Coarsening and energy landscapes:
Two examples

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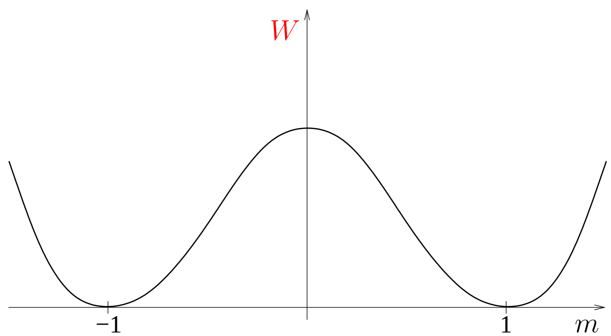
What is coarsening?

0^{th} Example: Cahn–Hilliard equation

$$\partial_t m - \triangle \frac{\partial E}{\partial m} = 0$$

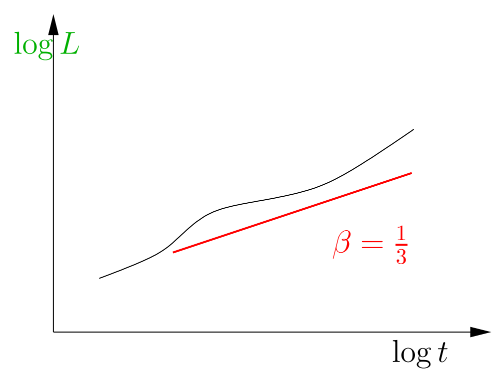
$$E(m) = \int \frac{1}{2}|\nabla m|^2 + W(m)\, dx$$



- periodic b.c. in $(0,\Lambda)^n$ with $\Lambda \gg 1$
- initial data: $m_0 = 0 +$ perturbation

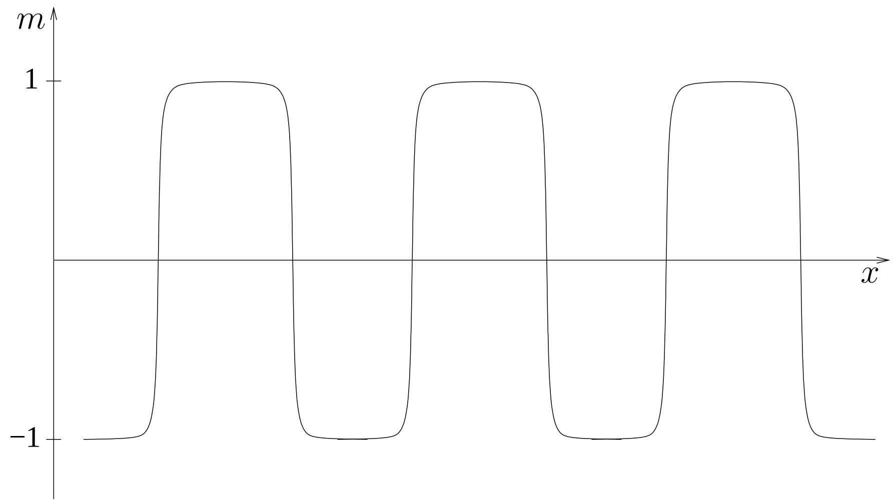
Statistically self–similar coarsening:

Characteristic exponent:



Bounds on coarsening?

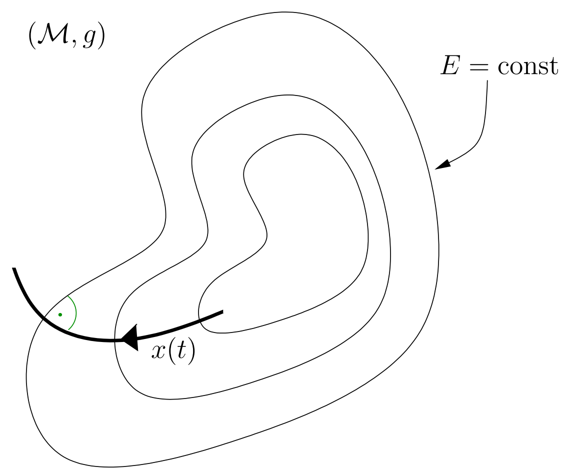
Cannot expect lower bounds: Too many stationary points of E



Upper bounds on coarsening?

... via lower bounds on energy!

