Asymptotic Analysis Of Phase Field Models Of Free Surfaces Driven By Surface Tension

Jie Wang
Adviser: Dr. Xiaoqiang Wang
Department of Scientific Computing
Florida State University

Abstract : We give an asymptotic analysis of the phase field Allen-Cahn and Cahn-Hilliard models of free surfaces with surface tension. Unlike the traditional approach to approximate the solution by the so called "matched asymptotic expansion" involving outer expansion, inner expansion and matching, our new approach uses a uniform "double asymptotic expansion" to expand the whole phase field function directly. The detailed structure of the phase field functions in the equilibrium state is given and the consistency of the phase field models with the corresponding sharp interface models is discussed, including the free surface Allen-Cahn model, Cahn-Hilliard model, and the Allen-Cahn model with volume constraint. The explicit asymptotic expansion of the phase field function reveals rich details of the phase field function structures. And it nicely explains some unusual phenomenon we observed in numerical experiments. The theory can be used to guide the future modeling and simulation of other moving boundary problems by phase field models.

Phase Field Model

A phase field function φ is introduced on a computational domain Ω to label the phases separated by surface Γ, which is given by the zero level set $\{x : \varphi(x) = 0\}$. The inside of Γ is represented by the positive part $\{x : \varphi(x) > 0\}$ and the outside by the negative part. As a typical diffusive interface description, let ϵ represent the length scale of the transition region from one phase to the other in the phase field model. When $\epsilon \to 0$, φ describes a sharp interface.

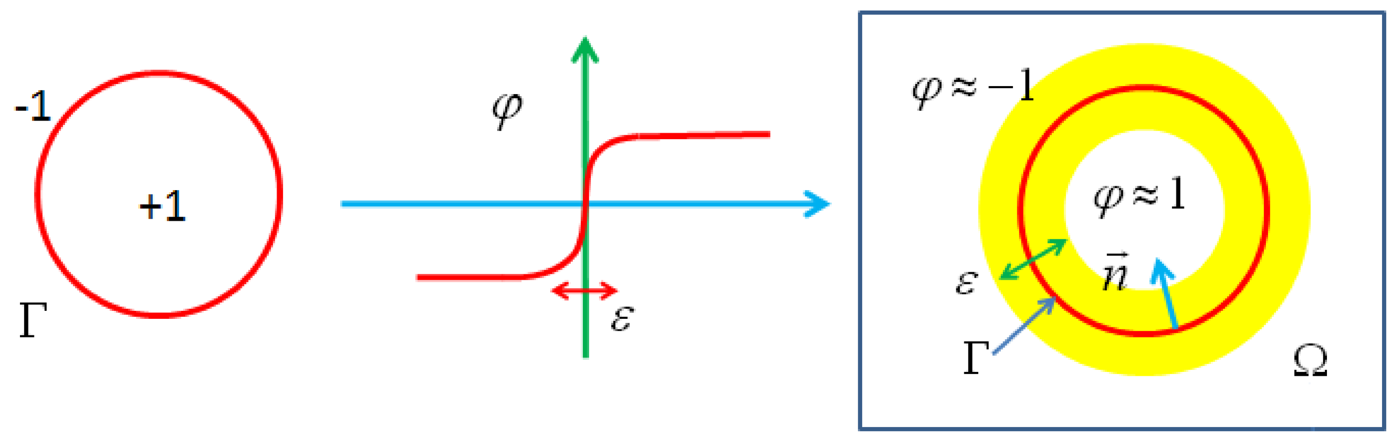

Figure 1: Illustration of phase field models.

Some important geometric features of free surface Γ can be nicely obtained by using the phase field function φ, *e.g.*,

area of Γ:

$$A(\varphi) = \int_\Omega \frac{\epsilon}{2}|\nabla\varphi|^2 + \frac{1}{4\epsilon}(\varphi^2-1)^2 dx \qquad (1)$$

normal direction of Γ:

$$\vec{n} = \frac{\nabla\varphi}{|\nabla\varphi|} \qquad (2)$$

mean curvature of Γ:

$$H_\Gamma = -\frac{1}{2}\nabla\cdot\vec{n} \qquad (3)$$

Phase field model is extensively used to track the free surfaces or moving boundaries emerging from the study of solidification dynamics, vesicle dynamics, fracture dynamics, viscous fingering *etc.*, because of its appealing features:

- explicit interface tracking is completely avoided;
- complex geometry and topology changes can be handled naturally;
- different driving forces, such as a reduction in bulk energy, interfacial energy and elastic energy, can be easily incorporated.

