Sharp interface limits of scalar and vectorial Allen-Cahn equations

Analysis and PDE Seminar jointly by CUHK, HKU and UNIST



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1 Phase field model for Mean Curvature Flow (MCF)

2 Phase transition for potentials of higher dimensional wells

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Mean Curvature flow

Consider the MCF $\{\Sigma_t\}_{t>0}$ parametrized by $\varphi_t(s)$ with s being the local coordinate:

 $\partial_t \boldsymbol{\varphi}_t(s) = \kappa(\boldsymbol{\varphi}_t(s), t) \boldsymbol{\nu}(\boldsymbol{\varphi}_t(s), t)$

Let $r = d_{\Sigma}(x, t)$ be the signed distance function (positive inside). Differentiating the identity $d_{\Sigma}(\varphi_t(s) + r\nu(s, t), t) \equiv r$ leads to

$$\nabla d_{\Sigma} = \boldsymbol{\nu}, \quad \partial_t d_{\Sigma} = -\partial_t \boldsymbol{\varphi}_t(s) \cdot \boldsymbol{\nu}$$

For fixed t, let $\pi(x)$ be the projection of x on Σ_t and $\{\kappa_i\}_{1 \leq i \leq d-1}$ are the principal curvatures,



$$\Delta d_{\Sigma}(x) = \sum_{i=1}^{d-1} \frac{-\kappa_i(\pi(x))}{1 - \kappa_i(\pi(x))d_{\Sigma}} = -\sum_{i=1}^{d-1} \kappa_i - d_{\Sigma} \sum_{i=1}^{d-1} \kappa_i^2 + o(d_{\Sigma})$$

Barrier formulation : $(\partial_t - \Delta)d_{\Sigma} = d_{\Sigma}|A|^2 + o(d_{\Sigma})$

Example: let $\Sigma_t = S_{R(t)}$ be the sphere of radius R(t) centered at 0 with $R(0) = R_0$,

$$\mathbf{d}_{\Sigma} = R(t) - |x|, \ \boldsymbol{\nu} = \nabla \mathbf{d}_{\Sigma} = -x/|x|, \ \operatorname{div} \boldsymbol{\nu} = \Delta \mathbf{d}_{\Sigma} = -(d-1)/|x|$$

If Σ_t evolves by MCF, then $R(t) = \sqrt{R_0^2 - 2(d-1)t}$.

The **phase–field models** are widely adopted in the description of the evolution of **interfaces** in continuum mechanics. They can be constructed to purposely reproduce a given **sharp interface model** when the thickness of their diffused interface, usually denoted by ε , trends to 0.



Other implicit representations: thresholding scheme, level–set method Typical phase models: Allen–Cahn (L^2 gradient flow) \rightarrow MCF, Cahn–Hilliard (H^1 gradient flow) \rightarrow Hele–Shaw, 4-th order Allen–Cahn \rightarrow Willmore flow.

Ginzburg-Landau equation

Consider Ginzburg-Landau equation under diffusive scaling $(x, t) \rightarrow (\varepsilon x, \varepsilon^2 t)$:

$$\partial_t c_{\varepsilon} = \Delta c_{\varepsilon} - \varepsilon^{-2} W'(c_{\varepsilon}) \tag{GL}$$

where $W(c) = (c^2 - 1)^2$. It is the gradient flow of $\int \frac{\varepsilon}{2} |\nabla c_{\varepsilon}|^2 + \frac{1}{\varepsilon} W(c_{\varepsilon}) dx =: d\mu_t^{\varepsilon}$:

$$\frac{d}{dt}\int d\mu_t^{\varepsilon} = -\int \varepsilon |\partial_t c_{\varepsilon}|^2 \, dx \tag{1}$$

Major challenge: ∇c_{ε} is not bounded in any L^p space due to concentration.

- Modica-Mortola '77, Bronsard-Kohn '91: $\mu_t^{\varepsilon} \xrightarrow{\varepsilon \to 0} \sigma \mathcal{H}^{d-1} \sqcup \Sigma_t$ under Γ -convergence. $\psi_{\varepsilon}(x,t) = \int_0^{c_{\varepsilon}(x,t)} \sqrt{2W(z)} dz$ is bounded in BV class.
- De Mottoni-Schatzman '95: <u>local</u>, asymptotic expansion $c_{\varepsilon} \approx c_A = \theta(\frac{d_{\Sigma}}{\varepsilon}) + o(\varepsilon^2).$
- Evans, Soner, Souganidis '92: global convergence to viscosity sol. to $\frac{\partial_t u}{|\nabla u|} = \operatorname{div} \left(\frac{\nabla u}{|\nabla u|} \right): \ (\partial_t - \Delta) \mathrm{d}_{\Sigma} > 0 \text{ in } \{ x \in \Omega : \mathrm{d}_{\Sigma}(x, t) > 0 \} \text{ as viscosity solu.}$
- Ilmanen '93, Chen '96, Röger-Schätzle '06: global, convergence to varifold solution Brakke '78: convergence of the localized energy law:

$$\frac{d}{dt}\int\phi(x)d\mu_t^{\varepsilon} = \int\varepsilon\left(-\Delta c_{\varepsilon} + \frac{1}{\varepsilon^2}W'(c_{\varepsilon})\right)\nabla c_{\varepsilon}\cdot\nabla\phi - \int\varepsilon\left(\Delta c_{\varepsilon} - \frac{1}{\varepsilon^2}W'(c_{\varepsilon})\right)^2\phi$$

