An isoperimetric problem with applications to diblock copolymer melts

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Regularity theory for elliptic and parabolic systems
and problems in continuum mechanics
Telč, May 1, 2014

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Polymer = a chain of many equal molecular structures,
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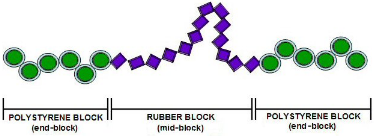
Multiplication of properties

An example

Three-block copolymer

Styrene-Butadiene-Styrene



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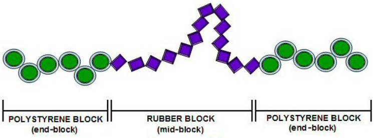
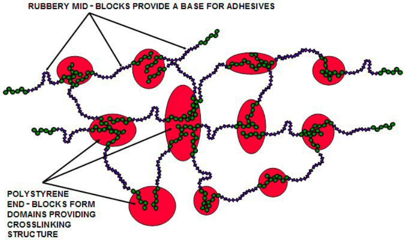


When cold, rigid – a little tacky – rigid



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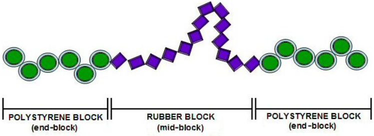

When hot, very fluid – viscous, adhesive – very fluid

Diblock copolymers

$$\cdots\text{-A-A-A-A-A-A-B-B-B-B-B-B-}\cdots$$

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Microscale phase separation
Nanostructures

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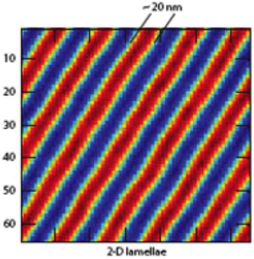
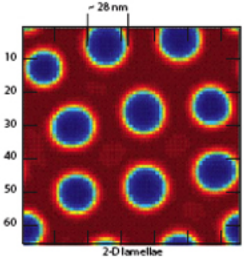
Proportion of components $\Longrightarrow$ different nanostructures
(also given by confinement, viewpoint disregarded here)

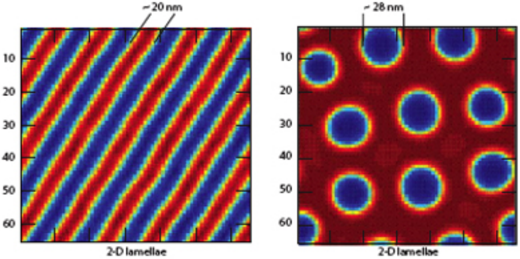
Lamellae



Spheres



Lamellae Spheres



Spheres Cylinders Gyroids Lamellae

Ability to self-assemble in different nanostructures according to proportion $\Rightarrow$ Applications in nanoengineering

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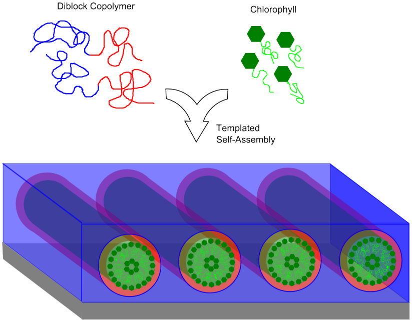

Building CHLOROSOMES

Mathematical model (Ohta-Kawasaki)

$u : \Omega \to \mathbb{R}$ describes density:

$$\begin{cases} u(x) = 1 & \text{in phase } A \\ u(x) = -1 & \text{in phase } B \end{cases} \qquad m = \frac{1}{|\Omega|} \int_\Omega u \, dx \quad \text{fixed}$$

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

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

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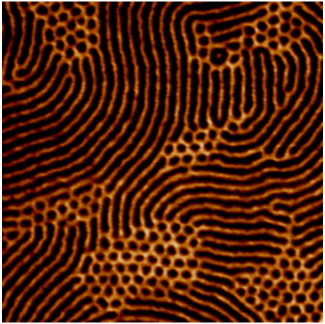

(Non homogeneous distribution at solidification time
$\Rightarrow$ Different nanostructures)

$G(x,y)$ Green's function for the Laplacian $\Rightarrow$

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

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Mathematically easier to handle: (Ren-Wei, 2003) as $\varepsilon \to 0$ the functionals $\frac{3}{16}\,\mathcal{E}_\varepsilon$ 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 $\gamma = 3\gamma_0/16 \geq 0$ (from Modica-Mortola),

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

For an easier handling . . .

Diffuse energy $\quad u \mapsto \mathcal{E}_\varepsilon(u)$

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Geometric version

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

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

. . . then we will try to get back

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Problem: are critical points at which $J'' > 0$ local minimizers?

