On minimizers of Helfrich energy for two-phase biomembranes

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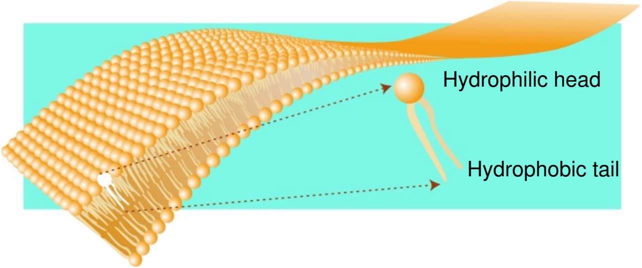
Biological membranes

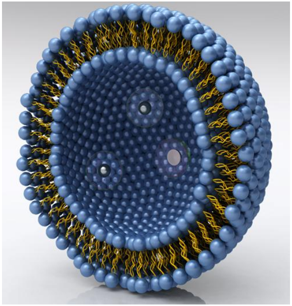
A lipid bilayer [Picture: M. A. Peletier and M. Röger]



Mechanical properties:

- in-plane fluid behaviour
- resistance to stretching
- bending elasticity

Artificial membranes



Section of an artificial liposome
[Picture: lyposphericnutrients.co.uk]

Applications:

- Pharmacology (deliverers of drugs)
- Bioengineering
- Gene-therapy
- Medical diagnostics

Modelling membranes

The model by Helfrich: elasticity "*as a special case of the well-established theory of thin elastic shells*"[1].

Helfrich's strain energy density

$$w = \frac{\kappa}{2}\left(\boxed{H} - H_0\right)^2 + \kappa_G \boxed{K}$$

Mean curvature
$H = k_1 + k_2$

Gauss curvature
$K = k_1 k_2$

[1] W. Helfrich, Elastic Properties of Lipid Bilayers: Theory and Possible Experiments, *Z. Naturforsch.*, vol. 28c (1973)

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Helfrich's strain energy density

$$w = \frac{\kappa}{2}\left(\boxed{H} - H_0\right)^2 + \kappa_G \boxed{K}$$

Mean curvature $H = k_1 + k_2$

Spontaneous curvature

Gauss curvature $K = k_1 k_2$

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Modelling membranes

Shape configurations are modeled as minimizers of

$$F(\mathcal{S}) := \sum_i \frac{\kappa}{2} \int_{S_i} (H - H_0)^2 \, d\sigma + \kappa_G \int_{S_i} K \, d\sigma$$

on $\mathcal{M}$:= systems of surfaces $\mathcal{S} = (S_1, \ldots, S_k)$ such that

- S_i is axisymmetric
- $\partial S_i = \emptyset$
- $\sum |S_i| = A$
- $\sum \mathrm{Vol}\,(S_i) = V$

Note: if $A \geq |\partial B_V|$, this set is not empty (w/ strict inequality, the set is infinite)

Axial symmetry

Question:

Find the maximal set Ω of parameters (H_0, A, V) such that the global minimizer, in the class of *embedded* surfaces, is axisymmetric.

(note: $(0, 4\pi r^2, 4\pi r^3/3) \in \Omega \subset \{A \geq |\partial B_V|\}$)

Gauss-Bonnet theorem

Let $\chi(S)$ be the Euler-Poincaré characteristic of the surface S ($\chi =$ Faces-Edges+Vertices, for any triangulation)

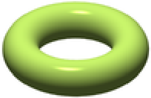
The genus is defined as

$$g(S) = \frac{2 - \chi(S)}{2}.$$

Gauss-Bonnet Theorem ($k_g :=$ geodesic curvature)

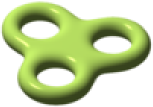
$$\int_S K \, d\sigma + \int_{\partial S} k_g \, ds = 2\pi\chi(S) \quad (= 4\pi(1 - g(S)))$$