An abstract framework:



$(\mathcal{M}, g)$	Riemannian manifold
E	functional on $\mathcal{M}$

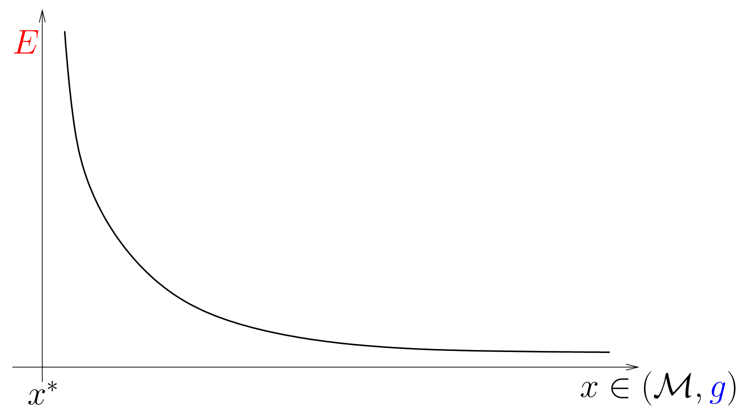
Gradient flow $\quad \dot{x} = -\text{grad}_g E(x)$

metric tensor $g_x(\delta x, \delta x)$ $\rightsquigarrow$ induced distance $d(x_0, x_1)$

local $\qquad\qquad$ global

Relating energy landscape to dynamics:

Proposition. (Kohn & O. '02)



Assume for $\alpha > 0$

$$E(x)\, d(x^*, x)^{\alpha} \gtrsim 1$$

provided $E(x) \leq 1$.

Then for $\sigma \in (1, \frac{\alpha+2}{\alpha})$

$$\int_0^T E(x(t))^{\sigma}\, dt \gtrsim \int_0^T (t^{-\frac{\alpha}{\alpha+2}})^{\sigma}\, dt$$

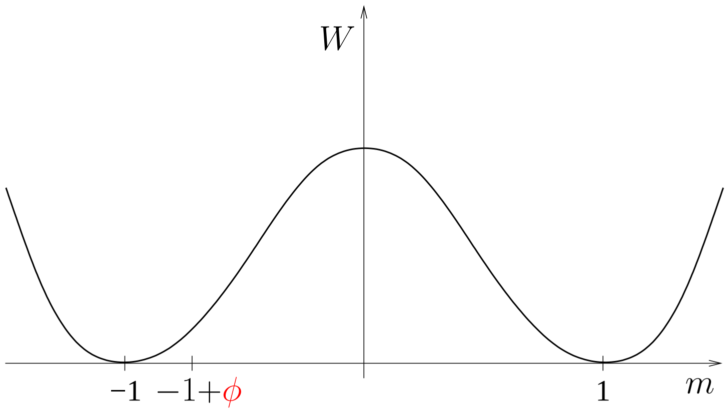
for $T \gg d(x^*, x(0))^{\alpha+2}$
and $E(x(0)) \leq 1$.

1^{st} **Example:** Ostwald ripening in mixtures

The model: Cahn–Hilliard equation

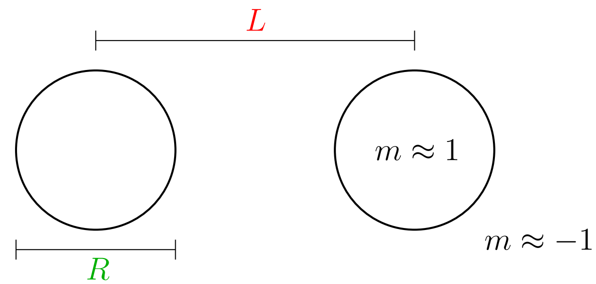
$$\partial_t m - \triangle \frac{\partial E}{\partial m} = 0$$

$$E(m) = \int \tfrac{1}{2}|\nabla m|^2 + W(m)\, dx$$

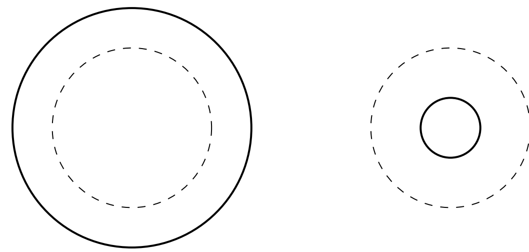


- periodic b.c. in $(0, \Lambda)^n$, $\Lambda \gg 1$
- $\Lambda^{-n} \int m\, dx = -1 + \phi$, $\phi \ll 1$

Typical configuration:



Coarsening proceeds by competetive growth and vanishing of particles



Heuristic predictions:

$R \sim t^{\frac{1}{3}}$ for $n \geq 3$ provided $R \gg \phi^{-1}$
(Lifshitz, Slyozov & Wagner '61 based on reduced model)

$R \sim \frac{1}{\ln^{\frac{1}{3}} \frac{1}{\phi}} t^{\frac{1}{3}}$ for $n = 2$ provided $R \gg \phi^{-1}$

... weak dependence on dimension.