Modulated energy method: Barrier

Recall $d\mu_t^{\varepsilon} = \left(\frac{\varepsilon}{2} |\nabla c_{\varepsilon}|^2 + \frac{1}{\varepsilon} W(c_{\varepsilon})\right) dx$ and the energy stress tensor $\mathbf{T} = \left(\frac{\varepsilon}{2} |\nabla c_{\varepsilon}|^2 + \frac{1}{\varepsilon} W(c_{\varepsilon})\right) \mathbf{I}_d - \varepsilon \nabla c_{\varepsilon} \otimes \nabla c_{\varepsilon}$

For any test function $\phi(x,t)$, one can derive

$$\frac{d}{dt} \int \phi(x,t) \, d\mu_t^{\varepsilon} = \int \partial_t \phi \, d\mu_t^{\varepsilon} + \int \underbrace{\varepsilon \left(-\Delta c_{\varepsilon} + \frac{1}{\varepsilon^2} W'(c_{\varepsilon}) \right) \nabla c_{\varepsilon}}_{\text{div T}} \cdot \nabla \phi \, dx$$
$$- \int \varepsilon \left(\Delta c_{\varepsilon} - \frac{1}{\varepsilon^2} W'(c_{\varepsilon}) \right)^2 \phi \, dx$$

Motivated by Ilmanen '93 (co-dim=1) and Lin '96, Jerrard–Soner '98 (co-dim=2), we choose $\phi = \frac{1}{2} d_{\Sigma}(x, t)^2$ in $\Sigma_t(\delta)$ and constant outside $\Sigma_t(2\delta)$:

$$\partial_t \phi - \Delta \phi + 1 \lesssim \phi \text{ in } \Sigma_t(2\delta),$$
(2)

This function will cut-off the singularity at Σ_t and lead to

$$\frac{d}{dt} \int \phi \underbrace{\left(\frac{\varepsilon}{2} |\nabla c_{\varepsilon}|^{2} + \frac{W(c_{\varepsilon})}{\varepsilon}\right) dx}_{d\mu_{t}^{\varepsilon}} \lesssim \int \phi \, d\mu_{t}^{\varepsilon} + \varepsilon \int \underbrace{\left(\frac{1}{2} |\nabla c_{\varepsilon}|^{2} - \frac{W(c_{\varepsilon})}{\varepsilon^{2}}\right) dx}_{d\zeta_{t}^{\varepsilon}}.$$

Modica '85, Ilmanen '93 use MP to show that the discrepancy $d\zeta_{\varepsilon}^{\varepsilon}$ preserves **negativity**. This implies the strong convergence of c_{ε} in $L^{2}_{loc}(\mathbb{R}^{d} \setminus \Sigma_{t})$.

Asymptotical Analysis

Inner solution is the expansion of c_{ε} near the interface in a stretched variable $z = d_{\Sigma}(x,t)/\varepsilon$, which is introduced to relax the sharp transition of c_{ε} near the interface. Outer solution determines the boundary condition of the inner solution at $z = \pm \infty$. We use the Ansatz

$$c_A(x,t) = c_0(\frac{\mathrm{d}_{\Sigma}}{\varepsilon}, x, t) + \varepsilon c_1 + \cdots \text{ near } \Sigma_t$$
 (inner solution)

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and look for c_A solving Allen-Cahn equations up to a tail:

$$\underbrace{\frac{\partial_t d_{\Sigma}}{\varepsilon} \partial_z c_0 + \partial_t c_0}_{=\partial_t c_A} \approx \underbrace{\frac{\Delta d_{\Sigma}}{\varepsilon} \partial_z c_0 + \frac{1}{\varepsilon^2} \partial_z^2 c_0 + \Delta c_0 + \dots - \frac{1}{\varepsilon^2} W'(c_0)}_{=\Delta c_A - \frac{1}{\varepsilon^2} W'(c_A)}$$

• $O(\varepsilon^{-2})$: we choose $c_0 = \theta(\frac{d_{\Sigma}}{\varepsilon})$, the optimal profile:

$$\begin{array}{ll} -\theta^{\prime\prime}(z) + W^{\prime}(\theta(z)) &= 0, \forall z \in \mathbb{R}, \\ \theta(0) = 0, \theta(\pm \infty) &= \pm 1. \end{array} \right\} \Rightarrow \theta(z) = \tanh(\frac{z}{\sqrt{2}})$$

• $O(\varepsilon^{-1})$: $(\partial_t - \Delta) d_{\Sigma} = 0$ on Σ_t leads to MCF.