$g = 0$



$g = 1$

$g = 2$



$g = 3$

Modelling membranes

Theorem

If $A \geq |\partial B_V|$, $\kappa > 0$ and $\kappa_G/\kappa > -2$, the minimization problem

$$\min_{\mathcal{S} \in \mathcal{M}} F(\mathcal{S})$$

has at least one solution.

where

$$F(\mathcal{S}) := \sum_i \frac{\kappa}{2} \int_{S_i} (H - H_0)^2 \, d\sigma + \kappa_G \int_{S_i} K \, d\sigma$$

$\mathcal{M}$:= systems of surfaces $\mathcal{S} = (S_1, \ldots, S_k)$ such that

- S_i is axisymmetric
- $\partial S_i = \emptyset$
- $\sum |S_i| = A$
- $\sum \text{Vol}\,(S_i) = V$

The direct method in the calculus of variations

General scheme: given $F : X \to \mathbb{R}$,

let $m := \inf \{F(u) : u \in X\}$, to prove: $\boxed{\exists\, u \in X : F(u) = m}$

- Step 0

  by definition: $\exists\, u_n \in X : F(u_n) \to m.$

- Step 1

  show that: $\exists\, u_{n_k}, u \in X : u_{n_k} \to u.$

- Step 2

  show that: $\liminf_{k\to\infty} F(u_{n_k}) \geq F(u).$

The direct method in the calculus of variations

Given Helfrich's functional $F : \mathcal{M} \to \mathbb{R}$,

- Step 1: F-bounded sequences are compact

$$\forall\, \mathcal{S}_n : F(\mathcal{S}_n) \le C \quad \Rightarrow \quad \exists\, \mathcal{S}_{n_k} \to \mathcal{S} \in \mathcal{M}.$$

- Step 2: F is lower-semicontinuous

$$\liminf_{n\to\infty} F(\mathcal{S}_n) \ge F(\mathcal{S}) \qquad \forall\, \mathcal{S}_n \to \mathcal{S}.$$

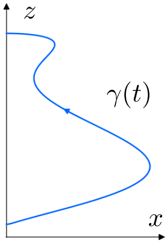
- Step 3: Continuity of constraints

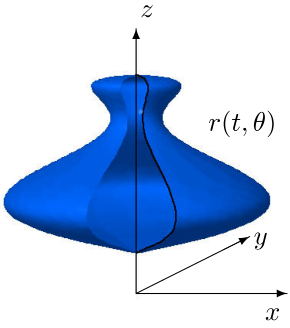
$$|\mathcal{S}_n| \to |\mathcal{S}|, \qquad \text{Vol}\,(\mathcal{S}_n) \to \text{Vol}\,(\mathcal{S})$$

Crucial point!

in which sense $\mathcal{S}_n \to \mathcal{S}$?

Surfaces of revolution





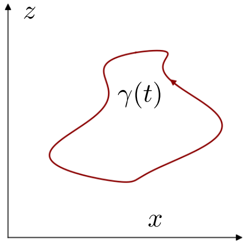
$\gamma : [0,1] \to \mathbb{R}^2$

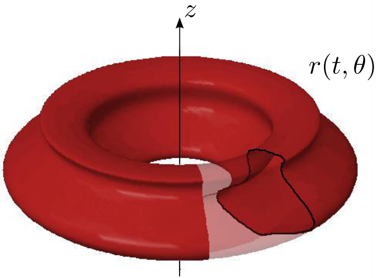
$\gamma(t) = [\gamma_1(t), \gamma_2(t)]$

$r : [0,1] \times [0, 2\pi] \to \mathbb{R}^3$

$r(t,\theta) = [\gamma_1(t)\cos(\theta), \gamma_1(t)\sin(\theta), \gamma_2(t)]$

Surfaces of revolution





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Surfaces of revolution

Principal curvatures:

