\partial E) \setminus \{0\}\,,$$

there exist δ, $C > 0$ s.t. for $F \subset \mathbb{T}^n$, with $|F| = |E|$ and $d(E,F) < \delta$

$$P_{\mathbb{T}^n}(F) \geq P_{\mathbb{T}^n}(E) + C[d(E,F)]^2\,.$$

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$$\int_{\partial E} \left(|D_\tau \varphi|^2 - |B_{\partial E}|^2 \varphi^2 \right) d\mathcal{H}^{n-1} > 0 \qquad \forall\, \varphi \in T^\perp(\partial E) \setminus \{0\}\,,$$

there exist δ, $C > 0$ s.t. for $F \subset \mathbb{T}^n$, with $|F| = |E|$ and $d(E,F) < \delta$

$$P_{\mathbb{T}^n}(F) \geq P_{\mathbb{T}^n}(E) + C[d(E,F)]^2\,.$$

The local minimality w.r.t. L^∞ perturbations (B.White, 1994) or w.r.t. L^1 perturbations ($\Rightarrow n \leq 7$, Morgan-Ros, 2010)
In both cases there was no quantitative estimate

Consequences: $\gamma = 0 \implies$ quantitative isop. ineq.

Corollary

Let $E \subset \mathbb{T}^n$ be smooth open set with constant mean curvature. If

$$\int_{\partial E} \left(|D_\tau \varphi|^2 - |B_{\partial E}|^2 \varphi^2 \right) d\mathcal{H}^{n-1} > 0 \qquad \forall\, \varphi \in T^\perp(\partial E) \setminus \{0\}\,,$$

there exist δ, $C > 0$ s.t. for $F \subset \mathbb{T}^n$, with $|F| = |E|$ and $d(E,F) < \delta$

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Corollary

$$P(F) \geq P(B) + C[d(B,F)]^2 \qquad \forall\, F \subset \mathbb{R}^n\,, \quad |F| = |B| = \omega_n$$

(Fusco-Maggi-Pratelli 2008, Figalli-Maggi-Pratelli 2010, Cicalese-Leonardi 2011)

Application: Global minimality of a single lamella

$$(\mathcal{P}) \qquad \text{Min} \left\{ J(E) = P_{\mathbb{T}^n}(E) + \gamma \int_{\mathbb{T}^n} |\nabla v_E|^2 \, dx \,, \qquad |E| = d \right\}$$

$$\begin{cases} -\Delta v_E = u_E - m \quad \text{in } \mathbb{T}^n \\ \int_{\mathbb{T}^n} v_E = 0 \end{cases}$$

$$u_E = \chi_E - \chi_{\mathbb{T}^n \setminus E}, \quad m = 2|E| - 1$$

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For $0 < d < 1$ set

$$L = \mathbb{T}^{n-1} \times [0, d]$$

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Theorem 4

Assume that L is the unique, up to translations and relabelling of coordinates, global minimizer of the periodic isoperimetric problem. Then L is also the unique global minimizer of $(\mathcal{P})$, provided γ is sufficiently small.

Let $n = 2$. Theorem 4 + Howards-Hutchings-Morgan, 1999

$$\Downarrow$$

If $\frac{1}{\pi} < d < 1 - \frac{1}{\pi}$, L is the unique global minimizer of $(\mathcal{P})$ in $\mathbb{T}^2$ provided γ is small (see also Sternberg-Topaloglu, 2011)

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If $\frac{1}{\pi} < d < 1 - \frac{1}{\pi}$, L is the unique global minimizer of $(\mathcal{P})$ in $\mathbb{T}^2$ provided γ is small (see also Sternberg-Topaloglu, 2011)

Let $n = 3$. Theorem 4 + a result of Hadwiger, 1972

$$\Downarrow$$

There exist $\varepsilon_0, \gamma_0 > 0$ s.t. if $\frac{1}{2} - \varepsilon_0 < d < \frac{1}{2} + \varepsilon_0$, $0 \leq \gamma < \gamma_0$

L is the unique global minimizer of $(\mathcal{P})$ in $\mathbb{T}^3$

Application: Local minimality of multiple strips lamellae

$$(\mathcal{P}) \qquad \text{Min} \left\{ J(E) = P_{\mathbb{T}^n}(E) + \gamma \int_{\mathbb{T}^n} |\nabla v_E|^2 \, dx \,, \qquad |E| = d \right\}$$

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For $0 < d < 1, k > 1$ and set

$$L_k = \mathbb{T}^{n-1} \times \cup_{i=1}^{k} \left[\tfrac{i-1}{k}, \tfrac{i-1}{k} + \tfrac{d}{k} \right]$$

Application: Local minimality of multiple strips lamellae

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Proposition

Fix d and $\gamma > 0$. Then there exists k_0 such that if $k \geq k_0$ the set L_k is a strict local minimizer for $(\mathcal{P})$

Extensions to the Neumann case

$$J_N(E) = P_\Omega(E) + \gamma \int_\Omega |\nabla v_E|^2 \, dx, \qquad |E| = d = \omega_n r^n < |\Omega|$$

$$\begin{cases} -\Delta v_E = u_E - m & \text{in } \Omega \\ \int_\Omega v_E = 0, \ \frac{\partial v_E}{\partial \nu} = 0 & \text{on } \partial\Omega \end{cases} \qquad u_E = \chi_E - \chi_{\Omega\setminus E}, \quad m = \fint_\Omega u_E$$

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Cicalese-Spadaro, 2013: If Ω is C^2 and bounded and

$$\gamma r^3 |\log r| \ll 1 \ (n = 2), \qquad \gamma r^3 \ll 1 \ (n \geq 3),$$

then the unique global minimizer is a convex set E such that

$$\partial E = \{x + (r + \varphi(\omega))\omega : \omega \in \mathbb{S}^{n-1}\}, \qquad \|\varphi\|_{C^1(\mathbb{S}^{n-1})} \leq c(n)\gamma r^{n+3}$$

Moreover E is a ball iff Ω is a ball.

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Julin-Pisante, 2014: Local minimality (with a quantitative estimate) for critical points of J_N with positive second variation

Application of Julin-Pisante local minimality result: Global minimality of multiple strips lamellae

Theorem 5 (Morini-Sternberg, 2014)

Fix $d \in (0,1)$. For any integer $k \geq 1$ there exists $\varepsilon(k,d) << 1$ such that if $0 < \varepsilon < \varepsilon(k,d)$ and

$$\frac{12k^2(k-1)^2}{2k-1} < \gamma < \frac{12k^2(k+1)^2}{2k+1},$$

then the horizontal multiple strips lamellae

$$L_k = (0,\varepsilon) \times \cup_{i=1}^{k} \left(\tfrac{i-1}{k}, \tfrac{i-1}{k} + \tfrac{d}{k}\right)$$

are the unique global minimizer in $\Omega_\varepsilon = (0,\varepsilon) \times (0,1)$ of the minimum problem

$$(\mathcal{P}_N) \qquad Min \left\{ J_N(E) = P_{\Omega_\varepsilon}(E) + \gamma \int_{\Omega_\varepsilon} |\nabla v_E|^2 \, dx \,, \qquad |E| = \varepsilon d \right\}$$