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ALLEN-CAHN DYNAMICS AND PHASE TRANSITIONS

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1. Introduction

An Allen-Cahn dynamics [3, 8] is a gradient flow of a free energy functional of the form

$$\mathbf{E}^\varepsilon(\mathbf{u}) = \int_{\mathbb{R}^N} \Big\{\frac{\varepsilon}{2}|\nabla \mathbf{u}|^2 + \frac{1}{\varepsilon}W(\mathbf{u})\Big\}dx \tag{1.1}$$

where $\mathbf{u} = (u_1, \cdots, u_m)$ is a phase order parameter, ε is a small positive constant, and W is a smooth potential of multiple wells of equal depth:

$$W = 0 \ \text{ on } \ A := \{\mathbf{a}_1, \cdots, \mathbf{a}_n\} \subset \mathbb{R}^m, \quad W > 0 \text{ on } \ A^c = \mathbb{R}^m \setminus A. \tag{1.2}$$

The gradient of the energy functional can be calculated as follows: for every direction $\mathbf{v}$,

$$\begin{aligned}\Big\langle \frac{\delta \mathbf{E}^\varepsilon}{\delta \mathbf{u}}, \mathbf{v}\Big\rangle &= \lim_{h\searrow 0} \frac{\mathbf{E}^\varepsilon(\mathbf{u}+h\mathbf{v}) - \mathbf{E}^\varepsilon(\mathbf{u})}{h} = \int_{\mathbb{R}^N} \Big\{\varepsilon \nabla \mathbf{u}\cdot\nabla \mathbf{v} + \frac{1}{\varepsilon}\mathbf{v}\cdot W_{\mathbf{u}}(\mathbf{u})\Big\}dx \\ &= \int_{\mathbb{R}^N} \Big(-\varepsilon\Delta \mathbf{u} + \frac{1}{\varepsilon}W_{\mathbf{u}}(\mathbf{u})\Big)\cdot \mathbf{v}\, dx = \Big(\text{grad } \mathbf{E}^\varepsilon,\ \mathbf{v}\Big)_{L^2(\mathbb{R}^N)}\end{aligned}$$

where grad $\mathbf{E}^\varepsilon := -\varepsilon\Delta\mathbf{u} + \frac{1}{\varepsilon}W_{\mathbf{u}}(\mathbf{u})$. Hence, in the $L^2(\mathbb{R}^N)$ space, the gradient flow $\mathbf{u}_t = -\text{grad } E^\varepsilon(\mathbf{u})$ leads to the Allen-Cahn equation in the vector form

$$\mathbf{u}^\varepsilon_t = \varepsilon\Delta\mathbf{u}^\varepsilon - \frac{1}{\varepsilon}\, W_{\mathbf{u}}(\mathbf{u}^\varepsilon). \tag{1.3}$$

Note that along a trajectory, there is the energy identity

$$\frac{d}{dt}\mathbf{E}^\varepsilon(\mathbf{u}^\varepsilon(t)) + \Big\|\mathbf{u}^\varepsilon_t\Big\|^2_{L^2(\mathbb{R}^N)} = 0.$$

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2. The Scalar Allen-Cahn Equation

Consider the Allen-Cahn equation of one component

$$\begin{cases} u^\varepsilon_t = \varepsilon\Delta u^\varepsilon - \frac{1}{\varepsilon} f(u^\varepsilon), & x\in\mathbb{R}^N, t>0,\\ u^\varepsilon(0,x) = g^\varepsilon(x), & x\in\mathbb{R}^N, t=0, \end{cases} \tag{2.1}$$

where f is smooth and non-degenerately **bistable**, i.e.,

$$f\in C^2(\mathbb{R}),\quad \{u\mid f(u)=0\}=\{-1,\alpha,1\},\quad f'(\pm1)>0>f'(\alpha). \tag{2.2}$$

The evolution of (2.1) undergoes two stages.

In the first stage, the gradient ∇u grows to $O(1/\varepsilon)$ size. Assume that initially $\nabla u^\varepsilon(\cdot,0)=O(1)$. Then in a short time the diffusion term $\varepsilon\Delta u^\varepsilon$ can be neglected, so the equation can be approximated by the ode

$$\frac{dw}{ds} = -f(w), \qquad s=\frac{t}{\varepsilon}.$$

As f is bistable, we see that

$$\lim_{s\to\infty} w(s) = \lim_{\varepsilon\searrow 0} w(t/\varepsilon) = \begin{cases} 1 & \text{if } w(0)>\alpha,\\ -1 & \text{if } w(0)<\alpha. \end{cases}$$

In terms of (2.1), in a very short time the space is divided into three regions: Two phase regions $\Omega^\pm$ in which $u^\varepsilon\approx\pm1$ and a thin interfacial region γ that connects the two phase regions. This behavior is commonly referred to as the generation of interface.

