The dynamics of boundary droplets for the mass-conserving Allen-Cahn equation with and without noise

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Two parts

Deterministic – Invariant manifolds

Stochastic – How does additive noise impact the system?

The Allen-Cahn equation has been used to model phase transition in binary alloys,

$$(AC) \quad u_t = \varepsilon^2 \Delta u - f(u) \quad (t,x) \in \mathbb{R} \times \Omega$$
$$\frac{\partial u}{\partial n} = 0 \quad \text{on } \partial\Omega$$

where $0 < \varepsilon << 1$ and $f(u) \sim u^3 - u$ is the derivative of a double well potential F, and Ω is a smoothly bounded domain.

Unfortunately, this equation does preserve species.

Two extensions: The Cahn-Hilliard equation, which is a fourth-order PDE, and

The Mass-conserving Allen-Cahn equation, which is second order but nonlocal, projecting the Allen-Cahn flow onto a constant mass surface:

$$(\dagger) \quad u_t = \varepsilon^2 \Delta u - f(u) + \frac{1}{|\Omega|} \int f(u) dx \quad (t,x) \in \mathbb{R} \times \Omega$$

$$\frac{\partial u}{\partial n} = 0 \quad \text{on } \partial\Omega$$

This is a gradient flow in an affine space for

$$J_\varepsilon(u) = \int_\Omega (\frac{\varepsilon^2}{2}|\nabla u|^2 + F(u))dx, \qquad (1)$$

$$u \in \{v \in H^1(\Omega) : \frac{1}{|\Omega|}\int v dx = m\}.$$

Stationary problem: Carr-Gurtin-Slemrod, DeGiorgi, Modica, Mortola, Sternberg, etc.

For the dynamic problem, the energy must decrease, so the state should quickly take on values near the minima of F (say ± 1) and then the interface, which must exist if the average is to be between ± 1, must reduce while maintaining enclosed volume.

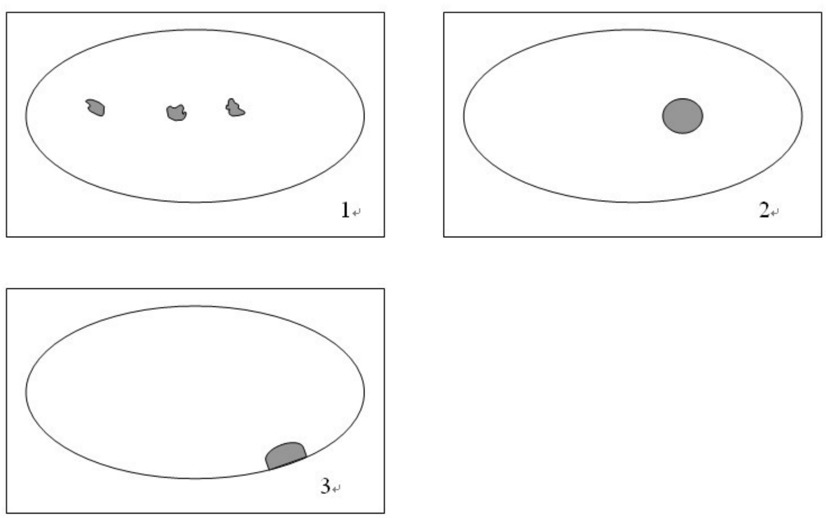


Figure 1: Three stages of the evolution in Ω.

We consider the case of $\Omega \subset \mathbb{R}^2$ and base our work on the important paper by Alikakos-Chen-Fusco (Calc. Var 2000) which gave a construction of approximate solutions to (†) as boundary 'droplets', of radius $\delta << 1$, moving along $\partial\Omega$ with a velocity that they determined to be

$$-\frac{4\varepsilon^2\delta}{3\pi}\mathcal{K}' + h.o.t.$$

Here, $\mathcal{K}$ is the curvature of $\partial\Omega$. Since ε is the thickness of the interface, it is necessary to have $\delta >> \varepsilon$.

A fundamental idea behind the approach can be found in work by Jack Hale and Giorgio Fusco and also Carr-Pego on 1-D Allen-Cahn dynamics for layered states:

Build a manifold of 'metastable states'

Enclose in small tubular neigborhood which is positively invariant

Compute the dynamics tangent to that manifold.

Here we go a little further:
Prove the existence of an invariant manifold as a graph over the first manifold.

PROBLEM: Given an

approximately invariant manifold, M,

is it possible to deduce the existence of a

true invariant manifold, $\tilde{M}$

nearby?