$$(\partial_t - \Delta)c_0 + \frac{1}{\varepsilon^2}W'(c_0) = (\partial_t d_{\Sigma} - \Delta d_{\Sigma})\theta'(\frac{d_{\Sigma}}{\varepsilon})$$
$$= \frac{\partial_t d_{\Sigma} - \Delta d_{\Sigma}}{d_{\Sigma}}\frac{d_{\Sigma}}{\varepsilon}\theta'\left(\frac{d_{\Sigma}}{\varepsilon}\right) \approx \sqrt{\varepsilon} \quad \text{in} \quad L^2(\Sigma_t(\delta))$$

Brakke's inequality

Let $\{\Sigma_t\}_{t>0}$ be a family of (d-1)-closed surface in \mathbb{R}^d with normal velocity V, then

$$\frac{d}{dt} \int_{\Sigma_t} f(x) \, \mathrm{d}\mathcal{H}^{d-1} = \int_{\Sigma_t} (V \cdot \nabla^\perp f - fV \cdot \mathbf{H}) \, \mathrm{d}\mathcal{H}^{d-1}.$$
(3)

Brakke's lemma

Assume V be normal, then $V = \mathbf{H}$ is equivalent to the Brakke's inequality:

$$\frac{d}{dt} \int_{\Sigma_t} f(x) \, \mathrm{d}\mathcal{H}^{d-1} \leqslant \int_{\Sigma_t} (\mathbf{H} \cdot \nabla f - f\mathbf{H} \cdot \mathbf{H}) \, \mathrm{d}\mathcal{H}^{d-1} \tag{4}$$

Subtracting (3) from (4):
$$0 \leq \int_{\Sigma_t} \nabla f \cdot (\mathbf{H} - V) - f\mathbf{H} \cdot (\mathbf{H} - V)$$
 (5)

To blow-up at $x_0 \in \Sigma_t$, we set $w = \mathbf{H} - V$ and replace f by $\lambda^{2-d} f(\frac{x-x_0}{\lambda})$.

$$\begin{split} & 0 \leqslant \lambda^{1-d} \int_{\Sigma_t} (\nabla f)(\frac{x-x_0}{\lambda}) \cdot w(x) dx + O(\lambda) \\ & = \int_{\frac{\Sigma_t - x_0}{\lambda}} \nabla f(y) \cdot w(x_0 + \lambda y) dy + O(\lambda) \xrightarrow{\lambda \to 0} \int_{T_{x_0} \Sigma_t} (\nabla_{\Sigma} f + \mathbf{n} \partial_r f) \cdot w(x_0). \end{split}$$

Since $T_{x_0}\Sigma_t \cong \mathbb{R}^{d-1}$ and w is normal, this implies $\mathbf{H} = V$. The book of Tonegawa' 2019 gives a friendly introduction of Brakke flow.

Phase-field approximation of Brakke's inequality

Writing $\mu_t = \mathcal{H}^{d-1} \sqcup \Sigma_t$ and $\mu_t^{\varepsilon}(A) \triangleq \int_A \left(\varepsilon |\nabla c_{\varepsilon}|^2 + \frac{1}{\varepsilon} W(c_{\varepsilon}) \right) dx$. The Brakke's inequality for MCF writes

$$\frac{d}{dt} \int f \, d\mu_t \leqslant \int \mathbf{H} \cdot \nabla^{\perp} f \, d\mu_t - \int |\mathbf{H}|^2 f \, d\mu_t,$$

$$\frac{d}{dt} \int f \, d\mu_t^{\varepsilon} = \int \varepsilon \left(-\Delta c_{\varepsilon} + \frac{1}{\varepsilon^2} W'(c_{\varepsilon}) \right) \nabla c_{\varepsilon} \cdot \nabla f \, dx - \int \varepsilon \left(\Delta c_{\varepsilon} - \frac{1}{\varepsilon^2} W'(c_{\varepsilon}) \right)^2 f \, dx$$

Based on Ilmanen '93, Chen '96, finally Röger-Schätzle '06 proved the following property under d = 2, 3: If $\mu_t^{\varepsilon} \to \mu_t$ weakly as Radon measure, then

• the lower-semicontinuity property holds:

$$\int f |\mathbf{H}|^2 \, d\mu_t \leqslant \liminf_{\varepsilon \to 0} \int \varepsilon \left(\Delta c_\varepsilon - \frac{1}{\varepsilon^2} W'(c_\varepsilon) \right)^2 f \, dx$$

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for f conti. Here a localization is needed to insert f in the inequality.

• μ_t is (d-1)-integral, i.e. $\mu_t = \theta_t \mathcal{H}^{d-1} \sqcup \Sigma_t$ with Σ_t being a countably (d-1)-rectifiable, \mathcal{H}^{d-1} -measurable set and $\theta \in L^1_{loc}(\mathcal{H}^{d-1} \sqcup \Sigma_t)$.