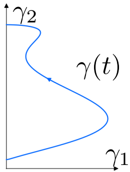
$$k_1 = \frac{\ddot{\gamma}_2\dot{\gamma}_1 - \ddot{\gamma}_1\dot{\gamma}_2}{|\dot{\gamma}|^3} \quad \text{(meridian)} \qquad k_2 = \frac{\dot{\gamma}_2}{\gamma_1|\dot{\gamma}|} \quad \text{(parallel)}$$

$$\text{Area:} \quad |S| = 2\pi \int_0^1 \gamma_1|\dot{\gamma}|\,dt \qquad \text{Volume:} \quad \text{Vol}\,(S) = \pi \int_0^1 \gamma_1^2\dot{\gamma}_2\,dt.$$

Helfrich energy:

$$F(S) = \int_S \frac{\kappa}{2}(H - H_0)^2 + \kappa_G K\,d\sigma$$

$$= \int_0^1 \Big[\frac{\kappa}{2}\,(k_1 + k_2 - H_0)^2 + \kappa_G k_1 k_2\Big] 2\pi\gamma_1|\dot{\gamma}|\,dt.$$



Compactness - bounds

Note:

- $k_1^2 + k_2^2 = H^2 - 2K$
- if $\kappa > 0$ and $\kappa_G/\kappa > -2$

$$\int_S k_1^2 + k_2^2 \, d\sigma \leq C\,(F(S) + |S|)$$

$$\Rightarrow \quad \int_0^1 k_1^2 + k_2^2 \;\; 2\pi\,\gamma_1|\dot{\gamma}|\,dt \leq C$$

On sequences γ^n

- vanishing control on curvatures (on e.g. $\{\gamma_1^n \leq 1/n\}$)
- need compactness and l.s.c. with respect to a *moving* measure

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On sequences γ^n

- vanishing control on curvatures (on e.g. $\{\gamma_1^n \leq 1/n\}$)
- need compactness and l.s.c. with respect to a *moving* measure

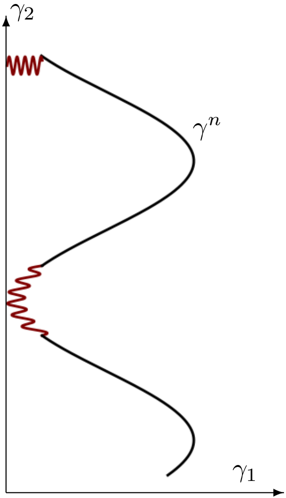
...or lack of bounds

Problem: γ_1 “close to 0"

Can there be $\{\gamma^n\}$ with

- $|\dot{\gamma}^n| \equiv L$
- $\dot{\gamma}^n \rightharpoonup \dot{\gamma}$?
- $|\dot{\gamma}| < L$

e.g.



Implication:

Area may not converge

...or lack of bounds

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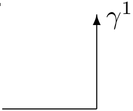

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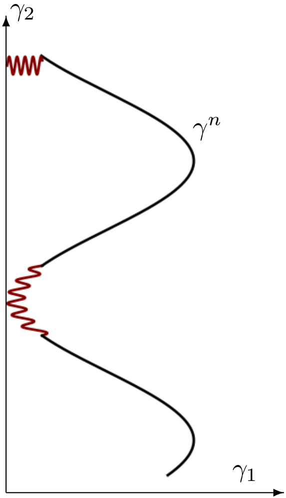

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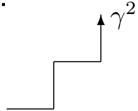

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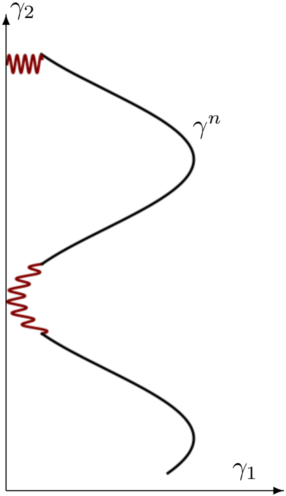

