Wetting and dewetting dynamics of anisotropic particles

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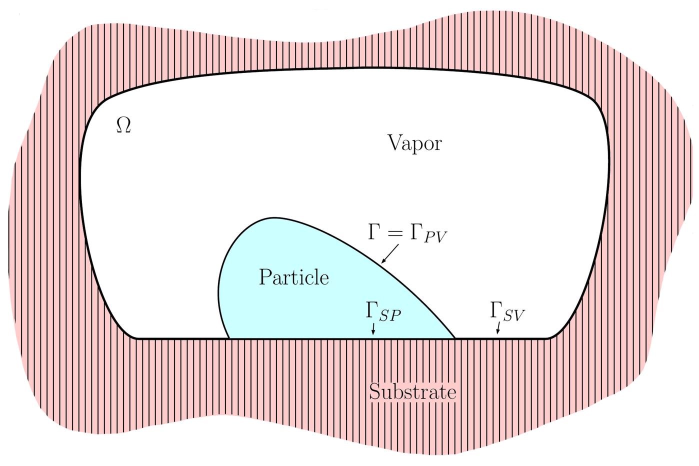
Setting



- Particle P
- Vapor V
- Substrate S
- $\Omega := \mathbb{R}^d \setminus S$ bounded and convex

Energy

$$E(P) = \int_\Gamma \gamma \, \mathrm{d}\mathcal{H}^{d-1}(x) + \int_{\partial P \cap \partial S} \sigma \, \mathrm{d}\mathcal{H}^{d-1}(x)$$

- $\gamma = \gamma(\nu) \in C^2(\mathbb{R}^d \setminus \{0\})$ with γ^2 convex, 1-homogeneous, and $c_\gamma|\nu| \le \gamma(\nu) \le C_\gamma|\nu|$
- $\sigma = \sigma(x) \in C^1(\mathbb{R}^d)$ with $\sigma := \gamma_{SP} - \gamma_{SV}$

Gradient flow

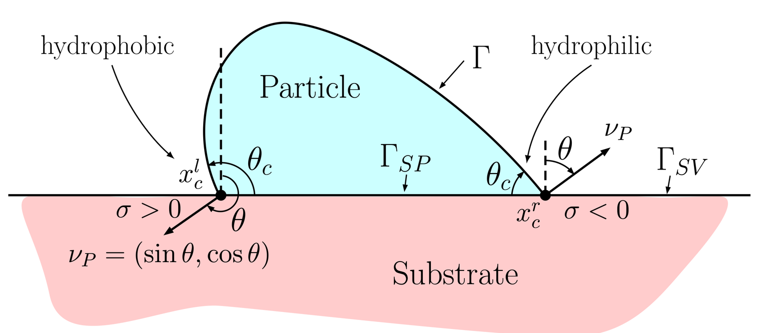
$H_\gamma(x) = \operatorname{div}(\nabla\gamma(\nu(x)))$ anisotropic mean curvature

Volume preserving gradient flow equation

$$V = \begin{cases} -\mu_\gamma(\nu)(H_\gamma - \Lambda) & \text{on } \Gamma \\ 0 & \text{on } \partial P \cap \partial S \end{cases}$$

Herring angle condition

$$\gamma(\nu) b_{PS} - (\nabla_\nu \gamma(\nu) \cdot b_P)\nu_{PS} + \sigma(x) b_S = 0 \quad \text{on } \partial\Gamma$$



- In dimension $d = 2$

$$\widetilde{\gamma}\cos\theta - \widetilde{\gamma}'\sin\theta + \sigma = 0$$

- Isotropic case (Young's equation)

$$\widetilde{\gamma}\cos\theta + \sigma = 0$$

Γ-convergence

Approximate energy

$$E(u) = \begin{cases} \int_\Gamma \gamma \, \mathrm{d}\mathcal{H}^{d-1}(x) + \int_{\partial P \cap \partial S} \sigma \, \mathrm{d}\mathcal{H}^{d-1}(x) & u = \mathbb{1}_P \in BV(\Omega;\{0,1\}) \\ \infty & \text{otherwise} \end{cases}$$

$$\Downarrow$$

$$E_h(u) = \frac{1}{\sqrt{h}}\int_\Omega u K_h * (\mathbb{1}_\Omega - u) \, \mathrm{d}\mathcal{H}^d(x) + \frac{1}{\sqrt{\pi h}}\int_\Omega \sigma u G_h * \mathbb{1}_S \, \mathrm{d}\mathcal{H}^d(x)$$

$K \in L^1(\mathbb{R}^d)$ suitable kernel representing the anisotropy γ

$G = (4\pi)^{-d/2} e^{-|x|^2/4}$ Gaussian kernel

$$G_h(x) := (h)^{-d/2} G\left(\frac{x}{\sqrt{h}}\right) \qquad K_h(x) := (h)^{-d/2} K\left(\frac{x}{\sqrt{h}}\right)$$

Theorem: Γ-convergence

Let Ω be convex, $\sigma \in C^1(\mathbb{R}^d)$. Under suitable assumptions on the kernel K, then

$$E_h \xrightarrow[s-L^1]{\Gamma} E$$

How is our result different from the result of [Esedoğlu-Otto]?

