Eighth workshop on random dynamical systems (Nov, 2015)

Local minima and energy barriers in the Cahn–Hilliard energy landscape

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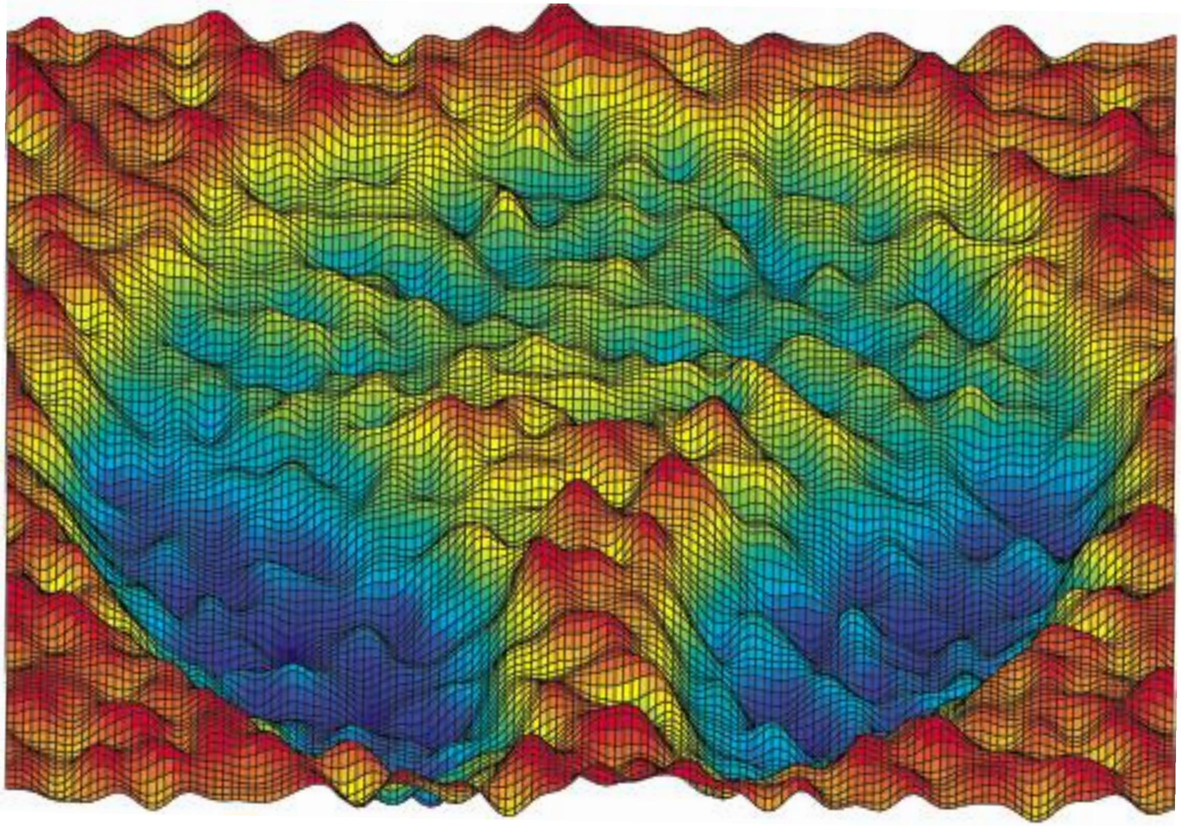
Joint work with Michael Gelantalis and Alfred Wagner (RWTH)

Switching and complex energy landscapes



From E, Ren, and Vanden-Eijnden, Phys Chem B (2005)

Model

Consider the energy

$$E(u) = \int_\Omega \frac{1}{2}|\nabla u|^2 + G(u)\, dx$$

For simplicity

$$G(u) = \frac{(1-u^2)^2}{4}$$

where Ω is the d-dimensional flat torus with side-length L. We study this energy subject to the fixed mean constraint

