The pinning effect of dilute defects

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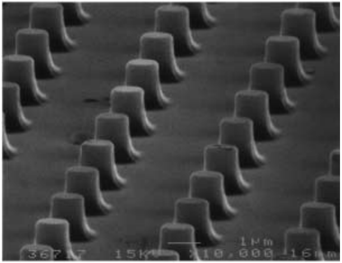
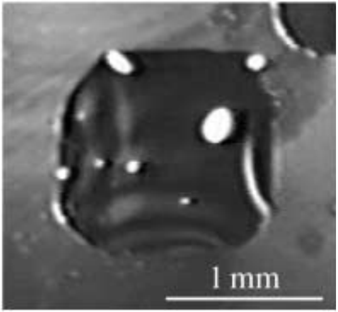
Joint work with Inwon Kim (UCLA)

Contact angle hysteresis





Marzolin, Smith, Prentiss and Whitesides *Adv. Mater.* (1998)
Bico, Tordeaux and Quéré *Euro. Phys. Lett.* (2001)

Model free boundary problem

Here I will study these issues in the context of the Bernoulli free boundary problem, in a domain U

$$\begin{cases} \Delta u = 0 & \text{in } \{u > 0\} \cap U \\ |\nabla u| = Q(x) & \text{on } \partial\{u > 0\} \cap U. \end{cases}$$

We assume $Q : \mathbb{R}^d \to (0, \infty)$ is continuous and $\mathbb{Z}^d$ periodic. Associated energy

$$J(u; U) = \int_U |\nabla u|^2 + Q(x)^2 \mathbf{1}_{\{u>0\}} \, dx.$$

This arises in a certain linearization of capillary energy near contact angle 0 or π, but mainly I am viewing it as a slightly simplified model still with many of the "nonlinear" issues of the capillary free boundary problem.

Pinning interval

For $p \in \mathbb{R}^d \setminus \{0\}$ and look for solution $u : \mathbb{R}^d \to [0, \infty)$ to

$$\begin{cases} \Delta u(x) = 0 \quad \text{in } \{u > 0\} \\ |\nabla u(x)| = Q(x) \quad \text{on } \partial\{u > 0\} \\ \sup_{\{u>0\}} |u(x) - p \cdot x| < \infty. \end{cases} \tag{1}$$

These are called plane-like solutions. Call a slope pinned if there exists a plane-like solution with slope p. Define for $e \in S^{d-1}$

$$Q_{\text{rec}}(e) = \inf\{\alpha : \ \alpha e \text{ is pinned}\} \ \text{ and } \ Q_{\text{adv}}(e) = \sup\{\alpha : \ \alpha e \text{ is pinned}\}.$$

Example: laminar media and discrete model

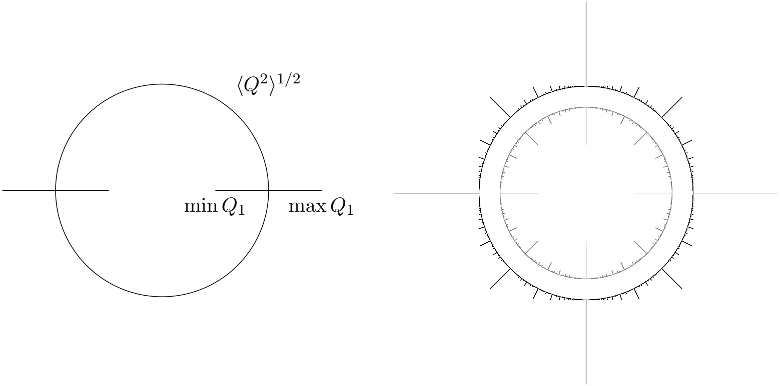


Figure: Pinning interval plotted as a graph $e \mapsto [Q_{\mathrm{rec}}(e), Q_{\mathrm{adv}}(e)]$ over $e \in S^1$. Left: Pinning interval for laminar medium $Q(x_1, x_2) = Q_1(x_1)$. Right: pinning interval from a related discrete Bernoulli free boundary problem.

[F. and Smart, ARMA '19]

Known results and open issues

Theorem (Caffarelli and Lee '08, Kim '08, F. '21)

- *For all* $\alpha \in [Q_{\text{rec}}(e), Q_{\text{adv}}(e)]$ *there exists a strong Birkhoff plane-like solution of (1) with slope* α. *The energy minimizing slope* $\langle Q^2 \rangle^{1/2}$ *is pinned.*
- *(*$d = 2$*)* $e \mapsto [Q_{\text{rec}}(e), Q_{\text{adv}}(e)]$ *is upper semicontinuous, continuous at irrational directions, left and right limits at rational directions.*
- *Homogenization of minimal supersolutions for convex data.*

Some challenging open issues, tough to address at this level of generality:

- Computing the pinning interval analytically
- Are jumps at rational directions generic?
- Does $[Q_{\text{rec}}(e), Q_{\text{adv}}(e)]$ have nonempty interior generically?
- Pinning interval in random media?