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Keller–Rubinstein–Sternberg problem

We consider the vectorial (or matrix-valued) Ginzburg–Landau equation with potentials of higher dimensional wells.

$$\partial_t Q_\varepsilon = \Delta Q_\varepsilon - \varepsilon^{-2} \partial W(Q_\varepsilon) \qquad Q_\varepsilon : \Omega \subset \mathbb{R}^d \mapsto \mathbb{R}^n \tag{GL}$$

where $\operatorname{Argmin} W(Q) = \mathbb{M} \triangleq \mathbb{M}^+ \sqcup \mathbb{M}^- \subset \mathbb{R}^n$ are two disjoint submanifolds.

Conjecture of Rubinstein–Sternberg–Keller '89

For well-prepared initial data, the gradient of Q_{ε} will be concentrated on a moving interface Σ_t governed by MCF and as $\varepsilon \downarrow 0$,

$$\int_{\Omega} \left(\frac{\varepsilon}{2} \left| \nabla Q_{\varepsilon} \right|^2 + \frac{1}{\varepsilon} W(Q_{\varepsilon}) \right) \, dx \approx \sigma \mathcal{H}^{d-1}(\Sigma_t) + \varepsilon \sum_{\pm} \sigma^{\pm} \int_{\Omega_t^{\pm}} \left| \nabla Q^{\pm} \right|^2 \, dx \qquad (6)$$

Moreover $Q^{\pm}: \Omega_t^{\pm} \times (0, T) \mapsto \mathbb{M}^{\pm}$ satisfy harmonic map heat flow.

- 1 Lin–Pan–Wang '13: Establishing (6) in the steady case, \mathbb{M}^{\pm} hypersurfaces, $\Sigma_t = \Sigma$ unique smooth stable minimum surface. $Q^{\pm}|_{\partial\Omega^{\pm}}$ form a minimal pair.
- 2 Fei–Wang–Zhang-Zhang '18: dynamic case with $\mathbb{M} = \mathbb{CP}^2 \sqcup \{0^5\} \subset \mathbb{R}^5$ by Hilbert expansion. Laux–L. '21 by modulated energy.
- 3 Fei-Lin-Wang-Zhang 'arxiv : dynamic case with $\mathbb{M} = \mathbb{O}(n)$ by Hilbert expansion.

Consider the matrix-valued GL equation

$$\partial_t Q_{\varepsilon} = \Delta Q_{\varepsilon} - \frac{1}{\varepsilon^2} \partial W(Q_{\varepsilon})$$

where $Q_{\varepsilon} : \Omega \to \mathbb{Q}$ where

$$\mathbb{Q} \triangleq \{ Q \in \mathbb{R}^{3 \times 3} : Q = Q^T, \operatorname{tr} Q = 0 \},$$
$$W(Q) = \frac{a}{2} \operatorname{tr}(Q^2) - \frac{b}{3} \operatorname{tr}(Q^3) + \frac{c}{4} \left(\operatorname{tr}(Q^2) \right)^2$$

is the Landau's

expansion of the (molecular) free energy and a, b, c > 0 are temperature dependent constants. At the critical temperature

$$b^2 = 27ac, s_- = 0, s_+ = \frac{b + \sqrt{b^2 - 24ac}}{4c}.$$

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argmin
$$W(Q) = \mathbb{M} := \{s(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}\mathbf{I}_3) : \mathbf{n} \in \mathbb{S}^2, s = s_{\pm}\}.$$

where $Q(x) = \int_{\mathbb{S}^2} f(x, p)(p \otimes p - \frac{1}{3}I) \,\mathrm{d}\mathcal{H}^2(p)$

is the normalized second moment of the distribution $f(x, \cdot)$ for fixed $x \in \Omega$.

The quasi-distance is define by 1

$$d^{W}(Q) \triangleq \inf_{\gamma} \int_{0}^{1} \sqrt{2W(\gamma(t))} |\gamma'(t)| dt$$
 (7)

where γ is any curve satisfying $\gamma(1) = Q$ and

$$\gamma(0) \in \mathbb{M}^+ = \{s^+(\mathbf{n} \otimes \mathbf{n} - \mathbf{I}_3/3) : \mathbf{n} \in \mathbb{S}^2\}$$

Moreover, we define $\psi_{\varepsilon}(x,t) \triangleq d_{\varepsilon}^{W} \circ Q_{\varepsilon}(x,t)$ where $d_{\varepsilon}^{W}(Q) \triangleq (\phi_{\varepsilon} *_{\mathbb{Q}} d^{W})(Q)$, mollified by an isotropic function ϕ_{ε} in \mathbb{Q} . Motivated by Fischer–Laux–Simon '21 on the scalar case, we introduce

$$E_{\varepsilon}[Q_{\varepsilon}|\Sigma](t) \triangleq \int_{\Omega} \left(\frac{\varepsilon}{2} |\nabla Q_{\varepsilon}|^2 + \frac{1}{\varepsilon} W(Q_{\varepsilon}) + \varepsilon^5 - \boldsymbol{\xi} \cdot \nabla \psi_{\varepsilon}\right) dx,$$

where $\boldsymbol{\xi}$ is an extension of the normal of Σ_t whose modulus decay in d_{Σ}^2 . Note that $|\partial d^W(\cdot)| = \sqrt{2W(\cdot)}$ a.e. in \mathbb{Q} . So $(\mathbb{Q}, 2W)/\mathbb{M}$ is a (quotient) metric space with distance function (7).