$$⨍_\Omega u(x)\, dx = -1 + \phi$$

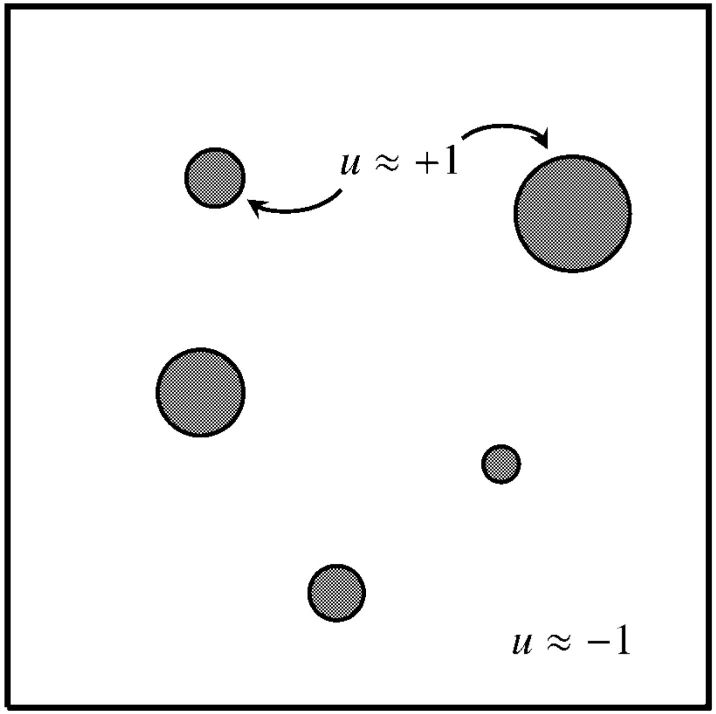
and in the scaling regime

$\phi \ll 1$ and $L \gg 1$ and

$\phi \gg L^{-d/(d+1)}$ (off-critical)

or $\phi \sim L^{-d/(d+1)}$ (critical)

Stochastic nucleation of “droplets”



Energy and the regime

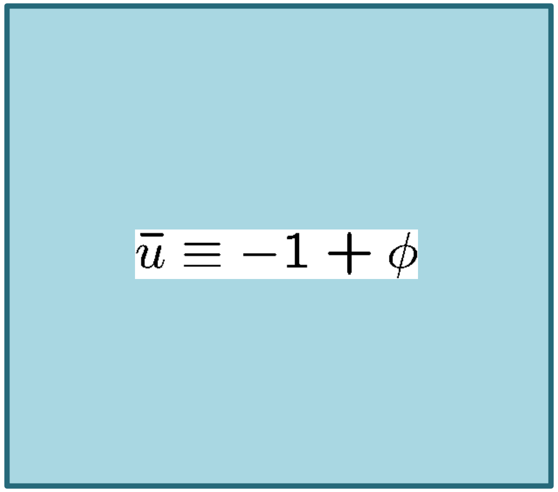
- Energetic preferences

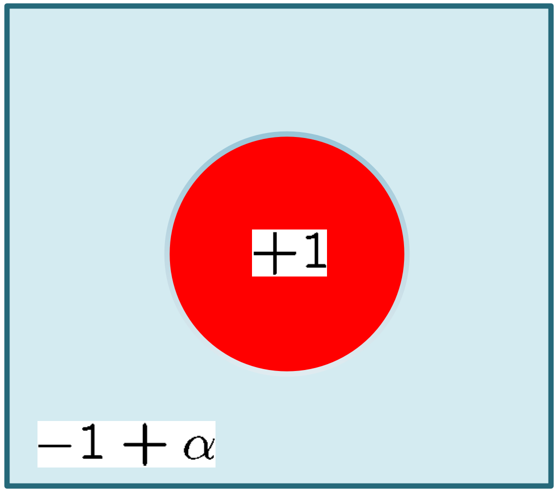
$$E(u) = \int_\Omega \frac{1}{2}|\underset{\substack{\uparrow \\ \text{prefers} \\ \text{u constant}}}{\nabla} u|^2 + G(\underset{\substack{\nwarrow \\ \text{prefers} \\ \text{u} =\pm 1}}{u})\,dx$$

- For L$\gg$1, bounded energy $\Rightarrow$ u$\approx\pm$ 1 on most of $[-L/2,L/2]^d$.
- On the one hand, energy concentrates on boundary of u=+1.
- On the other hand, the mean constraint leads to a “bulk” cost.