Dilute defect problem

Let $q \in C_c(B_1)$, the single defect profile, let $\delta > 0$ be the defect size to defect spacing ratio:

$$\begin{cases} \Delta u = 0 & \text{in } \{u > 0\} \\ |\nabla u| = Q_\delta(x) := 1 + \sum_{z \in \mathbb{Z}^d} q(\frac{x-z}{\delta}) & \text{on } \partial\{u > 0\}. \end{cases} \tag{2}$$

This is similar to the setting of Joanny and de Gennes' ('84) influential approach to modelling contact angle hysteresis.

Asymptotic expansion

Theorem (F. and Kim, preprint)

Let $\xi \in \mathbb{Z}^d$ irreducible and $e := \frac{\xi}{|\xi|}$. Then as $\delta \to 0$

$$\begin{aligned} Q^\delta_{\mathrm{adv}}(e) &= 1 + \gamma_d \delta^{d-1} |\xi|^{-1} k_{\mathrm{adv}}(e) + o(\delta^{d-1}), \text{ and} \\ Q^\delta_{\mathrm{rec}}(e) &= 1 + \gamma_d \delta^{d-1} |\xi|^{-1} k_{\mathrm{rec}}(e) + o(\delta^{d-1}). \end{aligned} \tag{3}$$

- Constant $\gamma_2 = \pi$ and $\gamma_d = \frac{1}{2} d(d-2)|B_1|$ in $d \geq 3$.
- $|\xi|^{-1}$ is the density of $\mathbb{Z}^d$ lattice sites on the hyperplane $\{x \cdot e = 0\}$.
- k_{adv} and k_{rec} measure the pinning effect of a single defect.

The single site problem

Single site problem

Consider viscosity solutions u of

$$\begin{cases} \Delta u = 0 & \text{in } \{u > 0\} \\ |\nabla u| = 1 + q(x) & \text{on } \partial\{u > 0\}. \end{cases} \tag{4}$$

Say that u is *proper* if it blows down to $(x_d)_+$

$$\lim_{r \to 0} \frac{u(rx)}{r} = (x_d)_+ \ \text{ locally uniformly.}$$

Far field asymptotics

Theorem

Let u be a proper solution of the single site problem (4). *Then:*

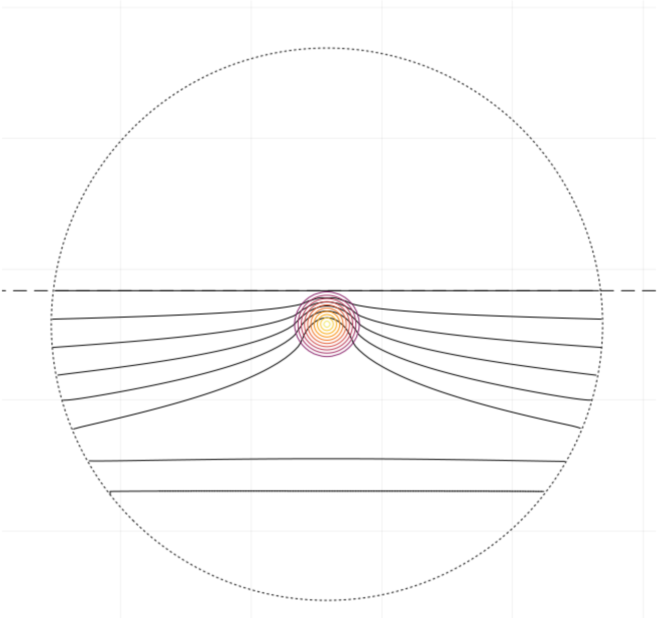
- *($d = 2$) There is $k \in \mathbb{R}$ so that*

$$u(x) = x_d + k \log |x| + O(1) \quad \text{for} \quad x \in \overline{\{u > 0\}} \setminus B_1.$$

- *($d \geq 3$) There are $s \in \mathbb{R}$ and $k \in \mathbb{R}$ so that*

$$u(x) = x_d + s - k \frac{1}{|x|^{d-2}} + O(\frac{1}{|x|^{d-1}}) \quad \text{as} \quad \overline{\{u > 0\}} \ni x \to \infty.$$

Pinning on a single site in $d = 2$



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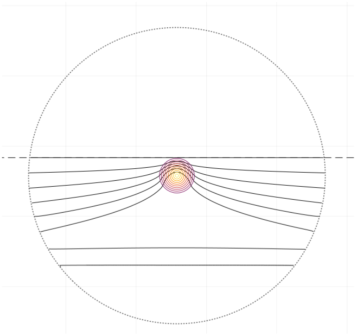