After the initiation, the $\varepsilon\Delta u^\varepsilon$ term will be of similar size to the $\varepsilon^{-1}f(u^\varepsilon)$ term. Indeed, after balance each other, they produce a net force that drives the propagation of interface.

The propagation can be characterized by a planar traveling wave $u^\varepsilon(x,t)=Q\Big(\dfrac{x\cdot\mathbf{n}-c\,t}{\varepsilon}\Big)$, where $\mathbf{n}\in\mathbb{S}^{N-1}$ is a unit vector and (c,Q) solves

$$c\,\dot Q + \ddot Q - f(Q) = 0 \quad\text{on }\ \mathbb{R},\qquad Q(\pm\infty)=\pm1,\quad Q(0)=\alpha. \tag{2.3}$$

For this traveling wave problem, the following is well-known [26, 15]:

Theorem 1 (**Traveling Waves).** *Assume that f is bistable, i.e. satisfies* (2.2). *Then* (2.3) *admits a unique solution $(c,Q)\in\mathbb{R}\times C^2(\mathbb{R})$. In addition, there holds* $c=\dfrac{\int_{-1}^1 f(u)du}{\int_{\mathbb{R}}\dot Q^2(z)\,dz}$.

Note that

$$\lim_{\varepsilon\searrow0} Q\Big(\frac{x\cdot\mathbf{n}-ct}{\varepsilon}\Big) = \begin{cases} 1 & \text{if } x\cdot\mathbf{n}>ct,\\ -1 & \text{if } x\cdot\mathbf{n}<ct. \end{cases}$$

The above formal argument on the evolution of interface can be made rigorous as follows.

Theorem 2 (**Generation of Interface**). *Assume that f is bistable and $\{g^\varepsilon\}$ is uniformly bounded.*

There is a positive constant $K = K(f, \|g^\varepsilon\|_{L^\infty})$ such that for every sufficiently small positive ε,

$$|u^\varepsilon(x, T^\varepsilon) \mp 1| \quad \leqslant \quad \varepsilon \qquad \forall\, x \in \Omega_\varepsilon^\pm(0),$$

where $T^\varepsilon = \sqrt{K}\varepsilon|\ln\varepsilon|$ and, denote by $B(p,r)$ the ball of radius r with center p,

$$\Omega_\varepsilon^+(0) := \{x \mid g^\varepsilon > \alpha + K\varepsilon|\ln\varepsilon| \text{ in } B(x, K\varepsilon|\ln\varepsilon|)\},$$
$$\Omega_\varepsilon^-(0) := \{x \mid g^\varepsilon < \alpha - K\varepsilon|\ln\varepsilon| \text{ in } B(x, K\varepsilon|\ln\varepsilon|)\}.$$

Theorem 3 (**Propagation of Interface**). *Let f be bistable. Assume that $\{g^\varepsilon\}_{0<\varepsilon<1}$ is uniformly bounded and for some open sets $\Omega^\pm(0)$,*

$$\text{(2.4)} \quad \liminf_{y\to x, \varepsilon\searrow 0} g^\varepsilon(y) > \alpha \ \forall\, x \in \Omega^+(0), \qquad \limsup_{y\to x, \varepsilon\searrow 0} g^\varepsilon(y) < \alpha \ \forall\, x \in \Omega^-(0).$$

Then the set

$$\Omega^\pm(t) := \Big\{x \in \mathbb{R}^N \ \Big|\ \lim_{y\to x, \varepsilon\searrow 0} u^\varepsilon(y,t) = \pm 1\Big\} \quad \forall\, t > 0,$$

together with $\Omega^\pm(0)$, evolves according to the **extended law of motion by constant speed***:*

$\Omega^\pm(t)$ shrinks/expands with normal velocity at most/least c.

In the classical sense, the motion law means that if $\partial\Omega^+(0) = \partial\Omega^-(0)$ is a smooth hypersurface, then before the formation of singularity, $\gamma(t) = \partial\Omega^+(t) = \partial\Omega^-(t)$ is a smooth hypersurface that moves with constant normal velocity c.

To explain the extended motion law, consider for definiteness the case $c \geqslant 0$. That $\{\Omega^-(t)\}$ expands with speed at least c means that

$$x \in \Omega^-(t) \Rightarrow B(x, c\tau) \in \Omega^-(t+\tau) \quad \forall \tau > 0.$$

Analogously, that $\{\Omega^-(t)\}$ shrinks with speed at most c means that

$$B(x,r) \subset \Omega^-(t) \Rightarrow B(x, r - c\tau) \subset \Omega^+(t+\tau) \quad \forall \tau > 0.$$

Here $B(x,r) = \emptyset$ if $r \leq 0$. The case $c < 0$ can be similarly described.