Heuristic picture of regimes

Two candidates for the global minimizer





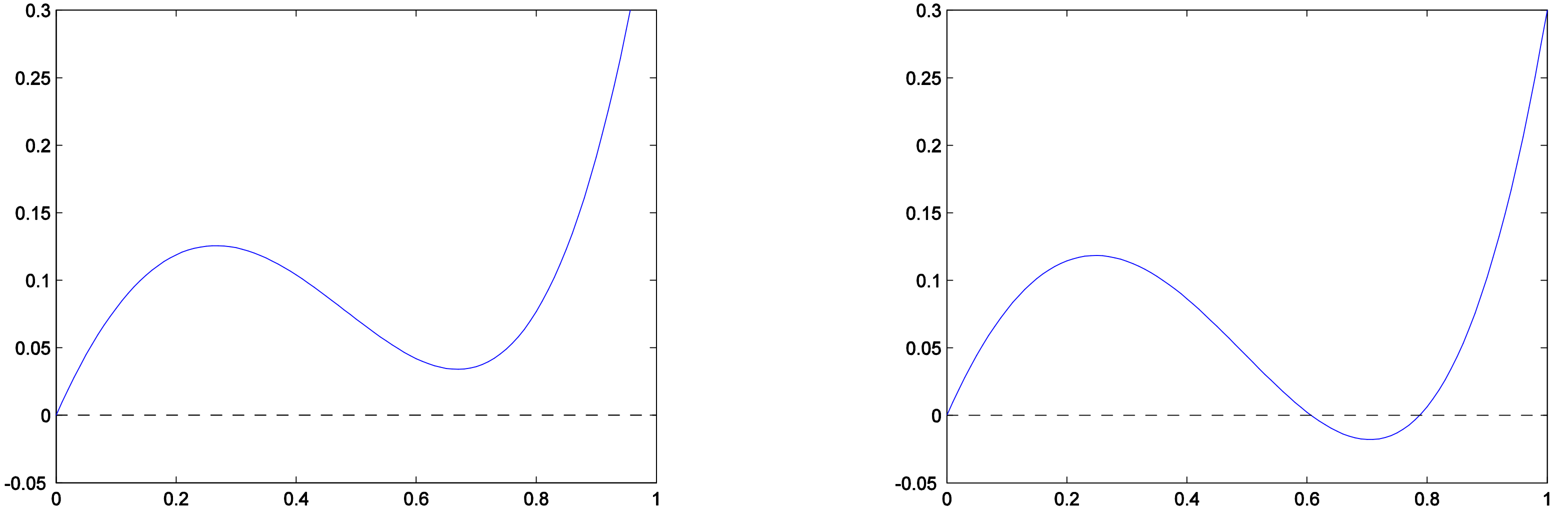
Wins for

$$\phi \ll L^{-d/(d+1)}$$

Wins for

$$\phi \gg L^{-d/(d+1)}$$

Heuristics for energy landscape



Energy as a function of “droplet radius” for different parameter values

Previous results on global min

- Biskup, Chayes, and Kotecky (2002)
- Carlen, Carvalho, Esposito, Lebowitz, and Marra (2006)
- Bellettini, Gelli, Luckhaus, Novaga (2006)

Critical constant

$$\phi = \xi_d L^{-d/(d+1)}$$

Energy barrier around constant state

- In the off-critical regime

$$\Delta E = C_* \phi^{-d+1} + o(\phi^{-d+1}).$$

- In critical regime with

$$\phi \, L^{d/(d+1)} = \xi \quad \text{(above critical value } \xi_d\text{)},$$

we obtain

$$\Delta E = C(\xi) \phi^{-d+1} + o(\phi^{-d+1}).$$

- Gives also a saddle point u_s with precisely that energy.

Γ-limit

- Rescaled energy gap

$$\begin{aligned}\mathcal{E}^{\xi}_{\phi}(u) :&= \frac{E(u)-E(\bar{u})}{\phi^{-d+1}}\\ &= \int_{\mathbb{T}_{\phi L}} \frac{\phi}{2}|\nabla u|^2 + \frac{1}{\phi}\Big(G(u) - G(-1+\phi)\Big)\,dx\end{aligned}$$

- Limit functional of the form

$$\mathcal{E}^{\xi}_{0}(u) := c_0 \mathrm{Per}(\{u=1\}) - 4|\{u=1\}| + \frac{4|\{u=1\}|^2}{\xi^{d+1}},$$