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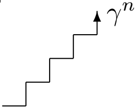

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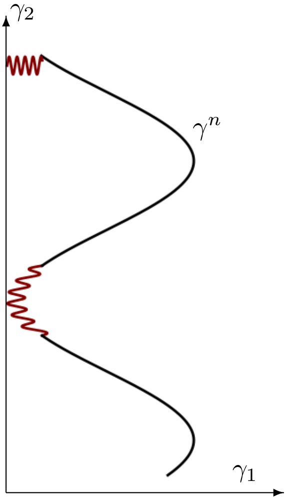

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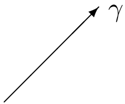

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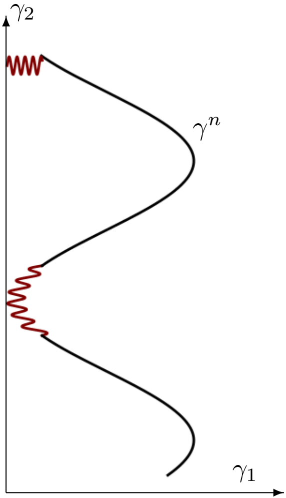


[Hutchinson, *Indiana Univ. Math. J.*, 1986]

Compactness and lower-semicontinuity for sequences of functions $\{f_n\}$ and measures $\{\mu_n\}$ such that $\int (f_n)^2 d\mu_n < C$.

- Define: (weak) convergence of function-measure pairs

$$(f_n, \mu_n) \rightharpoonup (f, \mu) \quad \text{iff} \quad \begin{cases} \mu_n \overset{*}{\rightharpoonup} \mu & \text{in } RM(\mathbb{R}) = (C_c^0(\mathbb{R}))' \\ \int f_n \phi \, d\mu_n \to \int f \phi \, d\mu & \forall\, \phi \in C_c^0(\mathbb{R}) \end{cases}$$

- (Generalized compactness) If $\mu_n \overset{*}{\rightharpoonup} \mu$ and $\int (f_n)^2 d\mu_n < C$

$$\Rightarrow \quad \exists\, (f_{n_k}, \mu_{n_k}) \rightharpoonup (f, \mu)$$

- (Generalized lower-semicontinuity) If $(f_n, \mu_n) \rightharpoonup (f, \mu)$

$$\Rightarrow \quad \liminf_{n\to\infty} \int (f_n)^2 d\mu_n \geq \int (f)^2 d\mu$$

Compactness - bounds

Bound on length

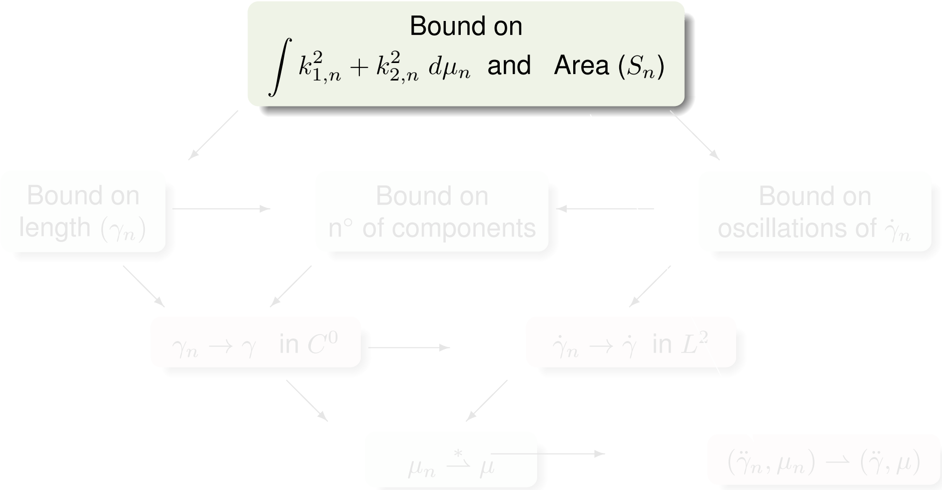
$$\text{length}(\gamma) \leq \frac{\sqrt{|S|}}{2\pi} \left\{ \left(\int_S k_1^2 \, d\sigma \right)^{1/2} + \left(\int_S k_2^2 \, d\sigma \right)^{1/2} \right\}.$$