This is similar to the

PROBLEM: Given

an invariant manifold, M, for a dynamical system T_t

is it possible to deduce the existence of

an invariant manifold, $\tilde{M}$, near M

for a dynamical system $\tilde{T}_t$, which is close to T_t?

• Invariant Manifolds

Let X be a Banach space.

Consider a map (e.g. the time-t map of a parabolic PDE)

$T \in C^k(X, X)$, $k \geq 1$.

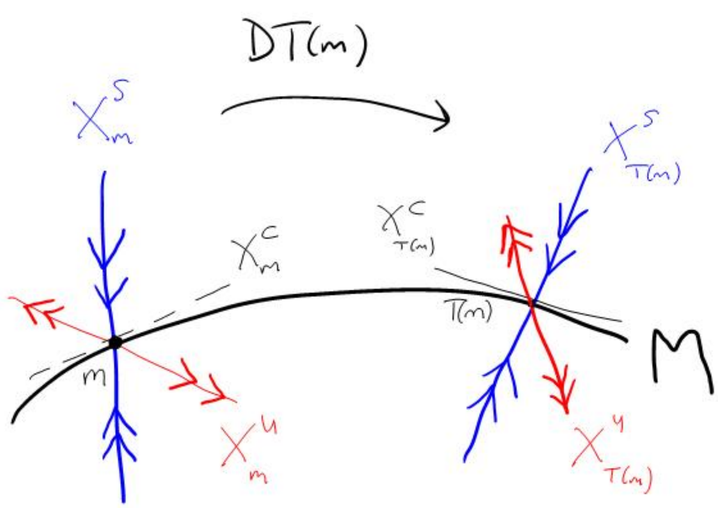
$M \subset X$: a C^k submanifold

M is *INVARIANT* under T if $T(M) \subset M$.

• Conditions for unique persistence of smooth invariant manifolds?

Stability is not sufficient (or necessary).

NORMAL HYPERBOLICITY



Approximately invariant manifolds

- M is approximately invariant if $d(T(M), M)$ is small.

- M is approximately normally hyperbolic if at any $m \in M$, there is a splitting

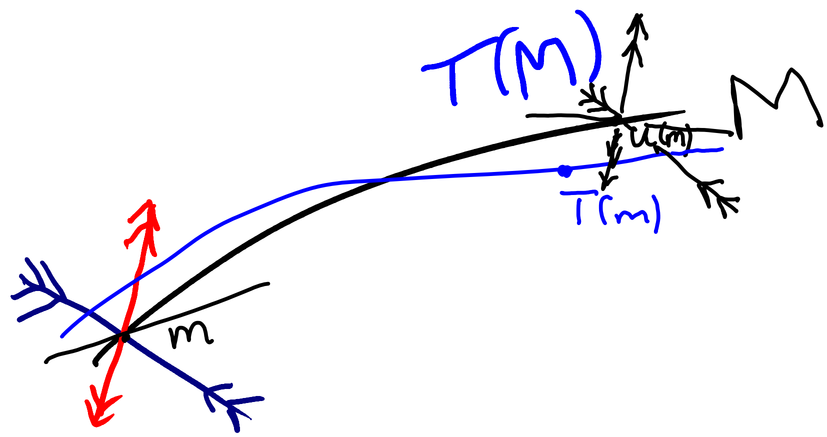
$$X = X_m^s \oplus X_m^u \oplus X_m^c$$

such that

1. $X_m^{s,u,c}$ are Lipschitz in m and the 'angles' between them are uniformly bounded below.

2. X_m^c is approximately $T_m M$ and X^s and X^c are approximately invariant under DT

3. $\Pi^u DT|_{X^u}$ isomorphically expands and does so to a greater degree than does $DT|_{X^c}$ while $\Pi^s DT|_{X^s}$ contracts and does so to a greater degree than does $DT|_{X^c}$.


T(M)
M
U(m)
T(m)
m

- Parameters:
  - r: radius of the working neighborhood around M;
  - σ: Error between $X^c_{T(m)}$ and $DT(X^c_m)$ and bound on $||\Pi^{\alpha}_{T(m)} DT(m)|_{X^{\beta}_m}||$, $\alpha \neq \beta$;
  - η: The error between $T(M)$ and M;
  - λ: Measurement of expansion in X^u; $\frac{1}{\lambda}$, the contraction in X^s;
  - B: Measurement of the lower bound of the 'angles' between X^c and X^u and X^s;
  - B_1: Upper bound of D^jT, $1 \leq j \leq k$, in the r-neighborhood of M;
  - L: Lipschitz constant of $X^{u,s,c}_m$ in m;