¹In the scalar case $d^W(z) = \int_0^z \sqrt{2W(s)} \, ds$. Yuning LIU (NYU Shanghai)



Modulated energy method: Calibration

Recall
$$s_{-} = 0, s_{+} = \frac{b + \sqrt{b^2 - 24ac}}{4c}, \psi_{\varepsilon}(x, t) \triangleq \mathbf{d}_{\varepsilon}^{W} \circ Q_{\varepsilon}(x, t)$$
 and the quasi-distance
 $E_{\varepsilon}[Q_{\varepsilon}|\Sigma](t) \triangleq \int_{\Omega} \left(\frac{\varepsilon}{2} |\nabla Q_{\varepsilon}|^{2} + \frac{1}{\varepsilon}W(Q_{\varepsilon}) + \varepsilon^{5} - \boldsymbol{\xi} \cdot \nabla \psi_{\varepsilon}\right) dx$

Laux–L. ' 21

Let Σ_t be a smooth MCF on [0,T] and $\varepsilon \|Q_{\varepsilon}^{in}\|_{L^{\infty}(\Omega)} + E_{\varepsilon}[Q_{\varepsilon}|\Sigma](0) \lesssim \varepsilon$,

then we have $E_{\varepsilon}[Q_{\varepsilon}|\Sigma](t) \lesssim \varepsilon$ for any $t \in [0, T]$.

Moreover, up to the extraction of a subsequence $\varepsilon = \varepsilon_k$,

$$Q_{\varepsilon_k} \xrightarrow{k \to \infty} Q = s_{\pm} \left(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3} \mathbf{I}_3 \right) \text{ weak-star in } L^{\infty}_t(H^1_{loc}(\Omega^{\pm}_t))$$

where $\mathbf{n}: \Omega_t^+ \mapsto \mathbb{S}^2$ is a weak solution of harmonic heat flow with 0-Neumann boundary condition on $\partial \Omega_t^+ = \Sigma_t$.

By L.' preprint, one can derive, for some $\beta > 0$, a quantitative estimate $\|\psi_{\varepsilon} - \sigma \mathbf{1}_{\Omega^+_{\varepsilon}}\|_{L^1(\Omega)} \lesssim \varepsilon^{\beta}$

under an assumption on the initial data. This follows from a Gröwall inequality, rather than the BV compactness of ψ_{ε} .

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Calibration and discrepancy: scalar case

In the scalar case $\psi_{\varepsilon}(x,t) = \int_{0}^{c_{\varepsilon}(x,t)} \sqrt{2W(z)} dz$, $n_{\varepsilon} = \frac{\nabla \psi_{\varepsilon}}{|\nabla \psi_{\varepsilon}|}$, and $\boldsymbol{\xi}$ satisfies $\partial_{t}\boldsymbol{\xi} + (\mathbf{H}\cdot\nabla)\boldsymbol{\xi} + (\nabla\mathbf{H})^{T}\boldsymbol{\xi} = O(\mathbf{d}_{\Sigma}).$

We can write the modulated energy by:

$$E_{\varepsilon}[c_{\varepsilon}|\Sigma](t) = \int_{\Omega} \frac{\varepsilon}{2} |\nabla c_{\varepsilon}|^{2} + \frac{1}{\varepsilon} W(c_{\varepsilon}) - \overbrace{\boldsymbol{\xi}} \cdot \frac{\nabla \psi_{\varepsilon}}{|\nabla \psi_{\varepsilon}|} |\nabla c_{\varepsilon}| \sqrt{2W(c_{\varepsilon})}$$
$$= \int_{\Omega} \underbrace{\frac{\varepsilon}{2} |\nabla c_{\varepsilon}|^{2} + \frac{1}{\varepsilon} W(c_{\varepsilon}) - |\nabla c_{\varepsilon}| \sqrt{2W(c_{\varepsilon})}}_{\text{discrepancy}^{2}} + \int_{\Omega} \underbrace{(1 - \boldsymbol{\xi} \cdot \mathbf{n}_{\varepsilon})}_{\geq \min(\mathrm{d}_{\Sigma}^{2}, 1)} |\nabla \psi_{\varepsilon}|$$
By $\varepsilon |\nabla c_{\varepsilon}|^{2} = |\nabla \psi_{\varepsilon}| + \sqrt{\varepsilon} |\nabla c_{\varepsilon}| \underbrace{\left(\sqrt{\varepsilon} |\nabla c_{\varepsilon}| - \frac{1}{\sqrt{\varepsilon}} \sqrt{2W(c_{\varepsilon})}\right)}_{\text{discrepancy}}$

and the Cauchy-Schwarz inequality, one can show

$$E_{\varepsilon}[c_{\varepsilon}|\Sigma](t) \gtrsim \int_{\Omega} \varepsilon |\nabla c_{\varepsilon}|^2 \min(\mathrm{d}_{\Sigma}^2, 1)$$

One can show $E_{\varepsilon}[c_{\varepsilon}|\Sigma](t)$ satisfies a Grönwall inequality and thus with appropriate initial data we have $E_{\varepsilon}[c_{\varepsilon}|\Sigma](t) \leq \varepsilon$. This recovers the estimate of Lin '96 when co-dim = 1 without employing MP.