Length scales $\leftrightarrow$ energy

- most excess volume in particles

  $\Rightarrow \quad (R/L)^n \approx \phi$

- most energy = interfacial energy

  $$\Rightarrow \quad E \sim \underbrace{L^{-n}}_{\substack{\text{number}\\ \text{density}}} \times \underbrace{R^{n-1}}_{\substack{\text{individual}\\ \text{interfacial area}}} \sim \phi R^{-1}$$

Induced distance = H^{-1}–norm

$$\begin{aligned} d(m_0, m_1)^2 &= \int |\nabla\varphi|^2 \, dx \quad \text{where } m_1 - m_0 + \triangle\varphi = 0 \\ &= \inf_J \left\{ \int |J|^2 \, dx \,\middle|\, m_1 - m_0 + \nabla \cdot J = 0 \right\} \\ &= ||m_1 - m_0||^2_{H^{-1}} \end{aligned}$$

Reference state: $m^* \equiv -1 + \phi$.

Proposition. (Conti, Niethammer & O. '04)

$$\Lambda^{-n} E(m) \left(\Lambda^{-n} ||m - m^*||^2_{H^{-1}}\right)^{\frac{1}{2}} \gtrsim \left\{ \begin{array}{ll} \phi^{\frac{3}{2}} & n \geq 3 \\ \phi^{\frac{3}{2}} \ln^{\frac{1}{2}} \frac{1}{\phi} & n = 2 \end{array} \right\}$$

provided $\Lambda^{-n} E(m) \ll \phi^2$.

Corollary. For $\sigma \in (1,3)$

$$\int_0^T \left(\Lambda^{-n} E(m(t))\right)^\sigma \, dt \;\gtrsim\; \phi \left\{ \begin{array}{ll} \int_0^T (t^{-\frac{1}{3}})^\sigma \, dt & n \geq 3 \\ \int_0^T (\ln^{\frac{1}{3}} \frac{1}{\phi} \, t^{-\frac{1}{3}})^\sigma \, dt & n = 2 \end{array} \right\}$$

provided $T \gg \phi^{-\frac{3}{2}} (\Lambda^{-n} ||m - m^*||^2_{H^{-1}})^3$ and $\Lambda^{-n} E(m(0)) \ll \phi^2$.

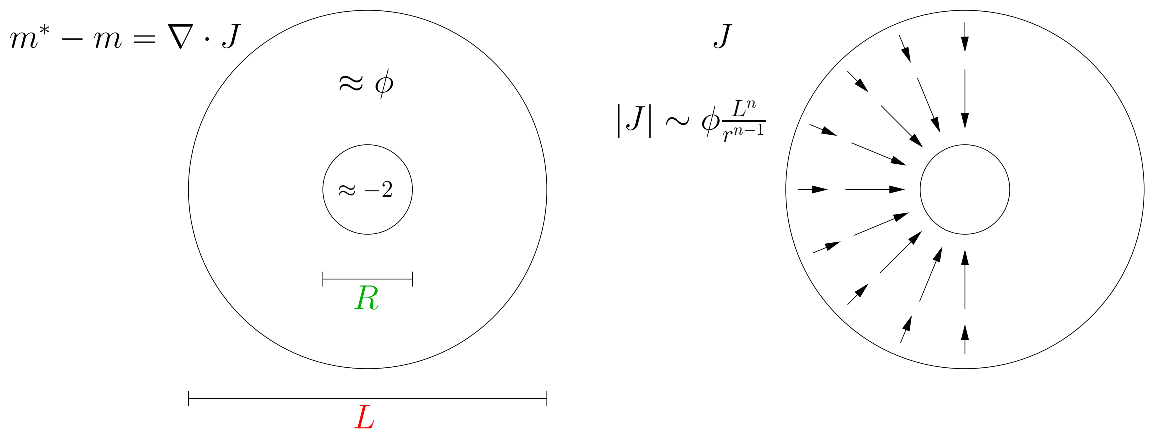
Interpretation:

$$R \quad \lesssim \quad \left\{ \begin{array}{ll} t^{\frac{1}{3}} & n \geq 3 \\ \ln^{-\frac{1}{3}} \frac{1}{\phi} \, t^{\frac{1}{3}} & n = 2 \end{array} \right\}$$