Choksi-Sternberg: computation of J'' at critical points

Ren-Wei: for spheres, cylinders and lamellae $J'' > 0$ (under certain restrictions)

Ross: gyroids are strictly stable constant mean curvature surfaces

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E.L. equation for (smooth) minimizers of $J(E)$ under volume constraint

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

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a regular critical point is a solution $E \in C^2$ of $(E.L.)$
(Spheres, cylinders, gyroids and lamellae are r.c.p.)

Translation invariance

We shall see that on r.c.p. the second variation depends on normal displacement on the boundary of E, thus a function of the type

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

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

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

Remark:

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Consequence: Regularity of local minimizers

Sternberg-Topaloglu 2011 for $N = 2$

Local minimizers of

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

are (ω, R)-minimizers of the area functional:

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

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Theorem

If $E \subset \mathbb{T}^n$ is a local minimizer of J, then $\partial^* E \setminus \Sigma$ is $C^{3,\alpha}$ for all $\alpha < 1$, and the closed set Σ satisfies $\dim_{\mathcal{H}}(\Sigma) \leq n - 8$

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consider $\quad T = \mathcal{L}\{\nu_1, \dots \nu_n\}$

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

so

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

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

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

Good decomposition; indeed

$$J''(E) > 0 \quad \Rightarrow \quad J''(E)[\varphi] \geq m_0 \|\varphi\|_{H^1} \qquad \forall \varphi \in T^{\perp}$$

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

Theorem 1 (A.-Fusco-Morini; Choksi-Sternberg 2007)

If $X(x) := \dfrac{\partial \Phi}{\partial t}(x,0)$, *we have*

$$\frac{d^2}{dt^2} J(E_t)\Big|_{t=0} = \int_{\partial E} \Big(|D_\tau (X\cdot\nu)|^2 - |B_{\partial E}|^2 (X\cdot\nu)^2 \Big)\, d\mathcal{H}^{n-1}$$

$$+ 8\gamma \int_{\partial E}\int_{\partial E} G(x,y)(X\cdot\nu)(x)(X\cdot\nu)(y)\, d\mathcal{H}^{n-1}(x)\, d\mathcal{H}^{n-1}(y)$$

$$+ 4\gamma \int_{\partial E} \partial_\nu v_E (X\cdot\nu)^2\, d\mathcal{H}^{n-1}$$

$$- \int_{\partial E} (4\gamma v_E + H_{\partial E})\,\mathrm{div}_\tau\big(X_\tau (X\cdot\nu)\big)\, d\mathcal{H}^{n-1}$$

$$+ \int_{\partial E} (4\gamma v_E + H_{\partial E})(\mathrm{div} X)(X\cdot\nu)\, d\mathcal{H}^{n-1}$$

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

Simplifications:

If Φ is volume preserving, that is $|E_t| = |E|$,

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Then (↑) the second variation reduces (Choksi-Sternberg) to

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

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Remark: $\int_{\partial E} X \cdot \nu\, d\mathcal{H}^{n-1} = \frac{d|E_t|}{dt}\Big|_{t=0} = 0$ if volume-preserving

For every critical point E of class C^2 set

$$\partial^2 J(E)[\varphi] = \int_{\partial E} \Big(|D_\tau \varphi|^2 - |B_{\partial E}|^2 \varphi^2 \Big)\, d\mathcal{H}^{n-1} + 8\gamma \int_{\partial E} \int_{\partial E} G(x,y)\varphi(x)\varphi(y) d\mathcal{H}^{n-1}(x)\, d\mathcal{H}^{n-1}(y) + 4\gamma \int_{\partial E} \partial_\nu v_E\, \varphi^2\, d\mathcal{H}^{n-1}$$

for all $\varphi \in \widetilde{H}^1(\partial E)$

A first quantitative result:

Theorem 2 ($W^{2,p}$ perturbations — A.-Fusco-Morini)

Let E be a C^2 critical point with

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

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

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

and

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

then

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

Key points:

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Construction of a volume-preserving flow:

in a neighbourhood of ∂E there exists a smooth field X with $\operatorname{div} X = 0$ s.t. the associated flow

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

satisfies

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

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Removal (control) of the translation part:

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

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

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

Theorem 3 (L^1 perturbations — A.-Fusco-Morini)

Let $E \subset \mathbb{T}^n$ be a regular critical point of J such that

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

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 appearing in the $W^{2,p}$ theorem)

Consequences: Ohta-Kawasaki energy

Proposition

If E regular critical point of J with $J''(E) > 0$, there exists a family $\{u_\varepsilon\}_{\varepsilon<\varepsilon_0}$ of isolated local minimizers of the diffuse energy $\mathcal{E}_\varepsilon$ with prescribed volume $m = \int_{\mathbb{T}^n} u_E \, dx$ such that

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

as $\varepsilon \to 0$.