- We can consider different kernels K and G
- The substrate energy density σ is space dependent
- We can consider $\gamma = \gamma(x,\nu)$ (but not in the MBO scheme)
- It should be possible to drop the convexity of Ω

The MBO scheme

Given $u_k := \mathbb{1}_{P^k}$ and $V^k := \Omega \setminus P^k$ at time step $t_k = kh$

$u_{k+1} := \mathbb{1}_{P^{k+1}}$ and $V^{k+1} := \Omega \setminus P^{k+1}$ are obtained as follows:

The thresholding scheme

- Convolution:

$$\varphi^k(x) = \frac{1}{\sqrt{h}} K_h * (\mathbb{1}_\Omega - 2u_k) + \frac{1}{\sqrt{\pi h}} \sigma G_h * \mathbb{1}_S.$$

- Thresholding:

$$P^{k+1} = \left\{ x \in \Omega \mid \varphi^k(x) < \delta^k \right\}, \quad V^{k+1} = \Omega \setminus P^{k+1}$$

where δ^k is such that the mass of P^{k+1} is equal to the one of P^k.

Define $\quad u_h(t) = u^0 \quad$ if $t \le 0$, $\quad u_h(t) = u^k \quad$ if $t \in [kh, (k+1)h)$.

Convergence of the scheme

Theorem: Existence of a mean curvature flow

Let $u^0 = \mathbb{1}_{P^0} \in BV(\Omega;\{0,1\})$ with ∇u^0 a bounded measure and consider a sequence $h \to 0$. Then there exists $u : (0,T) \times \Omega \to \{0,1\}$ such that

$$u_h \to u \quad \text{in } L^1((0,T)\times\Omega).$$

and ∇u is a bounded measure, which is equi-integrable in t. If we assume

$$\limsup_h \int_0^T E_h^K(u_h(t)) \, \mathrm{d}t \le \frac{1}{2}\int_0^T \int_{\mathbb{R}^d} \gamma(\nu)\left(|\nabla u| + |\nabla(\mathbb{1}_\Omega - u)| - |\nabla \mathbb{1}_\Omega|\right) \mathrm{d}t,$$

then u moves by anisotropic volume-preserving mean curvature flow with obstacle S. Namely, there exist $H_\gamma : [0,T] \times \Omega \to \mathbb{R}$ with

$$\int_0^T \int_\Omega |H_\gamma|^2 |\nabla u| \, \mathrm{d}t < \infty,$$

mean curvature in the sense that it satisfies

$$\int_0^T \int_\Omega H_\gamma \xi \cdot \nu |\nabla u| \, \mathrm{d}t = \int_0^T \int_\Omega \left(\gamma(\nu) \operatorname{div}\xi - \nu \nabla\xi \cdot \nabla_\nu \gamma(\nu)\right) |\nabla u| \, \mathrm{d}t$$

for all $\xi \in C^\infty\left((0,T)\times\Omega;\mathbb{R}^d\right)$ with $\xi|_{\partial S} \cdot \nu_S = 0$;

there exist $V : [0,T] \times \Omega \to \mathbb{R}$ with

$$\int_0^T \int_\Omega |V|^2 |\nabla u| \, \mathrm{d}t < \infty,$$

normal velocity in the sense that it satisfies

$$\int_\Omega \zeta(s,x) u(s,x) \, \mathrm{d}\mathcal{H}^d(x) - \int_\Omega \zeta(0,x) u^0(x) \, \mathrm{d}\mathcal{H}^d(x)$$
$$= \int_0^s \int_\Omega \partial_t \zeta(t,x) u(t,x) \, \mathrm{d}\mathcal{H}^d(x) \, \mathrm{d}t + \int_0^s \int_\Omega \zeta(t,x) V(t,x) |\nabla u| \, \mathrm{d}t$$

for all $\zeta \in C^\infty([0,T]\times\Omega)$ and $s \in (0,T]$.

Moreover, they satisfy the

Energy inequality

$$E(u(T)) + \frac{1}{2}\int_0^T \int_\Omega \frac{V^2}{\mu_\gamma(\nu)} + \mu_\gamma(\nu)(H_\gamma - \Lambda)^2 \left(|\nabla u| + |\nabla(\mathbb{1}_\Omega - u)| - |\nabla \mathbb{1}_\Omega|\right) \mathrm{d}t \le E(u^0)$$

for all $\xi \in C^\infty([0,T]\times\Omega)$ with $\xi|_{\partial S} \cdot \nu_S = 0$.

References

[1] G. Bellettini, M. Paolini. Anisotropic motion by mean curvature in the context of Finsler geometry. *Hokkaido Math. J.* 25 (1996), no. 3

[2] S. Esedoğlu, F. Otto. Threshold dynamics for networks with arbitrary surface tensions. *Comm. Pure Appl. Math.* 68 (2015), no. 5

[3] S. Gavhale, K. Švadlenka. Dewetting dynamics of anisotropic particles: a level set numerical approach. *Appl. Math.* 67 (2022), no. 5

[4] T. Laux, F. Otto. Convergence of the thresholding scheme for multi-phase mean-curvature flow. *Calc. Var.* 55 (2016), no. 5