Pulling a free boundary past a defect

$$\begin{cases} \Delta u = 0 \ \text{ in } \ \{u > 0\} \cap B_R(0) \\ |\nabla u| = 1 + q(x) \ \text{ on } \partial\{u > 0\} \cap B_R(0) \\ u(x) = (x_d + k \log R)_+ \ \text{ on } \partial B_R(0). \end{cases}$$

Pinning thresholds at scale R

$$\begin{cases} \Delta u = 0 & \text{in } \{u > 0\} \cap B_R(0) \\ |\nabla u| = 1 + q(x) & \text{on } \partial\{u > 0\} \cap B_R(0) \\ u(x) = (x_d + k \log R)_+ & \text{on } \partial B_R(0). \end{cases} \quad (5)$$

Definition

Define $u_{\text{adv}}^{k,R}$ to be the minimal supersolution of (5) above $(x_d - 1)_+$. Define

$$\kappa_{\text{adv}}^R := \sup\{k : \ \{u_{\text{adv}}^{k,R} = 0\} \cap \overline{B_1(0)} \neq \emptyset\} \geq 0. \quad (6)$$

This is the largest value of k such that some solution of (5) is pinned on the defect.

Pinning thresholds at scale R

$$
\begin{cases}
\Delta u = 0 & \text{in } \{u > 0\} \cap B_R(0) \\
|\nabla u| = 1 + q(x) & \text{on } \partial\{u > 0\} \cap B_R(0) \\
u(x) = (x_d + k \log R)_+ & \text{on } \partial B_R(0).
\end{cases}
\tag{5}
$$

Definition

Define $u_{\text{rec}}^{k,R}$ to be the maximal subsolution of (5) below $(x_d + 1)_+$.
Define

$$
\kappa_{\text{rec}}^R := \inf\{k : \overline{\{u_{\text{rec}}^{k,R} > 0\}} \cap \overline{B_1(0)} \neq \emptyset\} \leq 0. \tag{6}
$$

This is the most negative value of k such that some solution of (5) is pinned on the defect.

Limit as $R \to \infty$

Definition

$$k_{\text{adv}} := \sup \{k : \exists \text{ a proper solution } u \text{ of (4) with capacity } k\}$$
$$k_{\text{rec}} := \inf \{k : \exists \text{ a proper solution } u \text{ of (4) with capacity } k\}.$$

Theorem

- *The limits hold*

$$\lim_{R\to\infty} \kappa^R_{\text{adv}} = k_{\text{adv}} \quad \textit{and} \quad \lim_{R\to\infty} \kappa^R_{\text{rec}} = k_{\text{rec}}.$$

- *For every $k \in [k_{\text{rec}}, k_{\text{adv}})$ there exists a proper solution of (4) with capacity k.*

Description of proper single single site solutions is a bit different in $d \geq 3$, I will skip that here.

The periodic array of defects

Asymptotic expansion: first thoughts

We want to establish the expansion

$$Q^{\delta}_{\mathsf{adv}}(e) = 1 + \gamma_d \delta^{d-1} |\xi|^{-1} k_{\mathsf{adv}}(e) + o(\delta^{d-1}).$$

We do it by proving asymptotic upper and lower bounds.

- To prove the lower bound

$$\liminf_{\delta \to 0} \frac{Q^{\delta}_{\mathsf{adv}}(e) - 1}{\delta^{d-1}} \geq \gamma_d k_{\mathsf{adv}}(e)$$

  it suffices to construct supersolution barriers almost achieving this slope.

Asymptotic expansion: first thoughts

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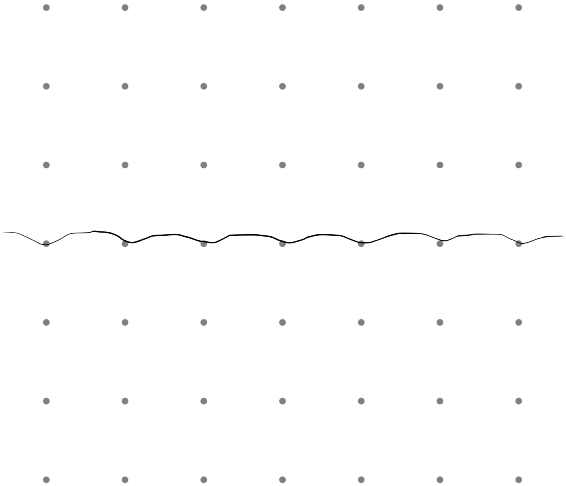
We do it by proving asymptotic upper and lower bounds.