Calibration and discrepancy: vectorial case

In the vectorial case, we shall derive a Grönwall inequality for $E_{\varepsilon}[Q_{\varepsilon}|\Sigma](t)$: Introducing an orthogonal projection in the direction $\partial d_{\varepsilon}^{W}(Q_{\varepsilon})$:

$$\Pi_{Q_{\varepsilon}}\partial_{x_{i}}Q_{\varepsilon} = \left(\partial_{x_{i}}Q_{\varepsilon} : \frac{\partial \mathrm{d}_{\varepsilon}^{W}(Q_{\varepsilon})}{|\partial \mathrm{d}_{\varepsilon}^{W}(Q_{\varepsilon})|}\right) \frac{\partial \mathrm{d}_{\varepsilon}^{W}(Q_{\varepsilon})}{|\partial \mathrm{d}_{\varepsilon}^{W}(Q_{\varepsilon})|}, \text{ with } x_{0} \triangleq t.$$

By Grönwall's inequality
$$\int_{\Omega} \left(\frac{1}{2} |\nabla Q_{\varepsilon}|^{2} + \frac{1}{\varepsilon^{2}} W(Q_{\varepsilon}) \right) (1 - \boldsymbol{\xi} \cdot \mathbf{n}_{\varepsilon}) \\ + \sum_{i=1}^{d} \int_{\Omega} |\partial_{x_{i}} Q_{\varepsilon} - \Pi_{Q_{\varepsilon}} \partial_{x_{i}} Q_{\varepsilon}|^{2} \lesssim \varepsilon^{-1} E_{\varepsilon}[Q_{\varepsilon}|\Sigma](t) \lesssim 1.$$

This leads to the modulated estimate of ∇Q_{ε} without employing MP:

$$\int_{\Omega} |\nabla Q_{\varepsilon}|^2 \min(\mathbf{d}_{\Sigma}^2, 1) \lesssim \varepsilon^{-1} E_{\varepsilon}[Q_{\varepsilon}|\Sigma](t)$$

Define the phase-field analogy of the mean curvature vector by $\mathbf{H}_{\varepsilon} = -\left(\varepsilon\Delta Q_{\varepsilon} - \varepsilon^{-1}\partial F(Q_{\varepsilon})\right) : \frac{\nabla Q_{\varepsilon}}{|\nabla Q_{\varepsilon}|}, \text{ one can derive a differential inequality:} \\
\frac{d}{dt}E_{\varepsilon}[Q_{\varepsilon}|I] + \frac{1}{2\varepsilon}\int \left(\varepsilon^{2}|\partial_{t}Q_{\varepsilon}|^{2} - |\mathbf{H}_{\varepsilon}|^{2} + \left|\mathbf{H}_{\varepsilon} - \varepsilon|\nabla Q_{\varepsilon}|\mathbf{H}\right|^{2}\right) dx \\
+ \frac{1}{2\varepsilon}\int \left|\varepsilon\partial_{t}Q_{\varepsilon} - (\operatorname{div}\boldsymbol{\xi})\partial \mathrm{d}_{\varepsilon}^{W}(Q_{\varepsilon})\right|^{2} dx \lesssim E_{\varepsilon}[Q_{\varepsilon}|I].$

Modulated estimates

To derive the compactness of $\partial_t Q_{\varepsilon}$, we use $\int_{\Omega} |\nabla Q_{\varepsilon}|^2 \min(d_{\Sigma}^2, 1) \lesssim 1$ and

$$\int_{\Omega_T} |\partial_t Q_{\varepsilon} + \mathbf{H} \cdot \nabla Q_{\varepsilon}|^2$$

$$\leqslant \ \varepsilon^{-2} \int_{\Omega_T} \varepsilon^2 |\partial_t Q_{\varepsilon}|^2 - |\mathbf{H}_{\varepsilon}|^2 + \left| \mathbf{H}_{\varepsilon} - \varepsilon |\nabla Q_{\varepsilon}| \mathbf{H} \right|^2 \lesssim 1$$

Formal asymptotic expansion shows $\partial_t Q_{\varepsilon} + \mathbf{H} \cdot \nabla Q_{\varepsilon} = \varepsilon^{-1} (\partial_t d_{\Sigma} + \mathbf{H} \cdot \nabla d_{\Sigma}) + O(1)$. Later we show $[\prod_{Q_{\varepsilon}} \partial_{x_i} Q_{\varepsilon}, Q_{\varepsilon}] = 0$ for $0 \leq i \leq d$. So we have

$$[\partial_i Q_\varepsilon, Q_\varepsilon] = [\partial_i Q_\varepsilon - \Pi_{Q_\varepsilon} \partial_i Q_\varepsilon, Q_\varepsilon] \xrightarrow{k \to \infty} \bar{S}_i(x, t) \text{ weakly in } L^2_t L^2_x(\Omega)$$