Theorem 1 *(***B-Lu-Zeng***) Let M be an approximately invariant, approximately normally hyperbolic manifold for the map T (or semiflow T_t). Suppose that $\partial M = \emptyset$ (this can be dropped).*
For $k > 1$ (or $k = 1$ and M is precompact) there exist

$$0 < \sigma_0 = \sigma_0(B, B_1, \lambda), \text{ and } 0 < \rho, \eta_0,$$

depending on $B,\ B_1,\ \lambda,\ r,\ L$, such that if $\sigma \in (0, \sigma_0)$, $\eta \in (0, \eta_0)$, then there exists a C^k normally hyperbolic invariant manifold $\tilde{M}$ in a ρ-neighborhood of M.

The application

Following Alikakos-Chen-Fusco, we scale space by a factor of δ:

$$\Omega_\delta \equiv \{x : \delta x \in \Omega\},$$

so that the droplet we seek has radius ~ 1. We also change $\varepsilon \to \delta\varepsilon$, so that (†) looks the same and the analysis becomes simpler.

$$(\dagger) \quad u_t = \varepsilon^2 \Delta u - f(u) + \frac{1}{|\Omega_\delta|} \int f(u)dx \quad (t,x) \in \mathbb{R} \times \Omega_\delta$$

$$\frac{\partial u}{\partial n} = 0 \quad \text{on } \partial\Omega_\delta.$$

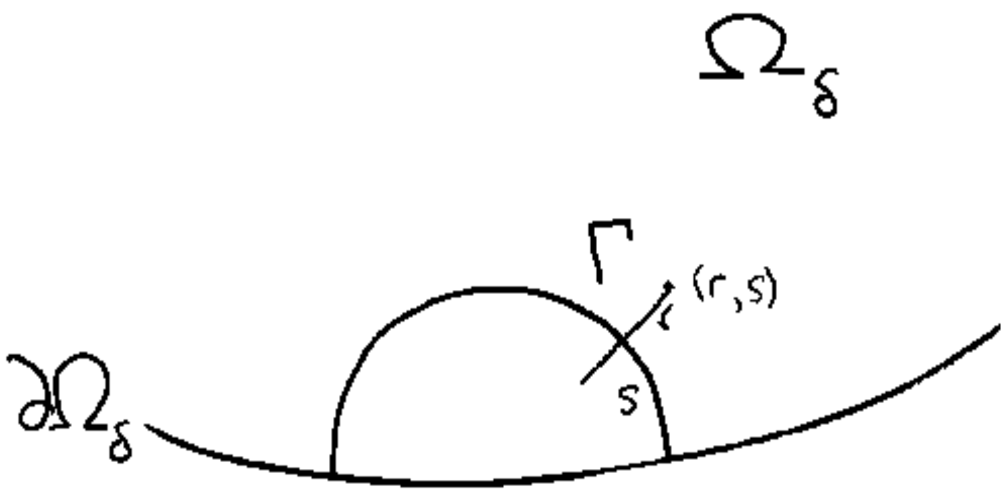
We parameterize $\partial\Omega_\delta$ using its arclength ξ and build an approximate droplet-like solution $u(\cdot, \xi)$ with its barycenter at the point of $\partial\Omega_\delta$ corresponding to ξ as follows:

$$u = u^I + u^B,$$

each of these being written as asymptotic expansions in ε, with u^I accounting for the state near the interface, and u^B accounting for it near where the interface meets $\partial\Omega_\delta$.

The leading order term in u^I is $U(r/\varepsilon)$, where U is the heteroclinic connection across the interface

$$\ddot{U} - f(U) = 0, \quad U(\pm\infty) = \pm 1, \quad U(0) = 0. \qquad (2)$$



Ω_δ
Γ
(r,s)
r
s
$\partial\Omega_\delta$

These functions are smoothly extended to the whole domain and the mass constraint, together with the demand that the residual be $O(\varepsilon^k)$ determines the interface Γ and the speed of the droplet

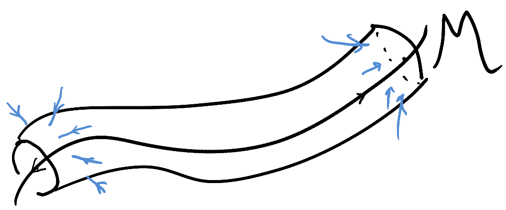
$$\dot{\xi} = -\frac{4\varepsilon^2}{3\pi}\mathcal{K}'_\delta.$$

All this is from A-C-F but they prove more.