- To prove the upper bound

$$\limsup_{\delta \to 0} \frac{Q^{\delta}_{\text{adv}}(e) - 1}{\delta^{d-1}} \leq \gamma_d k_{\text{adv}}(e)$$

  is trickier, we need to analyze a sequence of plane-like solutions achieving the maximal slope.

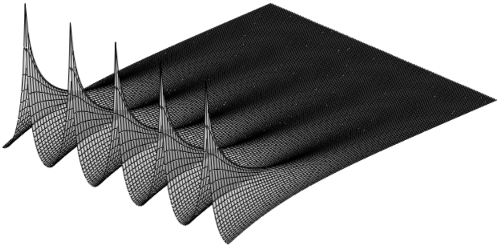
Intuition



Cell problem of semipermeable membranes

The following auxiliary problem describes the profile of u^δ away from the defects, here $\mathcal{Z} = \mathbb{Z}^d \cap \{x \cdot e = 0\}$ rotated to be on $\partial\mathbb{R}^d_+$,

$$\begin{cases} \Delta\omega = 0 & \text{in } \mathbb{R}^d_+, \\ \partial_{x_d}\omega = 1 & \text{on } \partial\mathbb{R}^d_+ \setminus \mathcal{Z} \\ \lim_{x\to z} \Phi(x-z)^{-1}\omega(x) = \frac{1}{\gamma_d} c_* & \text{for } z \in \mathcal{Z}, \\ \langle \partial_{x_d}\omega(\cdot, x_d)\rangle' = 0 & \text{for } x_d > 0. \end{cases} \tag{7}$$



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Lemma

There exists a solution of (7) bounded in $\{x_d \geq 1\}$ *if and only if* $c_* = |\square_{\mathcal{Z}}| = |\xi|$. *This solution is unique modulo adding a constant.*

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Here it is just a modified Green's function for a periodic Neumann problem:

$$\begin{cases} \Delta\omega = 0 & \text{in } \mathbb{R}^d_+, \\ \partial_{x_d}\omega = 1 - \sum_{z\in\mathcal{Z}} c_*\delta_z & \text{on } \partial\mathbb{R}^d_+ \\ \langle \partial_{x_d}\omega(\cdot, x_d)\rangle' = 0 & \text{for } x_d > 0. \end{cases} \tag{8}$$

Expansion of the plane-like solution

Theorem (F. and Kim, preprint)

Let $e \in \mathcal{S}^{d-1}$ rational. If u^δ are strong Birkhoff plane-like solutions with the maximal slope $Q^\delta_{\text{adv}}(e)$, then, modulo a period translation, there are $s_\delta \to 0$ so that

$$\lim_{\delta \to 0} \frac{1}{\delta^{d-1}} [Q^\delta_{\text{adv}}(e)\, x \cdot e + s_\delta - u^\delta(x)] = k_{\text{adv}}(e)\omega(x)$$

locally uniformly in $\{x \cdot e > 0\}$.

A parallel result holds for strong Birkhoff plane-like solutions with the minimal slope with Q^δ_{adv} and k_{adv} replaced by Q^δ_{rec} and k_{rec}.

Future directions

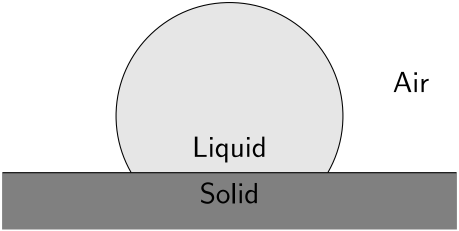
Future directions

- Irrational directions
- Is the pinning interval discontinuous in the normal direction e for finite δ?
- Random point process of defects
- Capillary free boundary problem for minimal surfaces

Thank you for your attention!

Contact angle hysteresis: phenomenological discussion

Slow condensation / evaporation or other slow volume forcing. Contact line only moves inwards below the receding angle θ_{rec}, only moves outward above the advancing angle θ_{adv}. Here consider $\theta_{rec} = \frac{\pi}{2}$ in an evaporating drop:



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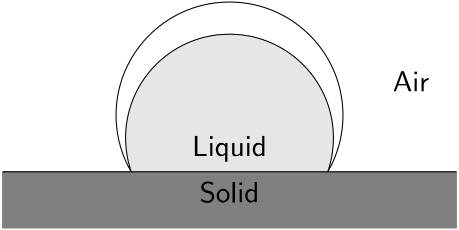

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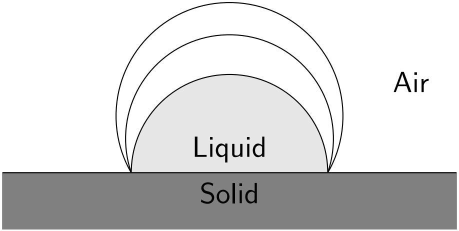

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