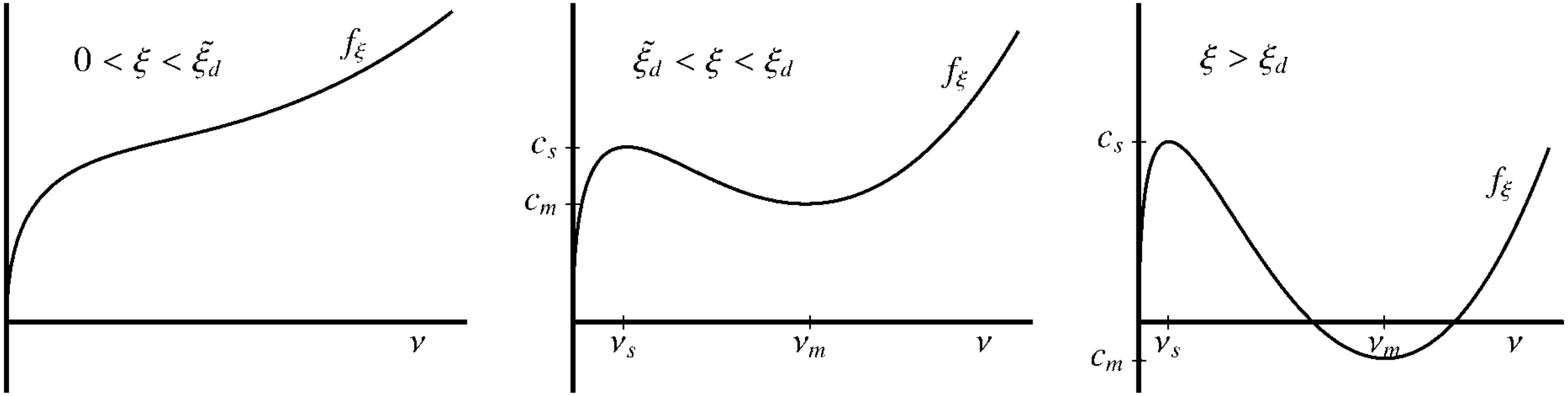
where

$$\xi = \lim \phi\, L^{d/(d+1)}.$$

Reflects the heuristic picture

Restriction to droplets of $\mathcal{E}_0^\xi$ yields

$$f_\xi(\nu) = C_1 \nu^{(d-1)/d} - 4\nu + \frac{4\nu^2}{\xi^{d+1}}$$



Notation, c_m, ν_m, c_s, ν_s, Ψ_m, Ψ_s

Going beyond the constant state

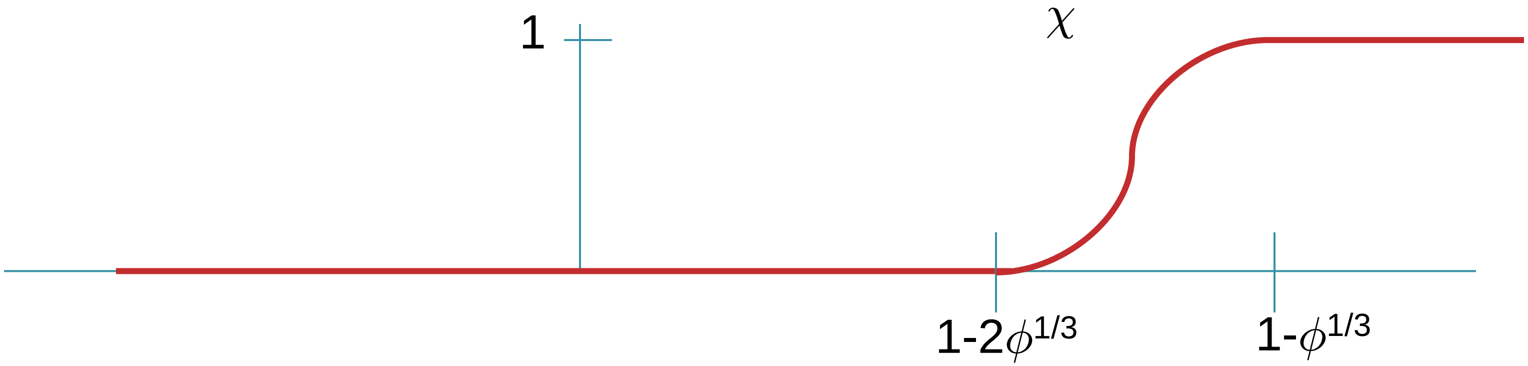
<u>Questions on the level of the CH model</u>

- Is there a local min with “volume” ν_{m}?
- What is the associated <u>energy barrier</u>?
- Can we characterize the local min as a droplet?
- The saddle point?

<u>Questions on the level of Gamma-limits</u>

- Info about limit $\Rightarrow$ info about original
- Local minima
- Saddle points?

“Volume”-type functional



$$\nu(u) := \int_{\mathbb{T}_{\phi L}} \chi(u(x))\,dx$$

Local min

Theorem. *For* $\xi \in (\tilde{\xi}_d, \xi_d]$, $\mathcal{E}_\phi^\xi$ *has a nonconstant local minimizer* $u_{m,\phi}$, *which minimizes* $\mathcal{E}_\phi^\xi$ *over*

$$|u - \Psi_m|_{\mathbb{T}_{\phi L}} \le \gamma_0.$$

The local minimizer $u_{m,\phi}$ *is well-approximated by* Ψ_m *in the sense that*

$|u_{m,\phi} - \Psi_m|_{\mathbb{T}_{\phi L}} \le \gamma$ *for all* $\gamma \le \gamma_0$ *and* $\phi \ll 1$, *and*

$\left|\mathcal{E}_\phi^\xi(u_{m,\phi}) - c_m\right| \lesssim \phi^{1/3}$,

$|\nu(u_{m,\phi}) - \nu_m| \le C(\xi)\phi^{1/6}$.