Free Surfaces Driven By Surface Tension

By using the phase field function φ, the surface tension energy can be formulated by:

$$W(\varphi) = \int_\Omega \frac{\epsilon}{2}|\nabla\varphi|^2 + \frac{1}{4\epsilon}(\varphi^2-1)^2 dx \qquad (4)$$

The second term $(\varphi^2-1)^2$ is a double-well potential which vanishes at -1 and $+1$. When we try to minimize $W(\varphi)$, phase field function φ tends to take values close to -1 and $+1$, while the first term $\frac{\epsilon}{2}|\nabla\varphi|^2$ penalizes the spatial inhomogeneity of φ. We say the system researches the equilibrium state when the surface tension energy $W(\varphi)$ is minimized.

The energy minimization process can be described by

1. Allen-Cahn equation:

$$\varphi_t = -\frac{1}{\epsilon}\frac{\partial W(\varphi)}{\partial\varphi} = \Delta\varphi - \frac{1}{\epsilon^2}(\varphi^2-1)\varphi \qquad (5)$$

with boundary condition

$$\frac{\partial\varphi}{\partial n} = 0 \text{ in } \partial\Omega, \quad \varphi(x,0) = \varphi_0(x) \text{ in } \Omega; \qquad (6)$$

2. Cahn-Hilliard equation:

$$\varphi_t = \Delta\frac{\partial W(\varphi)}{\partial\varphi} = -\Delta(\epsilon\Delta\varphi - \frac{1}{\epsilon}(\varphi^2-1)\varphi) \qquad (7)$$

with boundary condition

$$\frac{\partial\varphi}{\partial n} = \frac{\partial}{\partial n}(\epsilon\Delta\varphi - \frac{1}{\epsilon}(\varphi^2-1)\varphi) = 0 \text{ in } \partial\Omega, \quad \varphi(x,0) = \varphi_0(x) \text{ in } \Omega. \qquad (8)$$

Note, Cahn-Hilliard equation preserves the inside volume of Γ.

By using the Lagrange multiplier technique, we are able to develop the modified Allen-Cahn equation such that the volume is preserved.

The lagrange of equation (4) can be constructed as:

$$\begin{aligned} L(\varphi) &= W(\varphi) + \lambda\int_\Omega \varphi dx \\ &= \int_\Omega \frac{\epsilon}{2}|\nabla\varphi|^2 + \frac{1}{4\epsilon}(\varphi^2-1)^2 + \lambda\varphi dx \end{aligned} \qquad (9)$$

3. Modified Allen-Cahn equation with Volume Preserving Constraint:

$$\varphi_t = -\frac{1}{\epsilon}\frac{\partial L(\varphi)}{\partial\varphi} = \Delta\varphi - \frac{1}{\epsilon^2}(\varphi^2-1)\varphi - \frac{1}{\epsilon}\lambda \qquad (10)$$

with boundary condition (6).