Bound on oscillations

For all $(a, b) \subseteq (0, 1)$

$$4\pi |\dot{\gamma}_1(b) - \dot{\gamma}_1(a)| \leq |\dot{\gamma}|^2 \int_a^b \left(k_1^2 + k_2^2 \right) \, 2\pi \gamma_1 |\dot{\gamma}| \, dt.$$

Sketch of the proof



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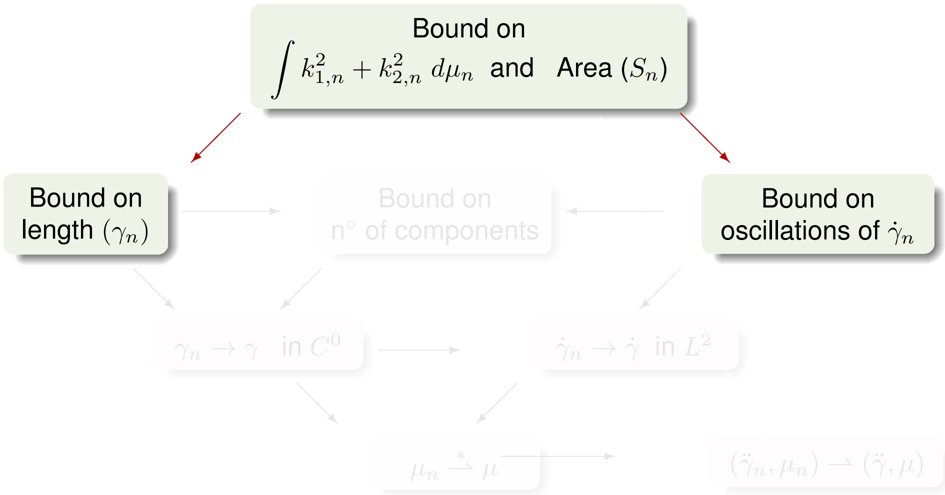

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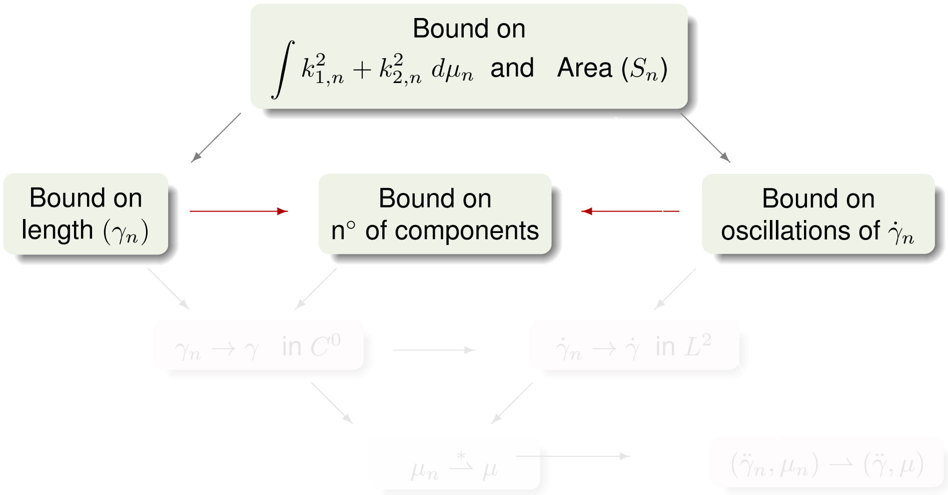