Ingredients

(1) Ψ_m strict L^2 local minimizer of

$$\mathcal{E}_0^\xi(u) = c_0 \mathrm{Per}(\{u=1\}) - 4|\{u=1\}| + \frac{4|\{u=1\}|^2}{\xi^{d+1}}$$

(2) For every γ, δ small and positive and for ϕ small enough,

$$\gamma \leq |u - \Psi_m|_{\mathbb{T}_{\phi L}} \leq \gamma_0$$

$$\Rightarrow \qquad \mathcal{E}_\phi^\xi(u) \geq \inf_{\gamma \leq |u-\Psi_m|_{\mathbb{R}^d} \leq \gamma_0} \mathcal{E}_0^\xi(u) - \delta.$$

(3) Good constructions.

Sketch of proof of theorem

Minimize $\mathcal{E}_\phi^\xi$ subject to $|u - \Psi_m| \leq \gamma_0$ via direct method.

Notice from (2) and (1) that

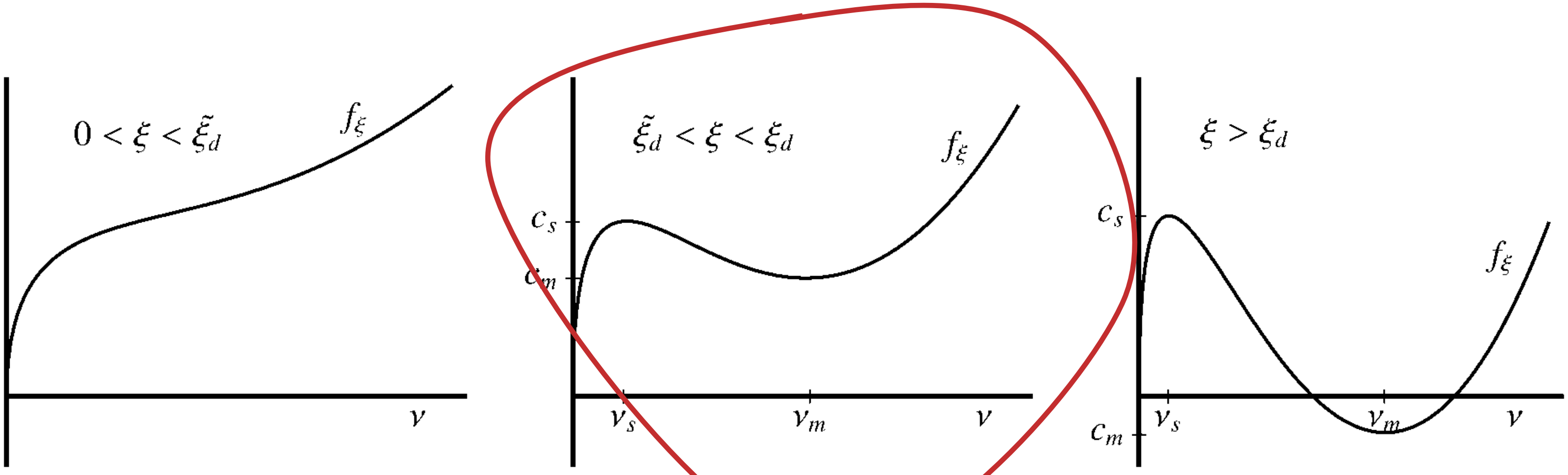
$$\gamma \leq |u - \Psi_m|_{\mathbb{T}_{\phi L}} \leq \gamma_0 \Rightarrow \mathcal{E}_\phi^\xi(u) \geq c_m + \delta.$$

On the other hand there is a construction close to Ψ_m in L^2 and energy.

Quantitative estimates rely on upper/lower bounds

$$\phi^{1/3} \gtrsim \mathcal{E}_\phi^\xi(u_{m,\phi}) - c_m \geq f_\xi(\nu(u_{m,\phi})) - c_m + O(\phi^{1/3}) \gtrsim \phi^{1/3}.$$

Energy barrier



For $\xi \in (\tilde{\xi}_d, \xi_d)$, natural to define barrier around $u_{m,\phi}$ via

$$\Delta E_1^{\phi,\xi} := \inf_{\psi} \max_{t \in [0,1]} \mathcal{E}_\phi^\xi(\psi(t)).$$

over paths $\psi \in C([0,1]; X_\phi)$ such that

$$\mathcal{E}_\phi^\xi(\psi(0)) < \mathcal{E}_\phi^\xi(u_{m,\phi}), \qquad \psi(1) = u_{m,\phi}.$$

Energy barrier (continued)

More modest goal: reach for $\varepsilon > 0$ small

$$\mathcal{N}_\varepsilon(u_{m,\phi}) := \left\{ u \in X_\phi \colon |u - u_{m,\phi}|_{\mathbb{T}_{\phi L}} + \mathcal{E}_\phi^\xi(u) - \mathcal{E}_\phi^\xi(u_{m,\phi}) < \varepsilon \right\}.$$