By Chen's formulation of GL, (under summation convention)

 $[\partial_t Q_\varepsilon - \Pi_{Q_\varepsilon} \partial_t Q_\varepsilon, Q_\varepsilon] = \partial_{x_i} [\partial_{x_i} Q_\varepsilon - \Pi_{Q_\varepsilon} \partial_{x_i} Q_\varepsilon, Q_\varepsilon].$

Converge locally $Q_{\varepsilon} \xrightarrow{\varepsilon \to 0} Q = s_{\pm}(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}\mathbf{I}_3) \in L^2_t L^2_{loc}(\Omega^{\pm}_t)$ and \mathbf{n} is a weak solution of harmonic heat flow into \mathbb{S}^2 with 0 Neumann bdy condition on Σ_t :

$$\int_0^T \int_{\Omega_t^+} \partial_t \mathbf{n} \wedge \mathbf{n} \cdot \boldsymbol{\varphi} + \int_0^T \int_{\Omega_t^+} (\partial_j \mathbf{n} \wedge \mathbf{n}) \cdot \partial_j \boldsymbol{\varphi} = 0, \quad \forall \boldsymbol{\varphi} \in C_c^1(\Omega)$$

Note that if \mathbf{n} is regular enough, we have

$$\partial_t \mathbf{n} - \Delta \mathbf{n} = |\nabla \mathbf{n}|^2 \mathbf{n} \text{ in } \Omega_t^+, \quad \partial_{\boldsymbol{\nu}} \mathbf{n}|_{\Sigma_t} = 0$$

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A commutator identity

For any
$$0 \leq i \leq d$$
, we have $[\prod_{Q_{\varepsilon}} \partial_{x_i} Q_{\varepsilon}, Q_{\varepsilon}] = 0$, $\forall x \in \Omega$.

Recall the orthogonal projection $\Pi_{Q_{\varepsilon}} \partial_{x_i} Q_{\varepsilon} \parallel \partial d_{\varepsilon}^W(Q_{\varepsilon})$. As $d_{\varepsilon}^W(Q)$ is isotropic (i.e. only depends on the eigenvalues of Q), there exists a smooth symmetric function $g_{\varepsilon}(\lambda_1, \lambda_2, \lambda_3)$ such that

$$\mathbf{d}_{\varepsilon}^{W}(Q) = g_{\varepsilon}(\lambda_{1}(Q), \lambda_{2}(Q), \lambda_{3}(Q))$$

Let Q_0 be a matrix having distinct eigenvalues, then $\lambda_i(Q)$ and the eigenvectors $\mathbf{n}_i(Q)$ are real-analytic functions of Q near Q_0 , and then by chain rule

$$\partial \mathbf{d}_{\varepsilon}^{W}(Q) = \sum_{k=1}^{3} \frac{\partial g_{\varepsilon}}{\partial \lambda_{k}} \frac{\partial \lambda_{k}}{\partial Q} = \sum_{k=1}^{3} \frac{\partial g_{\varepsilon}}{\partial \lambda_{k}} \mathbf{n}_{k}(Q) \otimes \mathbf{n}_{k}(Q)$$

in a neighborhood of Q_0 . We also have

$$Q = \sum_{k=1}^{3} \lambda_k(Q) \mathbf{n}_k(Q) \otimes \mathbf{n}_k(Q)$$

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So we have $\left[\partial d_{\varepsilon}^{W}(Q), Q\right] = 0$, holds in a neighborhood of Q_{0} having distinct eigenvalues, and thus for a general Q by continuity of $\partial d_{\varepsilon}^{W}(Q)$.

Boundary conditions on the free boundary

For any vector field $\varphi \in C_c^1(\Omega, \mathbb{R}^3)$, let Φ be the corresponding anti-symmetric matrix-valued function. Apply the anti-symmetric product $[\cdot, Q_{\varepsilon}]$ to the Q_{ε} equ:

$$\int_0^T \int_\Omega \left[\partial_t Q_\varepsilon, Q_\varepsilon \right] : \Phi + \int_0^T \int_\Omega \left[\partial_j Q_\varepsilon, Q_\varepsilon \right] : \partial_j \Phi = 0$$

We denote $\Sigma_t(\delta)$ the δ -neighborhood of Σ_t . Equivalently,

$$\sum_{\pm} \int_0^T \int_{\Omega_t^{\pm} \setminus \Sigma_t(\delta)} [\partial_t Q_{\varepsilon}, Q_{\varepsilon}] : \Phi + [\partial_j Q_{\varepsilon}, Q_{\varepsilon}] : \partial_j \Phi + \int_0^T \int_{\Sigma_t(\delta)} [\partial_t Q_{\varepsilon}, Q_{\varepsilon}] : \Phi + [\partial_j Q_{\varepsilon}, Q_{\varepsilon}] : \partial_j \Phi = 0$$