Heuristics for Proposition:

$$\Lambda^{-1}\,\|m-m^*\|^2_{H^{-1}} \;\sim\; \Lambda^{-n}\int |J|^2 dx \;\sim\; L^{-n}\int_R^L \left(\phi\frac{L^n}{r^{n-1}}\right)^2 r^{n-1}dr$$

$$\sim \left\{\begin{array}{ll} L^n\phi^2 R^{2-n} & n\geq 3 \\ L^n\phi^2 \ln\frac{L}{R} & n=2 \end{array}\right\} \sim \left\{\begin{array}{ll} \phi R^{2} & n\geq 3 \\ (\phi\ln\frac{1}{\phi})R^{2} & n=2 \end{array}\right\}$$



Recall $\quad \Lambda^{-n}E \;\sim\; \phi R^{-1}.$

Crucial geometric ingredient, applied to $\Omega = \{m \approx 1\}$.

Lemma. Assume

$$R\,\mathcal{H}^{n-1}(\partial\Omega) \;\le\; \mathcal{L}^n(\Omega).$$

Then $\exists\ \tilde{\Omega} \subset \Omega$ which

- covers substantial part of Ω, i. e.

$$\mathcal{L}^n(\tilde{\Omega}) \;\ge\; \tfrac{1}{2}\mathcal{L}^n(\Omega),$$

- behaves like union of balls of radius $\ge R$, i. e.

$$\mathcal{L}^n\big(\{\mathrm{dist}(\cdot,\tilde{\Omega}) \ge L\}\big) \;\le\; C(n)\,\big(1 + (\frac{R}{L})^n\big)\,\mathcal{L}^n(\tilde{\Omega})$$

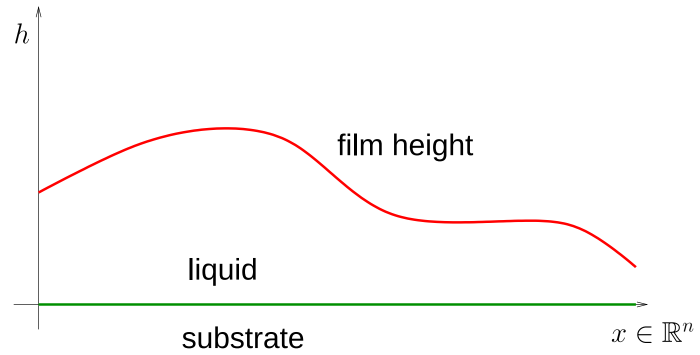
  for all L.

2^{nd} Example: Ostwald ripening in liquid films

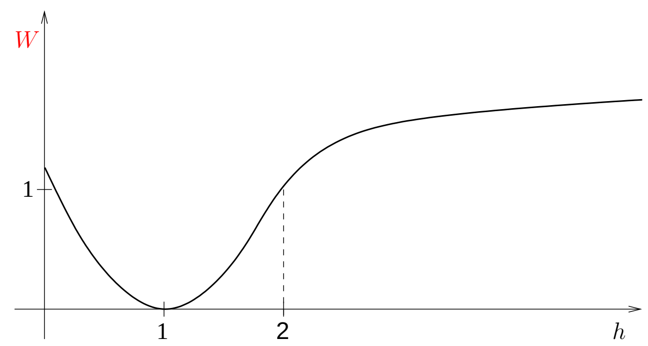
The model: Thin film equation

$$\partial_t h - \nabla \cdot \left(h \nabla \frac{\partial E}{\partial h}\right) = 0$$