We define

$$\Delta E_2^{\phi,\xi} := \inf_{\psi} \max_{t \in [0,1]} \mathcal{E}_\phi^\xi(\psi(t)),$$

over paths $\psi \in C([0,1]; X_\phi)$ such that

$$\mathcal{E}_\phi^\xi(\psi(0)) < \mathcal{E}_\phi^\xi(u_{m,\phi}), \qquad \psi(1) \in \mathcal{N}_\varepsilon(u_{m,\phi}).$$

Proposition. *There exists saddle points u_s^ϕ, $\tilde{u}_s^\phi$ of $\mathcal{E}_\phi^\xi$ such that*

$$\mathcal{E}_\phi^\xi(u_s^\phi) = \Delta E_1^{\phi,\xi} \geq c_s + O(\phi^{1/3}),$$
$$\mathcal{E}_\phi^\xi(\tilde{u}_s^\phi) = \Delta E_2^{\phi,\xi} = c_s + O(\phi^{1/3}).$$

Problem and partial resolution

Just fail to capture properties of u_s^ϕ, $\tilde{u}_s^\phi$.

Define "volume-constrained minimizers" $u_{\omega,\phi}$ such that

$$\nu(u_{\omega,\phi}) = \omega, \qquad \mathcal{E}_\phi^\xi(u_{\omega,\phi}) = \inf_{\{u:\, \nu(u)=\omega\}} \mathcal{E}_\phi^\xi(u) =: \hat{\mathcal{E}}_\phi(\omega).$$

Define the "weak" energy barrier surrounding $u_{m,\phi}$ as

$$\Delta E_{\omega,\phi}^\xi := \sup_{\omega\in[0,\nu_m]} \hat{\mathcal{E}}_\phi(\omega).$$

Properties of vol-constrained min

Choose (any) $\omega_* \in [0, \nu_m]$ such that

$$\widehat{\mathcal{E}}_\phi(\omega_*) = \Delta E^\xi_{\omega,\phi} + O(\phi^{1/3})$$

and denote by $u_{\omega_*,\phi}$ a corresponding volume-constrained minimizer.

Theorem. *The volume-constrained minimizer $u_{\omega_*,\phi}$ is well-approximated by the limit saddle point Ψ_s in the sense that*

$$|u_{\omega_*,\phi} - \Psi_s|_{\mathbb{T}_{\phi L}} \leq \gamma,$$

$$|\mathcal{E}^\xi_\phi(u_{\omega_*,\phi}) - c_s| \lesssim \phi^{1/3},$$

$$|\nu(u_{\omega_*,\phi}) - \nu_s| \leq C(\xi)\phi^{1/6}.$$

Proof similar to that for min

Here compactness takes the form

Lemma.

$$|\nu(u) - \nu_s| \le \beta_0 \text{ and } |u - \Psi_s|_{\mathbb{T}_{\phi L}} \ge \gamma$$
$$\Rightarrow \quad \mathcal{E}^{\xi}_{\phi}(u) \ge \inf_{\substack{|u-\Psi_s|_{\mathbb{R}^d} \ge \gamma \\ \nu_0(u)=\nu_s}} \mathcal{E}^{\xi}_{0}(u) - \delta.$$

Remark. *Notice that any approximately optimal path for* $\Delta E_2^{\phi,\xi}$ *stays within a* γ *neighborhood of* Ψ_s *for all volumes close to* ν_s*. The mountain pass around* Ψ_s *is "narrow" in this sense.*

Part II

THE DROPLET SHAPE

Isoperimetric inequalities

The limit energy

$$\mathcal{E}_0^\xi(u) = c_0 \mathrm{Per}(\{u=1\}) - 4|\{u=1\}| + \frac{4|\{u=1\}|^2}{\xi^{d+1}}$$

made us think of droplets because of the classical isoperimetric inequality.

Setting

$$\mathrm{P}_E(A) := \sigma_d^{1/d} d^{(d-1)/d} |A|^{(d-1)/d},$$

the classical isoperimetric inequality can be expressed

$$\mathrm{Per}(A) \geq \mathrm{P}_E(A),$$

for any Borel set $A \subset \mathbb{R}^d$.

Isoperimetric on the torus

For subsets of the torus that are not too large in the sense of $|A| \le \epsilon\,|\mathbb{T}_{\phi L}|$ for a known constant $\epsilon > 0$, there holds

$$\mathrm{Per}_{\mathbb{T}_{\phi L}}(A) \ge \mathsf{P}_E(A). \qquad (1)$$

Sphericity

Deviation from sphericity is measured in terms of the Fraenkel asymmetry.