Asymptotic Double Expansion

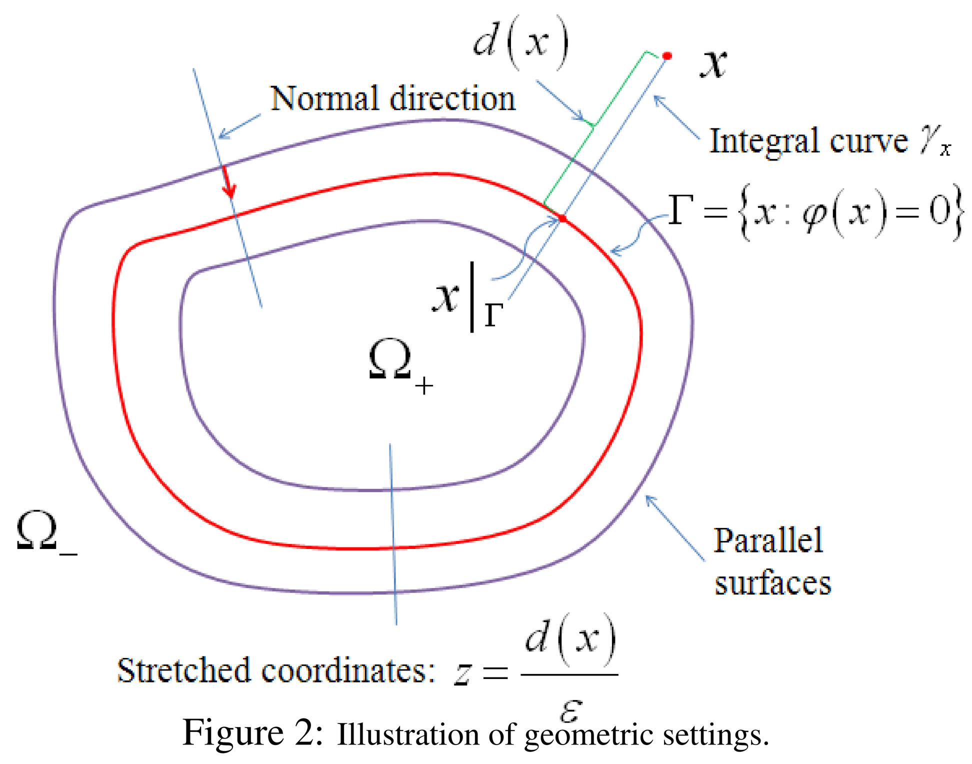

Figure 2: Illustration of geometric settings.

Denote the minimizer of $W(\varphi)$ by φ^* and Γ by $\{x : \varphi^*(x) = 0\}$, we give some assumptions:

(A1) Γ is smooth and compact and there exists a set of surfaces Γ_l which are parallel to Γ.

(A2) φ^* has an asymptotic expansion as

$$\varphi^*(x) = \sum_{n=0}^{\infty}\epsilon^n q_n(\frac{d(x)}{\epsilon}, x|_\Gamma),$$

where $q_i \in C^\infty(\bar{\mathbb{R}}\times\Gamma)$ are bounded smooth functions and independent of ϵ.

(A3) $\Phi(\epsilon, z, x) = \sum_{n=0}^{\infty}\epsilon^n q_n(z,x) \in C^\infty(\bar{\mathbb{R}}^2\times\Gamma)$, where $z \in \bar{\mathbb{R}}$, $x \in \Gamma$.

(A4) if $d(x) > 0$, $\lim_{\epsilon\to 0}\varphi^*(x) = 1$; otherwise, $\lim_{\epsilon\to 0}\varphi^*(x) = -1$. Moreover, $\nabla^n\varphi^*(x) = 0$ for $x \in \partial\Omega$ and $n > 0$. For each $q_n(z, x|_\Gamma)$ and integers $k \geq 0$, $m > 0$, $\lim_{z\to\pm\infty} z^k\frac{\partial^m q_n(z,x|_\Gamma)}{\partial z^m}$ are bounded.

Structure of Phase Field Functions in Equilibrium State

Based on the asymptotic double expansion assumptions, we can give a detailed description of the structure of phased field functions in equilibrium state by solving the first several terms of the asymptotic expansions.

1. Asymptotic Analysis of Allen-Cahn Models:

Theorem 1. *Suppose φ is the minimizer of (4) along the Allen-Cahn gradient flow, and φ satisfies assumptions (A1) to (A4), we have*

$$q_0(z) = \tanh(\frac{z}{\sqrt{2}}),\ q_1 = 0 \text{ and } H_\Gamma = 0.$$

Note, although assumption (A2) says $q_0 \in C^\infty(\bar{\mathbb{R}}\times\Gamma)$, the expression of q_0 implies q_0 only depends on the first parameter. Moreover, we can see that $\Gamma = \{x : \varphi(x) = 0\}$ is a minimal surface when the system is in the equilibrium state and q_1 vanishes constantly.