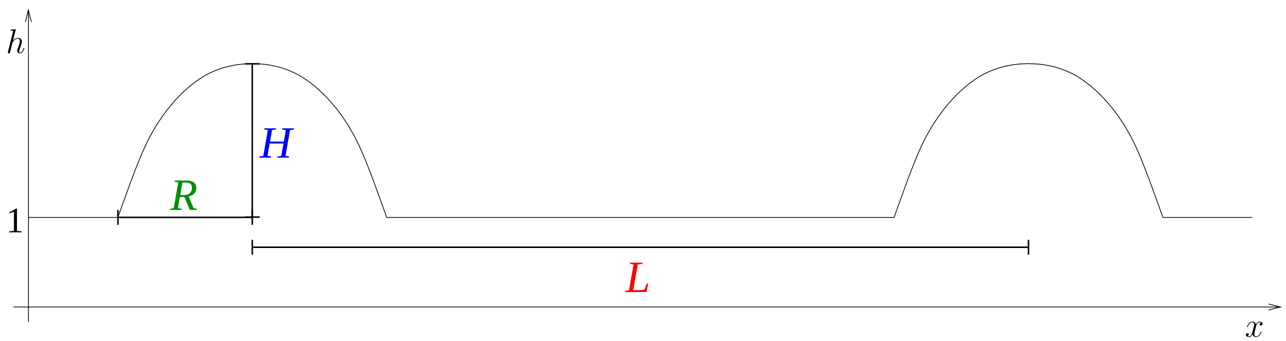
$$E(h) = \int \underbrace{\tfrac{1}{2}|\nabla h|^2}_{\text{capillary}} + \underbrace{W(h)}_{\text{short range interaction}} \quad dx$$



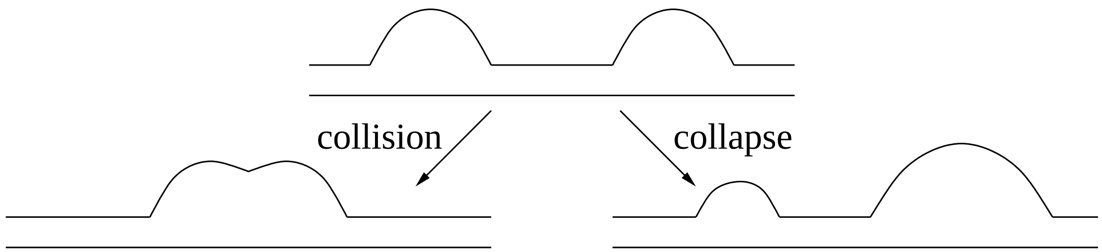
- periodic b.c. in $(0, \Lambda)^n$, $\Lambda \gg 1$
- $\Lambda^{-n} \int h \, dx = 2$



Typical configuration:



Two coarsening strategies:



Heuristic predictions:

$L \sim t^{\frac{2}{5}}$ for $n = 1$ (Glasner & Witelski '03 based on reduced model)

? for $n = 2$

Length scales $\leftrightarrow$ energy

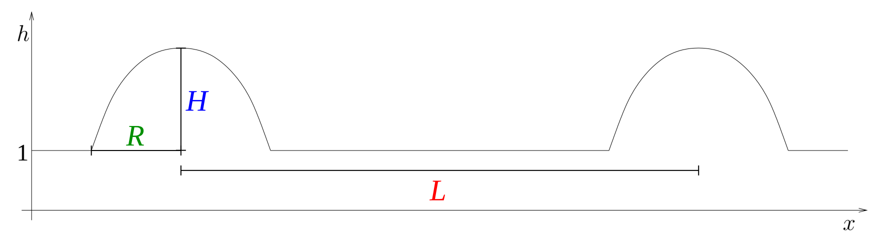
- Individual droplet in equilibrium

  $\Rightarrow$ equipartition of $\int \frac{1}{2}|\nabla h|^2 dx \sim (H/R)^2 R^n$ and $\int W(h)dx \sim R^n$

  $\Rightarrow H \sim R$

- Overall volume constraint

  $$\Rightarrow \quad \underbrace{L^{-n}}_{\text{number density}} \times \underbrace{R^n H}_{\text{individual volume}} \sim 1$$



- Specific energy

  $$\Rightarrow \Lambda^{-n} E \sim L^{-n} \times \underbrace{R^n}_{\text{individual energy}} \sim R^{-1} \sim L^{-\frac{n+1}{n}}$$

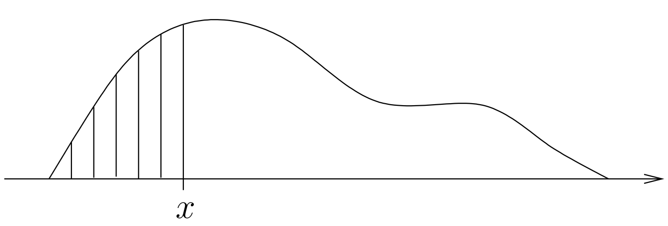
Induced distance = Wasserstein

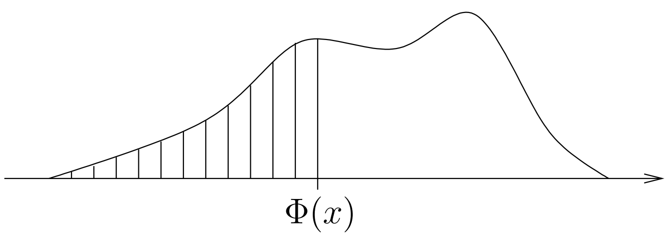
$$g_h(\delta h, \delta h) = \int h|\nabla\varphi|^2 \, dx \quad \text{where } \delta h + \nabla\cdot(h\nabla\varphi) = 0$$