Now assume that f is **balanced bistable**:

$$\text{(2.5)} \quad f = W' \in C^2(\mathbb{R}), \quad W(\pm 1) = 0 < W(u) \ \forall\, u \neq \pm 1, \quad W''(\pm 1) > 0.$$

Then

$$c = 0, \qquad \ddot{Q} = f(Q), \qquad \dot{Q} = \sqrt{2W(Q)}.$$

Note that in this case we have $\Omega^\pm(t) \supset \Omega^\pm(0)$ for all $t > 0$. In particular, if $\partial\Omega^+(0) = \partial\Omega^-(0)$, then $\Omega^\pm(t) = \Omega^\pm(0)$ for all $t > 0$ and we cannot see the evolution of the phase regions $\Omega^\pm$. To see the evolution, we use a faster time scale $\tau := \varepsilon t$, so (2.1) becomes

$$\text{(2.6)} \qquad \begin{cases} u_\tau = \Delta u - \frac{1}{\varepsilon^2} f(u), & x \in \mathbb{R}^N, \tau > 0, \\ u(x,0) = g^\varepsilon(x), & x \in \mathbb{R}^N, \tau = 0. \end{cases}$$

Formally, we can derive the evolution as follows. Assume that $u^\varepsilon = Q\Big(\frac{z(x,\tau)}{\varepsilon}\Big) + \cdots$. Then

$$0 = u^\epsilon_\tau - \Delta u^\varepsilon + \frac{1}{\varepsilon^2} f(u^\varepsilon) = \frac{1}{\varepsilon^2}\Big(f(Q) - |\nabla z|^2 \ddot{Q}\Big) + \frac{1}{\varepsilon}\Big(z_\tau - \Delta z\Big)\dot{Q} + \cdots .$$

(1) Since $\ddot{Q} = f(Q)$, the first term on the right-hand side vanishes if $|\nabla z| = 1$. This renders to

$$z(x,\tau) = \text{signed distance from } x \text{ to some hypersurface } \gamma(\tau).$$

(2) Since $|\dot{Q}| \le \varepsilon$ when $|z| \ge K\varepsilon|\ln\varepsilon|$, for the second term to be small, it is better to have

$$z_\tau = \Delta z \quad \text{on } \gamma(\tau) = \{x |\ z(x,\tau) = 0\}.$$

In differential geometry, it is known that when z is a signed distance,

$$\begin{aligned} z_\tau = V_{\gamma(\tau)} &= \text{normal velocity of } \gamma(\tau), \\ \tfrac{1}{N-1}\Delta z = H_{\gamma(\tau)} &= \text{mean curvature of } \gamma(\tau). \end{aligned}$$

Thus, the above formal derivation shows that the α-level set $\{\gamma(\tau)\}_{\tau \geqslant 0}$ of u^ε should evolve by the law of motion by mean curvature:

$$V_{\gamma(t)} = (N-1)H_{\gamma(t)}.$$

Theorem 4 (**Motion by Mean Curvature).** *Let f be balanced bistable, ie., satisfy* (2.5). *Assume that $\{g^\varepsilon\}_{0<\varepsilon\le 1}$ is uniformly bounded and satisfies (2.4) for some open sets $\Omega^\pm(0)$. Define*

$$\Omega^\pm(\tau) := \Big\{x \in \mathbb{R}^N \ \Big|\ \lim_{y\to x, \varepsilon\searrow 0} u^\varepsilon(y,\tau) = \pm 1\Big\} \quad \forall\,\tau > 0.$$

Then $\{(\Omega^+(\tau), \Omega^-(\tau))\}_{\tau\ge 0}$ is a weak solution to the motion by mean curvature flow.

Here by a classical solution $\{\gamma(\tau)\}_{\tau_1\le\tau<\tau_2}$ to the mean curvature flow, it means that

for each $\tau \in [\tau_1, \tau_2)$, the signed distance $z(x,\tau)$ from x to $\gamma(\tau)$ is smooth near $\gamma(\tau)$ and satisfies $z_\tau = \Delta z$ on $\gamma(\tau)$.

By a weak solution $\{(\Omega^+(\tau), \Omega^-(\tau))\}_{\tau\ge 0}$ to the mean curvature flow, it means the following:

(1) *For each $\tau \ge 0$, both $\Omega^+(\tau)$ and $\Omega^-(\tau)$ are open and $\Omega^+(\tau) \cap \Omega^-(\tau) = \emptyset$;*
(2) *Suppose $\tau_2 > \tau_1 \ge 0$ and $\{\gamma(\tau) := \partial\Omega(\tau)\}_{\tau_1\le\tau<\tau_2}$ is classical solution. Then*

$$\Omega(\tau_1) \subset \Omega^\pm(\tau_1) \quad \Longrightarrow \quad \Omega(\tau) \subset \Omega^\pm(\tau)\ \forall\,\tau \in [\tau_1, \tau_2).$$

The theorems stated here can be proven by the mathod developen in [10, 16]; see also [7, 11, 12, 20, 25, 36, 41, 42, 44, 47] and the references therein.