- A tubular L^2 neighborhood of radius ε^{k-2} around

$$M \equiv \{u(\cdot,\xi) : \xi \in [0, |\partial\Omega_\delta|]\}$$

is positively invariant.



Furthermore, an H^1_ε tube only expands slightly.

• The operator got by linearizing at $u(\cdot, \xi)$ has spectrum

$$\{\lambda_1\} \cup \sigma_-,$$

where all spectrum of σ_- is negative and

$$\lambda_1 = C\varepsilon^2\delta + h.o.t$$

with an explicit constant C which could be of either sign, depending on ξ.

Unfortunately, the top of σ_- is also $O(\varepsilon^2)$,
but
fortunately, there is no δ factor.
So, there is a weak spectral gap.

For each ξ, define

$$X^c_\xi \equiv \text{span}\{\partial_\xi u(\cdot, \xi)\} \quad \text{and} \quad X^s_\xi \equiv (X^c_\xi)^\perp.$$

With much of the groundwork laid by A-C-F, we prove that M is approximately invariant and approximately normally hyperbolic.

Applying the abstract theorem we get

Theorem (B-Jin) For each sufficiently small δ, there is an $\varepsilon_\delta > 0$ such that for all $\varepsilon < \varepsilon_\delta$ the mass-conserving Allen-Cahn equation (†) has an invariant manifold of droplet-like solutions

$$\tilde{M} = \{\tilde{u}(\cdot, \xi) : \xi \in [0, |\partial\Omega_\delta|]\}$$

with

$$||\tilde{u}(\cdot, \xi) - u(\cdot, \xi)||_\infty \to 0 \text{ as } \varepsilon \to 0.$$

The solutions $\tilde{u}(\cdot, \xi(t))$ exist for all $t \in \mathbb{R}$ and

$$\dot{\xi} = -\frac{4\varepsilon^2}{3\pi}\mathcal{K}_\delta' + h.o.t.$$

Clearly, there is a stationary droplet-like solution near every non-degenerate critical point of the curvature of the boundary.

The Stochastic Equation

(joint with D. Antonopoulou and G. Karali)

We now include additive noise:

$$(\ddagger) \quad u_t = \varepsilon^2 \Delta u - f(u) + \frac{1}{|\Omega_\delta|} \int f(u) dx + \dot{W}(x,t)$$

$$\frac{\partial u}{\partial n} = 0 \quad \text{on } \partial\Omega_\delta,$$

where $\dot{W}$ is the formal derivative of a Fourier series of independent Brownian motions in time.

A result by D. Antonopoulou, D. Blomker, and G. Karali shows that such additive noise which is algebraically strong in ε dominates the dynamics of interfaces of solutions for the 1-D Cahn-Hilliard equation.

The motion of boundary droplets here is also a 1-D motion.
Does algebraically strong noise also dominate in this case?

To be more precise about the noise, let Q be an operator on $L^2(\Omega_\delta)$ having an O.N. basis of eigenfunctions $\{e_k\}$ with corresponding eigenvalues a_k^2. Then

$$W(x,t) \equiv \sum_k a_k \beta_k(t) e_k(x),$$

where $\{\beta_k(t)\}$ is a sequence of independent Brownian motions. It is assumed that (to preserve mass)

$$\int_{\Omega_\delta} \dot{W} dx = 0.$$

We measure the strength of the noise through

$$\eta_0 \equiv \text{trace} Q = \sum_k a_k^2,$$

$$\eta_1 \equiv ||Q||,$$

and

$$\eta_2 \equiv \sum_k a_k^2 ||\nabla e_k||^2.$$

We assume that the noise is smooth in space.

In building the droplet states using the asymptotic expansion, we go far enough so that the residual is $O(\varepsilon^k)$ with $k \geq 5$.

With $u = u(\cdot, \xi)$ as a point on the approximate invariant manifold M, we write a solution to (‡) in a neighborhood of M as

$$w = u + v \quad \text{with} \quad v \perp \partial_\xi u.$$

Thus, if $||v(\cdot, t)||$ stays small, the dynamics of w is controlled by $u(\cdot, \xi(t))$. We therefore take ξ to satisfy the SDE

$$d\xi = b(\xi)dt + (\sigma(\xi), dW)$$

for some real-valued drift b and L^2-valued variance σ to be determined.

