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Partial Localisation in Lipid Bilayers

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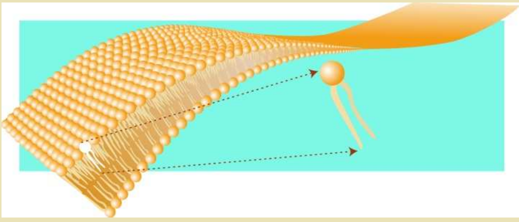
Lipid Bilayers

Biological membranes, two lipid molecules thick



A bilayer consisting of lipid molecules

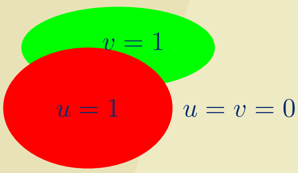
Properties of the Membranes

- ✶ Partial localisation: codimension-one objects
- ✶ Elastic properties: bending stiffness, stretching stiffness and resistance to fracturing

A Macroscopic Energy

Energy with two competing terms: interface and distance penalisation

$$F(u,v) = \sum_{i,j\in\{u,v,w\}}^{k} d_{ij}\,\text{Area}(\text{interface } i \leftrightarrow j) + \frac{1}{\delta}\|u-v\|^2_{H^{-1}},$$



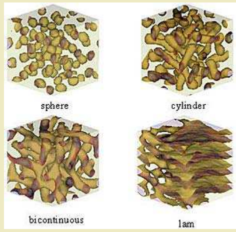
A configuration of heads ($v = 1$), tails ($u = 1$) and water ($u = v = 0$)

- ✶ $u, v : \mathbb{R}^N \supset \Omega \to \mathbb{R}$
  v is the volume fraction of heads, u of tails
  $w := 1/\delta - (u+v)$ is the volume fraction of the solvent (e.g. water)
- ✶ $u(x), v(x) \in \{0, 1/\delta\}$ almost everywhere
  $uv = 0$ almost everywhere
  Same mass of heads and tails: $\int_\Omega u = \int_\Omega v = m$
- ✶ Coefficients d_{ij} for interface penalisation, $\forall i,j,k\ :\ d_{ij} \le d_{ik} + d_{kj}$
- ✶ Scaling coefficient $\delta > 0$ gives typical thickness of the structures

We are interested in minimisers of F/m. What happens in the limit $\delta \downarrow 0$?

Origin of the Model

- ✶ Similar to diblock copolymers (Ohta-Kawasaki‡)



Some possible morphologies for diblock copolymers

- ✶ Our model follows in the sharp interface Γ-limit of the Ohta-Kawasaki energy

Results in One Dimension $(N = 1)$

- ✶ Heads and tails stay close together, forming layers
- ✶ These layers have a preferred width: stretching stiffness
- ✶ When monolayers combine the tails stick together

Theorem

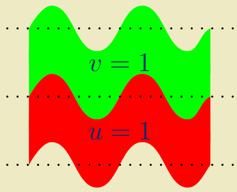
Let $d_{uw}, d_{vw} > 0$. Then for the energy of minimisers:

1. $d_{uv} = 0 \Rightarrow F \gtrsim m^{\frac{N-1}{N}}$ as $m \to \infty$
2. $d_{uv} > 0 \Rightarrow F \gtrsim m$ as $m \to \infty$

The scaling in 2 is the same as for a plate or cylinder. The plate has lowest energy of these two configurations.

Other Interesting Findings

- ✶ Fixed mass and $\delta \downarrow 0$ is equivalent to fixed δ and $m \to \infty$
- ✶ Calculation on monolayers suggests that the stability depends on the choice of d_{ij}



A critical point (dotted lines) for the energy on a two dimensional periodic strip, with perturbations to calculate stability

Ongoing Research

- ✶ Γ-limit for thin structures, $\delta \downarrow 0$
- ✶ Numerics on the L^2- or H^{-1}-gradient flow
- ✶ Geometrical methods to investigate the resulting patterns

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‡ T. Otha and K. Kawasaki, *Equilibrium morphology of block copolymer melts*, **Macromolecules**, 19:2621-2632, 1986

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