$$= \inf_u \left\{ \int h|u|^2 \, dx \;\middle|\; \delta h + \nabla\cdot(hu) = 0 \right\}$$

$$d(h_0, h_1)^2 = \inf_{(h,u)} \left\{ \int_0^1 \int h|u|^2 \, dxds \;\middle|\; \partial_s h + \nabla\cdot(hu) = 0, \; \begin{array}{l} h(0) = h_0 \\ h(1) = h_1 \end{array} \right\}$$

$$= \inf_\Phi \left\{ \int |\Phi(x) - x|^2 h_0(x) \, dx \;\middle|\; \Phi\# h_0 = h_1 \right\} =: W(h_0, h_1)^2$$





Reference state: $h^* \equiv 2$.

Proposition. (O., Rump & Slepcev '04)

$$\Lambda^{-n} E(h) \left[(\Lambda^{-n} W(h^*, h)^2)^{\frac{1}{2}} \right]^{\frac{n}{n+1}} \quad \gtrsim \quad 1 \qquad \text{provided } \Lambda^{-n} E(h) \ll 1.$$

Corollary. For $\sigma \in (1, \frac{3n+2}{n})$

$$\int_0^T \left(\Lambda^{-n} E(h(t)) \right)^\sigma \, dt \quad \gtrsim \quad \int_0^T (t^{-\frac{n}{3n+2}})^\sigma \, dt$$

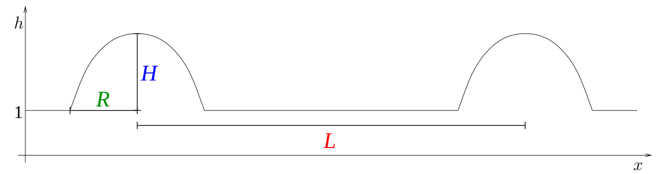
provided $T \gg W(h^*, h(0))^{2+\frac{n}{n+1}}$ and $\Lambda^{-n} E(h(0)) \ll 1$.

Interpretation:

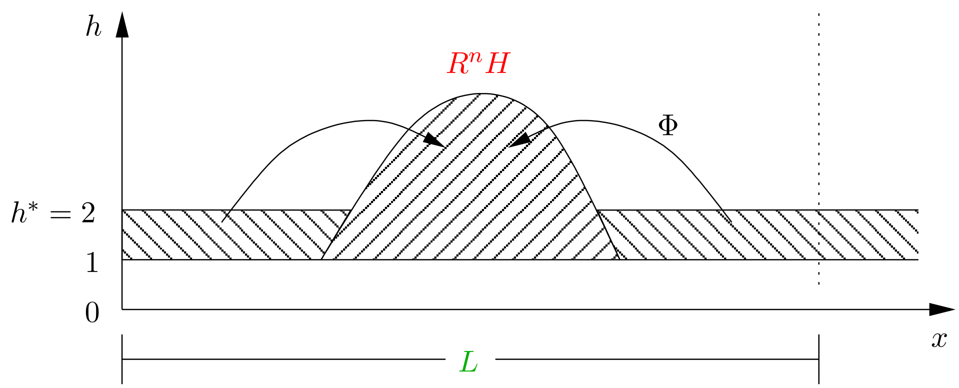
$$L \quad \lesssim \quad t^{\frac{n+1}{3n+2}} = \left\{ \begin{array}{ll} t^{\frac{2}{5}} & n = 1 \\ t^{\frac{3}{8}} & n = 2 \end{array} \right\}$$

... strong dependence on dimension.

Heuristics for Proposition:



$$\Lambda^{-n} \int |\Phi(x) - x|^2 h^* dx \sim \underbrace{L^{-n}}_{\text{number density}} \times \Big(\underbrace{L}_{\text{distance transported}} \Big)^2 \times \underbrace{R^n H}_{\text{individual volume}} \sim L^2$$



Recall $\quad \Lambda^{-n} E \sim L^{-\frac{n+1}{n}}$.