Coarsening mechanisms for Cahn-Hilliard equations with one and two-sided degenerate diffusion mobility

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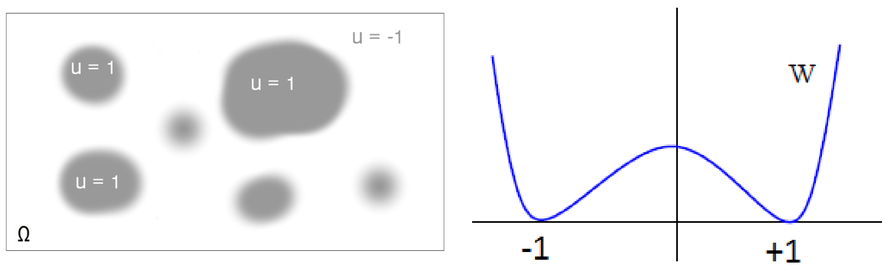
Cahn-Hilliard equation for phase separations

Let $\mathbf{u(x)}$ denote the density of components of a binary mixture and $\mathbf{W(u)}$ a double-well potential. A transition layer between the two phases has thickness of order ε.



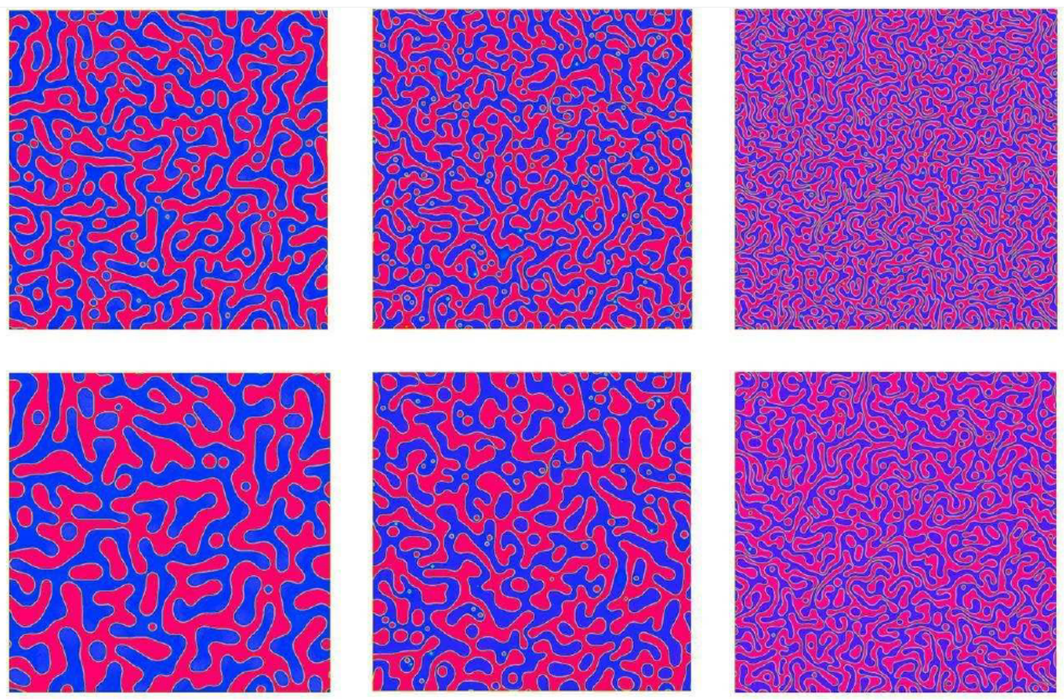
The Cahn-Hilliard energy is

$$\mathcal{E}(u) = \int_\Omega \frac{\varepsilon^2}{2}|\nabla u|^2 + W(u)\,dx.$$

The Cahn-Hilliard equation: H^{-1}— gradient flow

$$u_t = \nabla \cdot M(u)\nabla(-\varepsilon^2 \Delta u + W'(u))$$

Diffusion mobility dependent coarsening (Sheng et al. 2010)



(a) (b) (c)

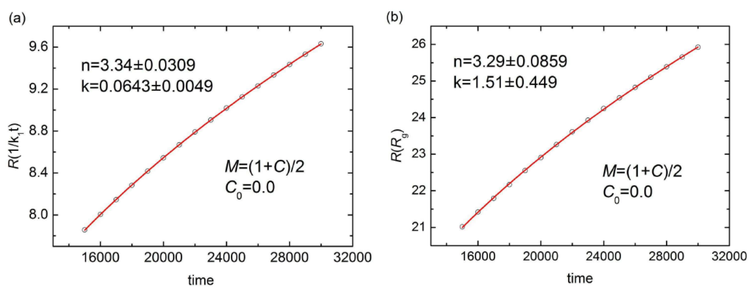
(a) $M = 1$ (b) $M = \frac{1+u}{2}$ (c) $M = 1 - u^2$

Coarsening Rates

A characteristic length scale $\mathbf{R(t)}$ grows in time, the growth rate depends on the diffusion mobility $\mathbf{M}$.

1. $M = 1$: $R(t) \sim t^{1/3}$
   Front migrates according to Mullins-Sekerka model (Pego '89).
2. $M = 1 - u^2$: $R(t) \sim t^{1/4}$.
   This rate is well known and is generally attributed to surface diffusion. But surface diffusion is not enough for coarsening to occur when there are disjoint branches of interfaces. What else is going on?
3. $M = \frac{1+u}{2}$: $R(t) \sim$????