By Ito calculus,

$$dw = \partial_\xi u d\xi + dv + \frac{1}{2}\partial_\xi^2 u d\xi d\xi.$$

Putting this into (‡) and using $dtdt = dtdW = 0$, we get

$$
\begin{aligned}
\Big[\|\partial_\xi(u)\|^2 - (v, \partial_\xi^2(u))\Big] d\xi = \\
\Big[(\mathcal{L}^\varepsilon(u), \partial_\xi(u)) - (Lv, \partial_\xi(u)) - (N(u,v), \partial_\xi(u))\Big] dt \\
+\Big[\frac{1}{2}(v, \partial_\xi^3(u)) - \frac{3}{2}(\partial_\xi^2(u), \partial_\xi(u))\Big](Q\sigma, \sigma)dt \\
+(\sigma, Q\partial_\xi^2(u))dt + (\partial_\xi(u), dW).
\end{aligned}
\tag{3}
$$

where $\mathcal{L}^\varepsilon$ is the nonlinear operator, etc, ... Now we use the fact that $||v||$ is small and $||\partial_\xi u||^2 \geq C\varepsilon$ for some $C > 0$. Examine the terms on the RHS. After some work we find, if $||v||_{H^1_\varepsilon} = \mathcal{O}(\varepsilon^{k-2})$,

$$
\begin{aligned}
d\xi = & -\frac{4}{3\pi}\mathcal{K}'_{\Omega_\delta}(\xi)\varepsilon^2[1 + \mathcal{O}(\delta)]dt + \mathcal{O}(\delta^3\varepsilon^2)dt \\
& + \mathcal{O}(\eta_1)\Big[1 + \mathcal{O}(\varepsilon^{k-\frac{5}{2}}) + \mathcal{O}(\delta)\Big]dt + (\mathcal{O}(\varepsilon^{\frac{1}{2}}), dW).
\end{aligned}
\tag{4}
$$

The expected value of the last term is 0 and so the question is whether or not the extra drift due to the noise, $\mathcal{O}(\eta_1)$, dominates the first term.

We know that in the deterministic setting, $||v||_{H^1_\varepsilon} = \mathcal{O}(\varepsilon^{k-2})$ remains true for all time if the initial data satisfies this. We need to extend this stability result to the stochastic case.

What we get is

Theorem 2 *If* $\eta_0, \eta_1 = o(\varepsilon^{2k-3})$ *then*

$$E[\|v(t)\|] \leq C\varepsilon^{k-2} \text{ for all } t > 0.$$

Idea behind the proof:

By Itô calculus we have

$$d\|v\|^2 = d(v,v) = 2(v,dv) + (dv,dv)$$

Since $v \perp u_\xi$

$$\begin{aligned}(v,dv) =& \Big(\Big[\mathcal{L}^\varepsilon(u) - Lv - N(u,v)\Big], v\Big)dt \\ & - \frac{1}{2}(\partial_\xi^2(u), v)d\xi d\xi + (dW, v) \\ & \leq C\varepsilon^k\|v\| - C^{-1}\varepsilon\|v\|^2 \\ & - \frac{1}{2}(\partial_\xi^2(u), v)d\xi d\xi + (dW, v).\end{aligned} \tag{5}$$

Also, since $dtdt = dtdW = 0$ and $(dW, dW) = \text{trace}(Q)dt$ we find

$$\begin{aligned}\|dv\|^2 =& \text{trace(Q)}dt - 2(Q\partial_\xi(u), \sigma)dt \\ & + \|\partial_\xi(u)\|^2(Q\sigma(\xi), \sigma(\xi))dt.\end{aligned} \tag{6}$$

Put these together, bound the RHS by an affine function of $\|v\|^2$, integrate and take expected value.

Remark

1. If the noise is larger, we still have that the solution stays in the $O(\varepsilon^{k-2})$ tubular neighborhood in L^2 with high probability for a long time.

2. However, we need to stay in the $O(\varepsilon^{k-2})$ tubular neighborhood in H^1_ε for a long time with high probability.

So far the best we have been able to do is

Theorem 3 *If* $\eta_2 = \mathcal{O}(\varepsilon^{2k-6})$ *and* $\eta_0 = \mathcal{O}(\varepsilon^{2k-3})$, *then*

$$||v(t)||_{H^1_\varepsilon} \leq \varepsilon^{k-2}$$

for a time interval $[0, T_\varepsilon] \to [0, \infty)$ *with probability* $P_\varepsilon \to 1$ *as* $\varepsilon \to 0$.

Unfortunately (?), $\eta_1 \leq \eta_0 = \mathcal{O}(\varepsilon^{2k-3}) = \mathcal{O}(\varepsilon^7)$.

So, if the noise is sufficiently strong to dominate the deterministic dynamics, then we cannot show that the H^1_ε tube is invariant long enough for us to deduce that the noise really does dominate the deterministic dynamics!