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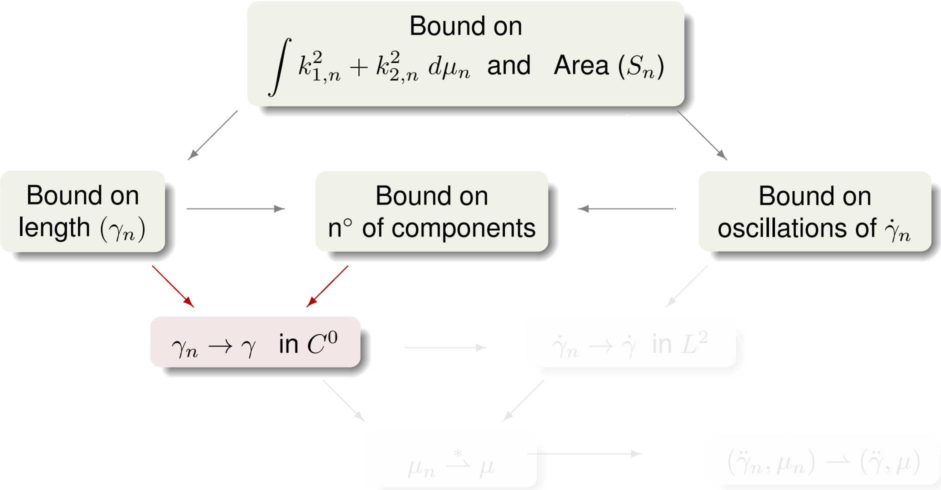

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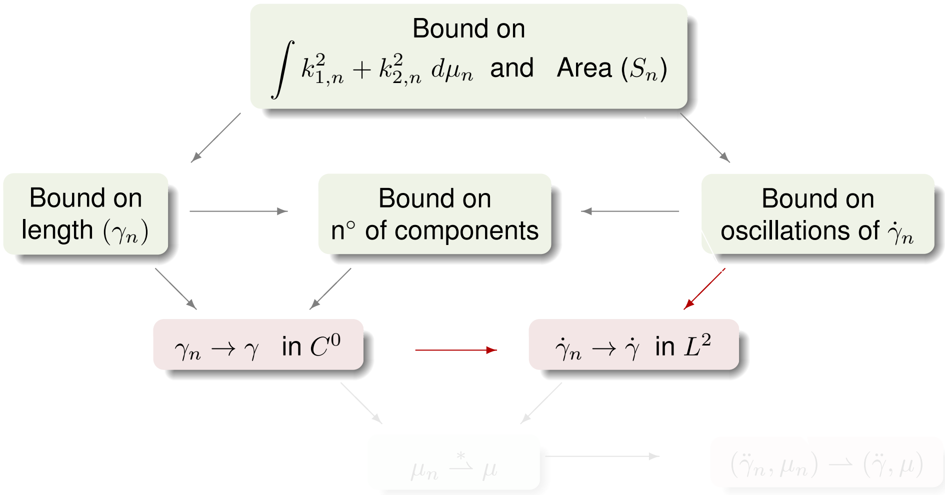

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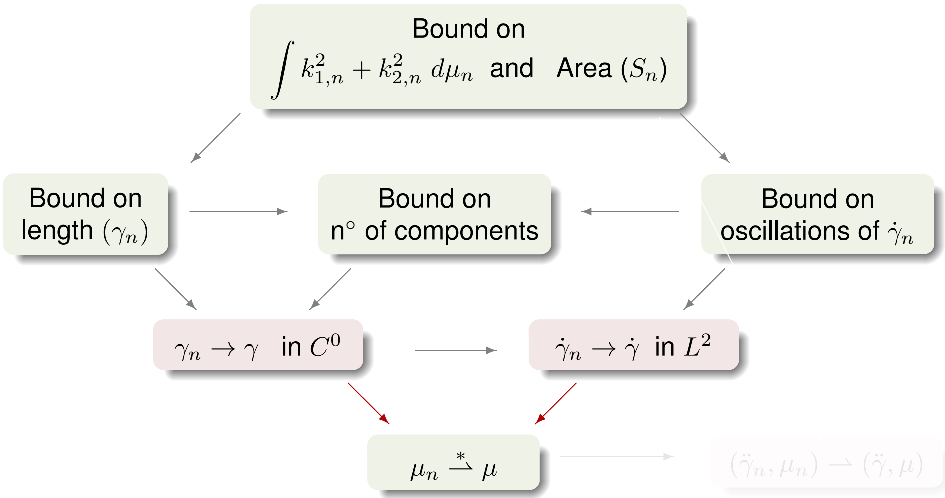