Definition. *For* $E \subset \mathbb{R}^d$ *defined as*

$$\lambda(A) := \min_{x \in \mathbb{R}^d} \frac{|A \triangle B(x)|}{|A|},$$

where $B(x) \subset \mathbb{R}^d$ *is a ball with center* x *and volume* $|A|$ *and* $A \triangle B$ *denotes the symmetric difference of* A *and* B*.*

Similarly, for $A \subset \mathbb{T}_{\phi L}$ *(not too large)*

$$\lambda(A) := \min_{x \in \mathbb{T}_{\phi L}} \frac{|A \triangle B(x)|}{|A|},$$

$B(x) \subset \mathbb{T}_{\phi L}$.

Sharp quantitative isoperimetric inequality

Fusco, Maggi, Pratelli (2008):

Theorem.

$$\mathsf{Per}(A) \geq \mathsf{P}_E(A) + C(d)\lambda(A)^2 \mathsf{P}_E(A),$$

Adaptation to the torus:

Corollary.

$$\mathsf{Per}_{\mathbb{T}_{\phi L}}(A) \geq \mathsf{P}_E(A) + C(d)\lambda(A)^2 \mathsf{P}_E(A) - \frac{4d|A|}{\phi L},$$

for any Borel set $|A| \subset \mathbb{T}_{\phi L}$ *with* $|A| < \epsilon |\mathbb{T}_{\phi L}|$.

Application to Cahn-Hilliard

Theorem. *The minimizer* $u_{m,\phi}$ *and any volume-constrained minimizer* $u_{\omega_*,\phi}$ *are approximately spherical in the sense that, for every* $s \in [-1+2\phi^{1/3}, 1-2\phi^{1/3}]$, *both* $u_{m,\phi}$ *and* $u_{\omega_*,\phi}$ *satisfy*

$$\lambda(\{u > s\}) \lesssim \phi^{\alpha} \qquad \textit{with} \quad \alpha = \min\{1/6, 1/(2d)\}$$

and consequently

$$|u_{m,\phi} - \Psi_m|^2_{\mathbb{T}_{\phi L}} + |u_{\omega_*,\phi} - \Psi_s|^2_{\mathbb{T}_{\phi L}} \begin{cases} \leq C(\xi)\phi^{1/6} & \textit{for} \quad d = 2,3 \\ \lesssim \phi^{1/(2d)} & \textit{for} \quad d \geq 4. \end{cases}$$

In fact, for any $\omega \in (0, \xi^{d+1}/2)$ *and* ϕ *sufficiently small, any associated volume-constrained minimizer* $u_{\omega,\phi}$ *satisfies*

$$\lambda(\{u_{\omega,\phi} > s\}) + |u_{\omega,\phi} - \Psi(\cdot,\omega)|^2_{\mathbb{T}_{\phi L}} \lesssim \frac{\phi^{\alpha}}{\omega}.$$

No EL eqn.

Part III

STEINER SYMMETRIZATION

Symmetrization on R^d and torus

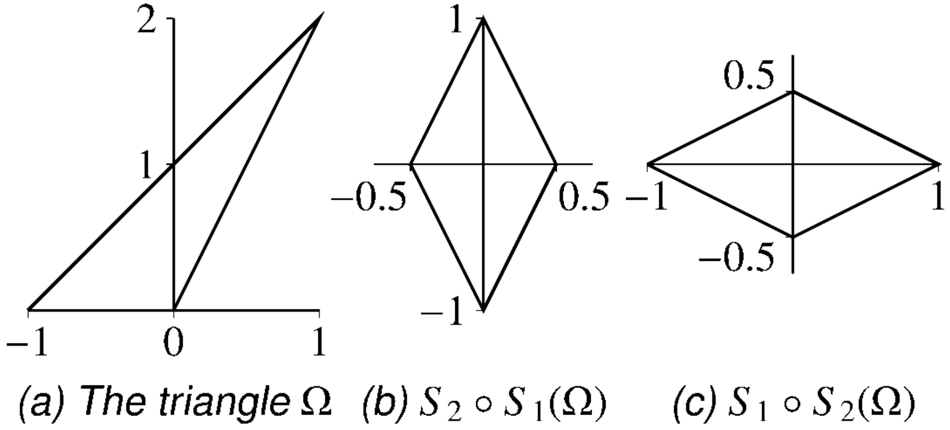


Figure. *(a) The triangle* Ω *(b)* $S_2 \circ S_1(\Omega)$ *(c)* $S_1 \circ S_2(\Omega)$

Kawohl (1985)

$$\int_{\mathbb{T}_{\phi L}} |\nabla u|^2 \, dx \geq \int_{\mathbb{T}_{\phi L}} |\nabla u^*|^2 \, dx$$

$$\int_{\mathbb{T}_{\phi L}} F(u) \, dx = \int_{\mathbb{T}_{\phi L}} F(u^*) \, dx \qquad \text{for measurable functions } F.$$