3. The Allen-Chan System

Now for W satisfying (1.2), consider the Allen-Cahn system (1.3) in the fast time scale

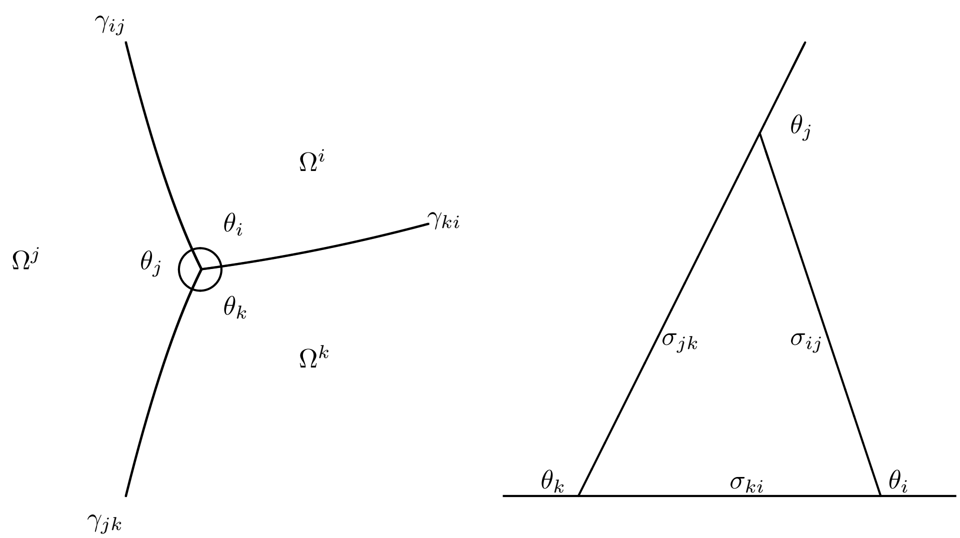
$$\mathbf{u}^\varepsilon_\tau = \Delta \mathbf{u}^\varepsilon - \frac{1}{\varepsilon^2} W_{\mathbf{u}}(\mathbf{u}^\varepsilon), \quad x \in \mathbb{R}^N, \quad \tau > 0.$$

Define, for each $\tau > 0$,

$$\begin{aligned} \Omega^i(\tau) &:= \Big\{ x \in \mathbb{R}^N \;\Big|\; \lim_{y \to x, \varepsilon \searrow 0} \mathbf{u}^\varepsilon(y,\tau) = \mathbf{a}_i \Big\}, \\ \gamma_{ij}(\tau) &= \partial\Omega^i(\tau) \cap \partial\Omega^j(\tau). \end{aligned}$$

Formally, one can drive the following

(1) Each γ_{ij} evolves according the mean curvature flow.
(2) The intersection angles among interfaces at their intersection are determined from the Allen-Cahn dynamics.



When $N = 2$, the most commonly seen intersections are triple Junctions [6, 8]. A triple junction is an intersection p_{ijk} of three interfaces $\gamma_{ij}, \gamma_{jk}, \gamma_{ki}$. The intersection angles obey the Herring Law (cf. figure):

$$\frac{\sin\theta_i}{\sigma_{jk}} = \frac{\sin\theta_j}{\sigma_{ki}} = \frac{\sin\theta_k}{\sigma_{ij}}$$

where σ_{ij}, called the **surface tension** between phases Ω^i and Ω^j, is defined by

$$\begin{gathered} \sigma_{ij} = \inf_{\mathbf{u} \in \mathbf{X}_{ij}} \int_{\mathbb{R}} \Big\{ \tfrac{1}{2}|\mathbf{u}_x|^2 + W(\mathbf{u}) \Big\} dx \\ \mathbf{X}_{ij} = \{ \mathbf{u} \in C(\mathbb{R} \to \mathbb{R}^m) \mid \mathbf{u}(-\infty) = \mathbf{a}_i, \mathbf{u}(\infty) = \mathbf{a}_j \}. \end{gathered}$$

The resulting evolution of the interface $\gamma = \cup \gamma_{ij}$ has been studied in [1, 8, 37, 39, 40].

Formally, one can show that $\mathbf{E}^\varepsilon$ defined in (1.1) converges (in so called Γ-limit sense) to

$$\mathbf{E}^0(\gamma) := \sum_{i\neq j}\int_{\gamma_{ij}} \sigma_{ij}dS$$

where dS is surface element and $\gamma = \cup_{i\neq j}\gamma_{ij}$ is the interface.

So far there are few rigorous analysis on the Allen-Cahn system.

For reader's convenience, we list some relevant references in this direction of research.

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