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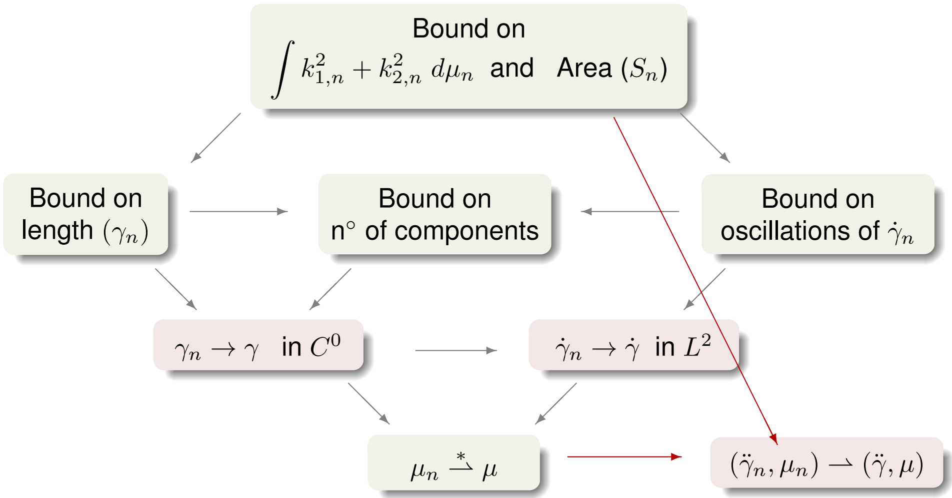
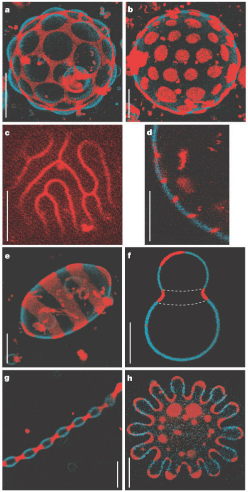
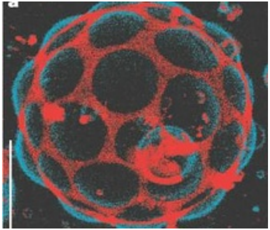


Multiphase membranes

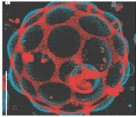


Phase separation of *rafts* on Giant Unilamellar Vesicles



[T. Baumgart, S. T. Hess, W. W. Webb, *Imaging coexisting fluid domains in biomembrane models coupling curvature and line tension*, Nature, 2003.]

Modelling multiphase membranes



Energy of a 2-domain shape $S = S_a \cup S_b$

$$F(S) = \int_{S_a} \frac{\kappa^a}{2}\left(H - H_0^a\right)^2 + \kappa_G^a K$$ Helfrich's energy on S_a

$$+ \int_{S_b} \frac{\kappa^b}{2}\left(H - H_0^b\right)^2 + \kappa_G^b K$$ Helfrich's energy on S_b

$$+ \int_{\Gamma} \sigma$$ Line tension[2]

$\Gamma = \partial S_a = \partial S_b$

[2] R. Lipowsky, Budding of membranes induced by intramembrane domains. *J. Phys. II France 2*, 1992.