Via progress on equality of gradients by Cianchi-Fusco (2006)

Theorem. *Let* $u \in C^1(\mathbb{T}_{\phi L})$ *satisfy*

$$\left|\left\{(\widehat{x}_i, y) \in \mathbb{T}_{\phi L} : \partial_y u(\widehat{x}_i, y) = 0,\ u(\widehat{x}_i, y) < M(\widehat{x}_i)\right\}\right| = 0$$

for all $i = 1, \ldots, d$, *where*

$$M(\widehat{x}_i) := \max\left\{u(\widehat{x}_i, y), y \in \left[-\frac{\phi L}{2}, \frac{\phi L}{2}\right]\right\}.$$

If

$$\int_{\mathbb{T}_{\phi L}} |\nabla u|^2 \, dx = \int_{\mathbb{T}_{\phi L}} |\nabla u^*|^2 \, dx,$$

then there exists $a \in \mathbb{T}_{\phi L}$ *such that* u *is Steiner symmetric about the point* a.

Consequences d $\geq$ 2

Proposition. *For any* $\omega \in [\omega_1, \xi^{d+1}/2]$, *any volume-constrained minimizer* $u_{\omega,\phi}$ *is (up to a translation) equal to its Steiner symmetrization about the origin. In particular, its superlevel sets are simply connected and* $u_{\omega,\phi}$ *is strictly decreasing in all directions away from the unique point of maximum.*

Additionally in d=2

Proposition. *For any volume-constrained minimizer* $u_{\omega,\phi}$ *with volume* $\omega \in [\omega_1, \xi^3/2]$ *and any* $\eta \in (-1,1)$*, there holds*

$$\rho_{out}(\{u_{\omega,\phi} > \eta\}) = r_\omega + \frac{O(\phi^{1/6})}{(1+\eta)},$$

and

$$\rho_{in}(\{u_{\omega,\phi} > \eta\}) = r_\omega + \frac{O(\phi^{1/6})}{(1-\eta)},$$

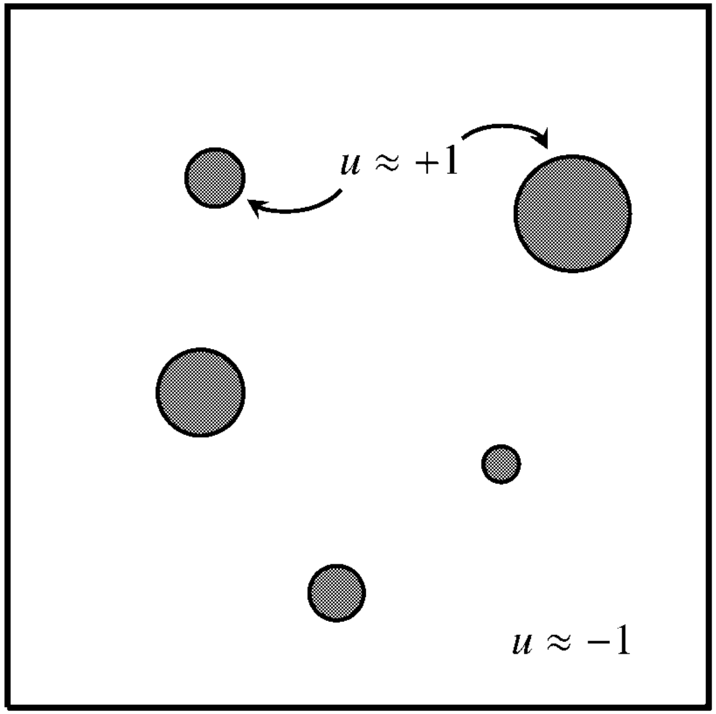
where

$$r_\omega := \sqrt{\frac{\omega}{\pi}}.$$

Consequently, there holds

$$\rho_{out}(\{u_{\omega,\phi} > \eta\}) - \rho_{in}(\{u_{\omega,\phi} > \eta\}) = \frac{O(\phi^{1/6})}{(1-\eta^2)}.$$

Input into stochastic model?



a la Vanden-Eijnden and Westdickenberg,
Rare events in stochastic partial differential equations on large spatial domains, (2008),

References

Gelantalis and Westdickenberg, *Energy barrier and Gamma-convergence in the d-dimensional Cahn-Hilliard equation*, Calc. Var. PDE, (2014).

Gelantalis, Wagner, and Westdickenberg, *Existence and properties of certain critical points of the Cahn-Hilliard energy,* submitted (2015).

Thank you for your attention.