The convergences $\lim_{\varepsilon \to 0} Q_{\varepsilon}$ are not up to the boundary Σ_t but $\nabla_{x,t} Q \in L^2_t L^2(\Omega^+_t)$:

$$\int_0^T \int_{\Omega_t^+ \setminus \Sigma_t(\delta)} \left[\partial_t Q, Q \right] : \Phi + \left[\partial_j Q, Q \right] : \partial_j \Phi + \int_0^T \int_{\Sigma_t(\delta)} \bar{S}_0 : \Phi + \bar{S}_j : \partial_j \Phi = 0$$

for some $\bar{S}_i \in L^2_{x,t}$ by modulated estimate. Take $Q = s_{\pm}(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}I_3) \in L^2_t L^2_x(\Omega^{\pm}_t)$:

$$\int_0^T \int_{\Omega_t^+} \partial_t \mathbf{n} \wedge \mathbf{n} \cdot \boldsymbol{\varphi} + \int_0^T \int_{\Omega_t^+} (\partial_j \mathbf{n} \wedge \mathbf{n}) \cdot \partial_j \boldsymbol{\varphi} = 0, \quad \forall \boldsymbol{\varphi} \in C_c^1(\Omega)$$

Convergence estimate of ψ_{ε}

We give a heuristic proof basic on the following result:

$$\partial_{x_i} f^+ = \partial_{x_i} f \mathbf{1}_{\{x \in \Omega: f(x) > 0\}}, \qquad \forall f \in W^{1,1}(\Omega).$$

Recall $\psi_{\varepsilon}(x,t) = d_{\varepsilon}^{W} \circ Q_{\varepsilon}(x,t)$. Differentiating $\int (\psi_{\varepsilon} - \sigma \mathbf{1}_{\Omega^{+}})^{+} dx$ leads to delta mass $\nabla \mathbf{1}_{\Omega^{+}}$. To avoid it, we introduce the weighted energy

$$g_{\varepsilon}(t) := \int (\psi_{\varepsilon} - \sigma \mathbf{1}_{\Omega^+})^+ \zeta(\mathbf{d}_{\Sigma}) dx$$

for a cut-off ζ and let $U_{\varepsilon} = \{x \in \Omega : \psi_{\varepsilon} > \sigma \mathbf{1}_{\Omega^+}\}$. Using $(\partial_t + \mathbf{H} \cdot \nabla) \zeta(\mathbf{d}_{\Sigma}) = O(\mathbf{d}_{\Sigma})$,

$$\begin{split} g'_{\varepsilon}(t) &= \int_{U_{\varepsilon}} \left(\partial_{t} Q_{\varepsilon} + (\mathbf{H} \cdot \nabla) Q_{\varepsilon} \right) : \partial \mathbf{d}_{\varepsilon}^{W}(Q_{\varepsilon}) \, \zeta(\mathbf{d}_{\Sigma}) \\ &- \underbrace{\int_{U_{\varepsilon}} \mathbf{H} \cdot \nabla \psi_{\varepsilon} \zeta(\mathbf{d}_{\Sigma})}_{= \int \mathbf{H} \cdot \nabla (\psi_{\varepsilon} - \sigma \mathbf{1}_{\Omega^{+}})^{+} \zeta(\mathbf{d}_{\Sigma})} + \int (\psi_{\varepsilon} - \sigma \mathbf{1}_{\Omega^{+}})^{+} \underbrace{\partial_{t} \zeta(\mathbf{d}_{\Sigma})}_{\approx -\mathbf{H} \cdot \nabla \zeta(\mathbf{d}_{\Sigma})} \end{split}$$

So we can derive a Grönwall inequality of $g_{\varepsilon}(t) \lesssim \varepsilon$. To get the desired estimate of ψ_{ε} , one simply employ standard trick to remove the weight $\zeta(\mathbf{d}_{\Sigma})$ at the price of a weaker convergence rate ε^{β} .

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Related works which (might) be (re)proved by the modulated energy method:

- Allen-Cahn/(3D)Navier-Stokes (Constant mobility) to MCF/Navier-Stokes, Hensel-L. 'preprint. Variable mobility case which converges to two-phase NSE, is open.
- 2 Cahn–Hilliard to Hele-Shaw. New proof of Alikakos–Bates–Chen '96 using modulated method ?
- 3 Allen–Cahn to triple junction dynamics. Fischer–Marveggio' preprint
- 4 Contact angle model. Abels–Moser '20, Moser–Hensel ' preprint
- 5 Anisotropic models (with anchoring boundary conditions): Lin–Wang '21 for Ericksen's models (static), L. 'preprint for a simplified Landau-De Gennes dynamics (planar case).

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6 Conjecture of Rubinstein–Sternberg–Keller for (two) closed hypersurfaces.