Modelling multiphase membranes

Alternative model - sharp interface: introduce a phase indicator $\varphi : S \to \{0,1\}$

$$F(S,\varphi) := \int_S \left\{ \frac{\kappa(\varphi)}{2} (H - H_0(\varphi))^2 + \kappa_G(\varphi)\, K \right\} + \sigma \mathscr{H}^1(\Gamma)$$

$$\begin{aligned} \kappa(0) &= \kappa^a \\ \kappa(1) &= \kappa^b \end{aligned} \qquad \begin{aligned} H_0(0) &= H_0^a \\ H_0(1) &= H_0^b \end{aligned} \qquad \begin{aligned} \kappa_G(0) &= \kappa_G^a \\ \kappa_G(1) &= \kappa_G^b \end{aligned}$$

$\mathscr{H}^1(\Gamma) =$ one-dimensional Hausdorff measure of Γ

Modelling multiphase membranes

Phases on a curve $\varphi : \gamma \to \mathbb{R}$

vs

parametrized phases $\tilde{\varphi} = \varphi \circ \gamma : [0,1] \to \mathbb{R}$

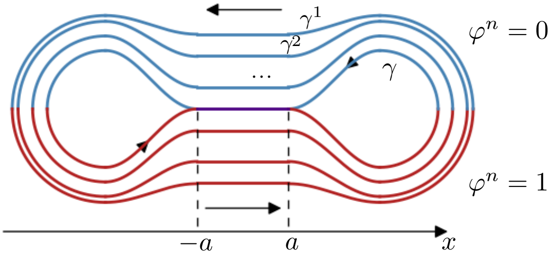


Figure: The problem of defining the phase on a curve when overlapping can arise as limit of well-defined configurations (γ^n, φ^n).

Modelling multiphase membranes

Theorem

If $A \geq |\partial B_V|$, $\kappa > 0$ and $\kappa_G/\kappa > -2$, the minimization problem

$$\min_{\mathcal{S} \in \mathcal{M}} F(\mathcal{S})$$

has at least one solution (for every fixed phase-area value).

where

$$F(\mathcal{S}) := \sum_i \int_{S_i} \left\{ \frac{\kappa(\varphi)}{2} (H - H_0(\varphi))^2 + \kappa_G(\varphi) K \right\} + \sigma \mathscr{H}^1(\Gamma_i)$$

$\mathcal{M}$:= systems of surface-phase couples $\mathcal{S} = ((S_1, \varphi_1), \ldots, (S_k, \varphi_k))$ with

- S_i is C^1, axisymmetric
- $\sum |S_i| = A$
- $\sum \mathrm{Vol}\,(S_i) = V$
- $\partial S_i = \emptyset$
- $\varphi_i \in BV_{\mathrm{loc}}((0,1); \{0,1\})$

Sketch of the proof

- Compactness
  - Surfaces: as for one-phase membranes

    Ascoli-Arzelà for curves on a fixed interval

  - Phases: BV compactness + L^∞ bound

$$\varphi^n \to \varphi \quad \text{in } L^p, \qquad \varphi \in BV_{\text{loc}}$$

- Lower semicontinuity
  - $\sigma \mathscr{H}^1(\Gamma)$:

    l.s.c. for $BV_{\text{loc}} + \ldots$

  - Mean and Gaussian curvatures:

    l.s.c. for function-measure pairs, with phase-dependent measures

References:

- R. Choksi, M. V.
  Global minimizers for the doubly-constrained Helfrich energy: the axisymmetric case (submitted).
- R. Choksi, M. Morandotti, M. V.
  Global minimizers for multi-phase axisymmetric membranes (submitted).
- M. Helmers.
  Convergence of an approximation for rotationally symmetric two-phase lipid bilayer membranes (submitted).

Thank you for your attention !!