2. Asymptotic Analysis of Allen-Cahn Equation with volume pre- serving constraint:

Theorem 2. *Suppose $\tilde{\varphi}$ is the minimizer of (9) following the modified Allen-Cahn gradient flow (10) and $\tilde{\varphi}$ satisfies assumptions (A1) to (A4), we have H_Γ is a constant and*

$$\tilde{q}_0(z) = \tanh(\frac{z}{\sqrt{2}}), \quad \tilde{q}_1(z, x|_\Gamma) = \frac{\sqrt{2}}{3}H_\Gamma\tilde{q}_0^2$$

Notice that H_Γ is a constant implies Γ is a constant mean curvature surface.

3. Asymptotic Analysis of Cahn-Hilliard Models:

Theorem 3. *Suppose Suppose $\hat{\varphi}$ is the minimizer of (4) and driven by the Cahn-Hilliard gradient flow, with assumptions (A1) to (A4), we have H_Γ is a constant and*

$$\hat{q}_0(z) = \tanh(\frac{z}{\sqrt{2}}), \text{ and } \hat{q}_1(z, x|_\Gamma) = \frac{\sqrt{2}}{3}H_\Gamma\hat{q}_0^2.$$

Note, although assumption (A2) said $\hat{q}_0 \in C^\infty(\bar{\mathbb{R}}\times\Gamma)$, the expression of $\hat{q}_0$ implies $\hat{q}_0$ only depends on the first parameter. Moreover H_Γ is a constant implies Γ is a constant mean curvature surface.

Numerical Experiments

Starting from the initial data, we simulate the evolution process of free surface driven by Cahn-Hilliard gradient flow, which preserves the inside volume.

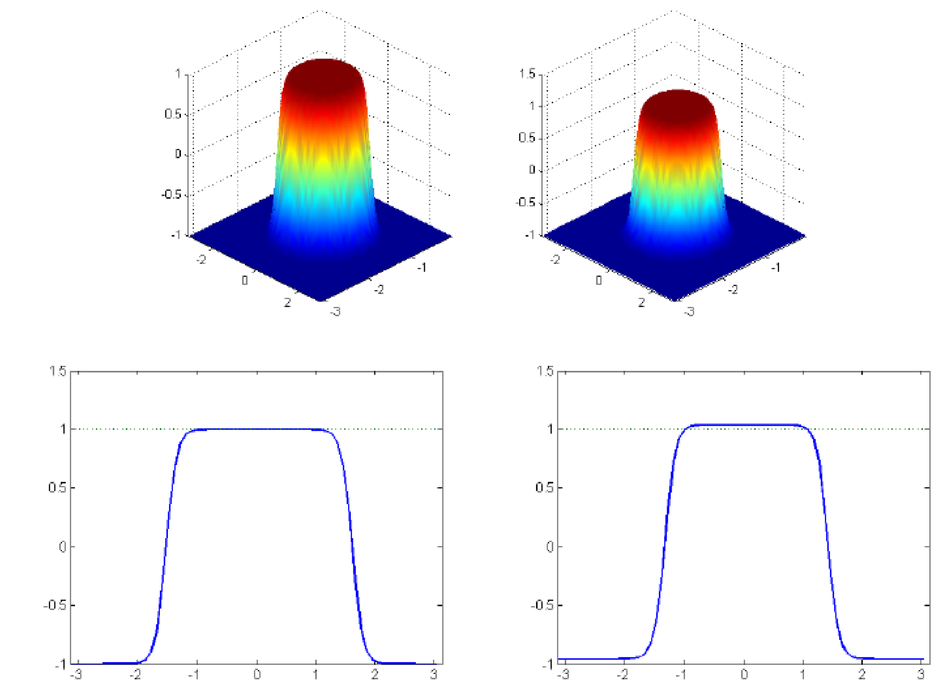

Figure 3: The cross section views of initial phase field function (left ones in two rows) and the ending phase field function (right ones in two rows).

References

[1] J. Wang and X. Wang, Asymptotic Analysis of Phase Field Models of Free Surfaces Driven by Surface Tension, submitted to *J. of Math. Anal. Appl.*.