$\gamma = 0$: area and quantitative isoperimetric inequality

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Corollary

If $E \subset \mathbb{T}^n$ is regular and has constant mean curvature, and 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 all $F \subset \mathbb{T}^n$ 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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Known only for L^∞ perturbations, or with minimal surface methods ($\Rightarrow n \leq 7$) but always with no quantitative estimate (Morgan-Ros, 2010)

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Corollary

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

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

Key points:

B. White (Almgren)'s theorem

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If some ω-minimizers E_h of the area functional converge in L^1 to a C^2 set, for large h the boundary ∂E_h is a graph on ∂E:

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with ψ_h of class $C^{1,1/2}$ and $\psi_h \to 0$ in $C^{1,\alpha}$ for $\alpha < 1/2$ (this implies closeness in L^∞).

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Extension: Neumann case

Minimality for Lamellae:

Corollary (Single lamella)

If a single lamella of volume m is the unique global minimizer (*) of the isoperimetric problem in $\mathbb{T}^n$ with volume constraint, then also of $P_{\mathbb{T}^n} + \gamma \cdot$nonlocal term, provided γ small.

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By contradiction, sequence (E_h, γ_h) with $\gamma_h \to 0$, but then

$$J_h = P_{\mathbb{T}^n} + \gamma_h N.L.T.$$

Γ-converges to $P_{\mathbb{T}^n}$

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(*) known to be true if $N = 2$ for $|m| < 1 - 2/\pi$; if $N = 3$ only for $m = 0$ (Hadwiger).

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In any dimension, the set of values m for which the lamella is the unique minimizer of the perimeter is open.

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Corollary (Cases $N = 2$ and $N = 3$)

If $N = 2$ and $|m| < 1 - 2/\pi$ or $N = 3$ and $|m| < m_3$ then for all $\gamma < \gamma_0$ the single lamella is the unique minimizer of $P_{\mathbb{T}^n} + \gamma \cdot N.L.T.$

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For any m and γ, there esists k_0 such that for $k \geq k_0$ the k-lamellar set with volume parameter m is an isolated local minimizer of $P_{\mathbb{T}^n} + \gamma \cdot N.L.T$.

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E.A., N. Fusco, M. Morini: Minimality via second variation for a nonlocal isoperimetric problem, Commun. Math. Phys. 322 (2013)

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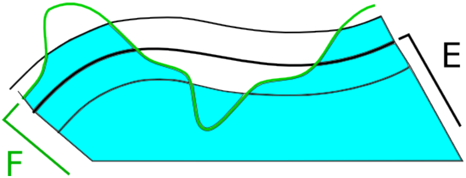
(Penalization + obstacle)

Compare $J(F)$ with $J(F_h)$, truncation at a distance h (on both sides) from ∂E



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(Penalization + obstacle)

Compare $J(F)$ with $J(F_h)$, truncation at a distance h (on both sides) from ∂E: for large h volume is preserved and F_h solves (another penalization) a problem without obstacle $\Rightarrow$ is a regular graph and (lots of computations ...) the curvatures are equibounded, so ψ_h equibounded in $W^{2,p}$ ... curvatures converge strongly in L^p

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Via penalization, one can apply Almgren's theorem (in particular $F_h \to E$ in $C^{1,\alpha}$), then needs a delicate comparison between the decay speeds of $d(E_h, E)$ and $J(E_h) - J(E)$.

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From $W^{2,p}$ to L^{∞} perturbations

From L^{∞} to L^{1} perturbations

Extension: Neumann case

Theorem 3 in the case $\gamma = 0$

Let $E \subset \mathbb{T}^n$ a C^2 open set with constant mean curvature s.t.

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

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Step 1 By Theorem 2, if $|F| = |E|$,

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

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We argue by contradiction, assuming that this is not true, i.e.

there exist E_h such that, $|E_h| = |E|$,

$$\varepsilon_h = d(E_h, E) \to 0, \qquad P_{\mathbb{T}^n}(E_h) < P_{\mathbb{T}^n}(E) + \frac{C_0}{4} d(E_h, E)^2$$

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Step 3 Consider the minimizers F_h of the following problems

$$(1) \quad \mathrm{Min}\left\{ P_{\mathbb{T}^n}(F) + \Lambda_1 \sqrt{\left(d(F,E) - \varepsilon_h\right)^2 + \varepsilon_h} + \Lambda_2 \big| |F| - |E| \big| \right\}$$

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One can prove:

- if Λ_2 is sufficiently large (independently on Λ_1), then $|F_h| = |E|$

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(2) $$J(F) + \Lambda_1 d(F,E) + \Lambda_2 \big| |F| - |E| \big|$$

- if Λ_1 is sufficiently large (independently on Λ_2), the only minimizer of the functional in (2), is E (up to a translation), hence

$$\chi_{F_h} \to \chi_E \quad \text{in } L^1(\mathbb{T}^n)$$

- each F_h is a (ω, R)-minimizer of the perimeter, hence

$\partial F_h = \{x+\psi_h(x)\nu(x) : x \in \partial E\}$, $\psi_h \to 0$ in $C^{1,\alpha}(\partial E)$, $\alpha \in (0, 1/2)$

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Impossible!

$$H_{\partial F_h} = \begin{cases} \dfrac{\Lambda_1\big(d(F_h,E)-\varepsilon_h\big)}{\sqrt{\big(d(F_h,E)-\varepsilon_h\big)^2+\varepsilon_h}}\,\mathrm{sign}\,(\chi_{F_h}-\chi_E)+\lambda_h & \text{on } \partial F_h\setminus\partial E, \\ \lambda & \text{on } \partial F_h\cap\partial E, \end{cases}$$

for some Lagrange multipliers $\lambda_h \to \lambda$.

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for some Lagrange multipliers $\lambda_h \to \lambda$. Since $\varepsilon_h^{-1} d(F_h,E) \to 1$,

$H_{\partial F_h} \to H_{\partial E}$ in $L^\infty(\partial E)$ $\Longrightarrow$ $\psi_h \to 0$ in $W^{2,p}(\partial E)\ \forall p \geq 1$

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$$H_{\partial F_h} \to H_{\partial E} \text{ in } L^\infty(\partial E) \quad \Longrightarrow \quad \psi_h \to 0 \text{ in } W^{2,p}(\partial E)\ \forall p \geq 1$$

But
$$\begin{aligned} P_{\mathbb{T}^n}(F_h) + \Lambda_1\sqrt{\varepsilon_h} &\leq P_{\mathbb{T}^n}(F_h) + \Lambda_1\sqrt{\big(d(E_h,E)-\varepsilon_h\big)^2+\varepsilon_h} \\ &\leq P_{\mathbb{T}^n}(E_h) + \Lambda_1\sqrt{\varepsilon_h} \leq P_{\mathbb{T}^n}(E) + \frac{C_0}{4}\varepsilon_h^2 + \Lambda_1\sqrt{\varepsilon_h} \\ &\leq P_{\mathbb{T}^n}(E) + \frac{C_0}{2} d(F_h,E)^2 + \Lambda_1\sqrt{\varepsilon_h} \end{aligned}$$

$$H_{\partial F_h} = \begin{cases} \dfrac{\Lambda_1\big(d(F_h,E)-\varepsilon_h\big)}{\sqrt{\big(d(F_h,E)-\varepsilon_h\big)^2+\varepsilon_h}}\,\mathrm{sign}\,(\chi_{F_h}-\chi_E)+\lambda_h & \text{on } \partial F_h\setminus\partial E, \\ \lambda & \text{on } \partial F_h\cap\partial E, \end{cases}$$

for some Lagrange multipliers $\lambda_h\to\lambda$. Since $\varepsilon_h^{-1}d(F_h,E)\to 1$,

$$H_{\partial F_h}\to H_{\partial E} \text{ in } L^\infty(\partial E) \quad\Longrightarrow\quad \psi_h\to 0 \text{ in } W^{2,p}(\partial E)\ \forall p\geq 1$$

But
$$\begin{aligned} P_{\mathbb{T}^n}(F_h)+\Lambda_1\sqrt{\varepsilon_h} &\leq P_{\mathbb{T}^n}(F_h)+\Lambda_1\sqrt{\big(d(E_h,E)-\varepsilon_h\big)^2+\varepsilon_h} \\ &\leq P_{\mathbb{T}^n}(E_h)+\Lambda_1\sqrt{\varepsilon_h}\leq P_{\mathbb{T}^n}(E)+\frac{C_0}{4}\varepsilon_h^2+\Lambda_1\sqrt{\varepsilon_h} \\ &\leq P_{\mathbb{T}^n}(E)+\frac{C_0}{2}d(F_h,E)^2+\Lambda_1\sqrt{\varepsilon_h} \end{aligned}$$

$$\Longrightarrow \quad P_{\mathbb{T}^n}(F_h)\leq P_{\mathbb{T}^n}(E)+\frac{C_0}{2}d(F_h,E)^2$$

Contradiction to the $W^{2,p}$-minimality of E!