Numerical simulation: data fitting ($M = \frac{1+u}{2}$, Sheng et al. 2010)



Assume a power law relation

$$R(t)^n - R_0^n = kt,$$

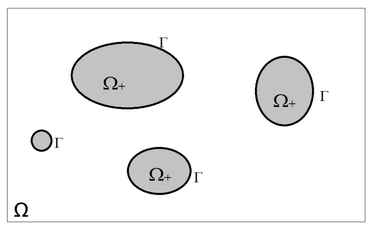
data fitting indicates $n = 3.3$, that is

$$R(t) \sim t^{1/3.3}.$$

Question: How do we have such a weird rate?

Explanation through asymptotic analysis

The two phases are separated by an interface.
We can directly describe the evolution of the interface.
Sharp interface models are connected to phase field models.



Free energy is related to interface area by Γ-limit:

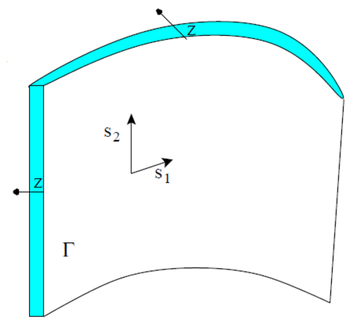
$$\lim_{\varepsilon\to 0}\int_\Omega \left(\frac{\varepsilon}{2}|\nabla u|^2 + \frac{1}{\varepsilon}W(u)\right)dx = \int_\Gamma a_1\,dS.$$

Under the mass conservation restriction, minimizers of $\mathcal{E}$ minimize the interface area.

Geometry of interfaces

The 0–level set of $\mathbf{u}$ is a hypersurface $\Gamma(t) \in \mathbb{R}^n$. Let $\rho(x,t)$ be the signed distance function from $\mathbf{x}$ to $\Gamma(t)$ and $z = \frac{\rho}{\varepsilon}$. Then $x \mapsto (s_1, s_2, z)$.

$-\frac{\partial \rho}{\partial t}$ is the normal velocity of Γ, and



$$\nabla_x = \sum_{i=1}^{2}(\nabla_x s_i)\frac{\partial}{\partial s_i} + \varepsilon^{-1}(\nabla_x \rho)\frac{\partial}{\partial z}.$$

$$\varepsilon^2\Delta_x = \partial_{zz} + \varepsilon\kappa\partial_z + \varepsilon^2(\Delta_s + z\kappa_1\partial_z) + \ + \varepsilon^3\Delta_1 + O(\varepsilon^4),$$

where in 3D:

$$\kappa = k_1 + k_2 = H,$$
$$\kappa_1 = -k_1^2 - k_2^2 = 2K - H^2.$$

Here k_1, k_2 are principal curvatures and H, K are mean and Gaussian curvatures.

Interface migration laws for the CH with $M = \frac{1+u}{2}$

- In time scale $t = O(\varepsilon^{-1})$: one-sided Mullins-Sekerka (or Hele-Shaw)

$$\Delta\mu_1 = 0 \quad \text{in } \Omega_+,$$
$$\mu_1 = H \quad \text{on } \Gamma,$$
$$V = \partial_n \mu_1^+ \quad \text{on } \Gamma.$$

  Disjoint components of Ω_+ do not communicate.
- In time scale $t = O(\varepsilon^{-2})$, a quasi-stationary porous medium diffusion process in Ω_- determines the normal velocity of Γ.

$$\nabla \cdot (\mu_1 \nabla \mu_1) = 0 \quad \text{in } \Omega_-, \tag{1}$$
$$\mu_1 = H \quad \text{on } \Gamma, \tag{2}$$
$$V = \mu_1^- \partial_n \mu_1^- \quad \text{on } \Gamma. \tag{3}$$

- Scaling arguments suggest $R \sim t^{1/3}$ in the $t = O(\varepsilon^{-1})$ dynamics and $R \sim t^{1/4}$ in the $t = O(\varepsilon^{-2})$ dynamics. So the numerical simulation is in a regime where a hybrid behavior, or a crossover of coarsening occurs.

Interface migration laws for CH with $M = 1 - u^2$

- In $t = O(\varepsilon^{-1})$ time scale, no migration of interface.
- In $t = O(\varepsilon^{-2})$ time scale, the normal velocity of the interface is determined by surface diffusion together with a quasi-stationary porous medium diffusion process in both phases.

$$\nabla \cdot (\mu_1 \nabla \mu_1) = 0 \quad \text{in } \Omega_\pm, \tag{4}$$
$$\mu_1 = H \quad \text{on } \Gamma, \tag{5}$$
$$V = \Delta_s H + \mu_1^+ \partial_n \mu_1^+ + \mu_1^- \partial_n \mu_1^- \quad \text{on } \Gamma. \tag{6}$$

- Our asymptotic analysis indicates that even though the diffusion mobility is degenerate in both phases, the quasi-stationary porous medium diffusion process provides the communication mechanism for disjoint components of the interface Γ, which makes coarsening possible.
- This mechanism depends on the fact that the double well potential $W(u)$ is smooth at $u = \pm 1$ with $W''(\pm 1) \neq 0$.