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Analysis of the Cahn–Hilliard Equation with a Relaxation Boundary Condition Modeling the Contact Angle Dynamics

Xinfu Chen, Xiaoping Wang & Xianmin Xu*

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Abstract

We analyze the Cahn–Hilliard equation with a relaxation boundary condition modeling the evolution of an interface in contact with the solid boundary. An L^∞ estimate is established which enables us to prove the global existence of the solution. We also study the sharp interface limit of the system. The dynamic of the contact point and the contact angle are derived and the results are compared with the numerical simulations.

1. Introduction

Wetting and spreading are of critical importance in many applications such as microfluidics, inkjet printing, surface engineering and oil recovery [4,12]. The subject has attracted much interest in physics and applied mathematics communities. The phenomena of wetting and spreading are governed by the surface and interfacial interactions, acting usually at small scale. The fundamental concept that characterizes the wetting property of the solid surface is the static contact angle, which is defined as the measurable angle that a liquid makes with a solid. The contact angle of liquid with a flat, homogenous surface is given by the Young's equation [23]

$$\cos\theta = \frac{\nu_{\mathrm{SV}} - \nu_{\mathrm{SL}}}{\nu}, \tag{1}$$

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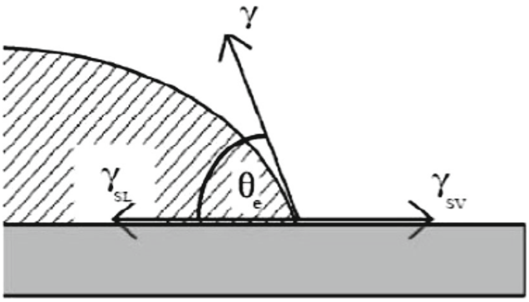

Fig. 1. Contact angle formed by the liquid air interface with the solid boundary

where ν_{SV}, ν_{SL} and ν are the surface tension of the solid-vapor interface, the solid-liquid interface and the liquid-vapor interface respectively (see Fig. 1). Mathematically, the wetting phenomena and the equilibrium state of the two phase fluid on a solid surface can be described by the phenomenological Cahn–Landau theory [4,6], which uses the interfacial free energy in a squared-gradient approximation, with the addition of a surface energy term in order to account for the interaction with the solid wall (see also [15])

$$\mathcal{F} = \int_\Omega \frac{1}{2}\varepsilon|\phi|^2 + \frac{1}{\varepsilon}F(\phi)\,\mathrm{d}r + \int_{\partial\Omega} \nu(\phi, x)\,\mathrm{d}S, \tag{2}$$

where ε is a small parameter, ϕ is the composition field, $F(\phi)$ is the double well potential for the bulk free energy density in Ω. The simplest double well potential is given by $F(\phi) = (1-\phi^2)^2$. $\nu(\phi, x)$ is the free energy density at the solid boundary $\partial\Omega$ which interpolates between ν_{SL} and ν_{SV} and it is locally x dependent for rough surfaces [20,21]. The equilibrium interface structure is obtained by minimizing the total free energy $\mathcal{F}$, which results in the following Cahn–Landau equation

$$-\varepsilon\Delta\phi + \frac{1}{\varepsilon}F'(\phi) = 0, \qquad \text{in} \quad \Omega \tag{3}$$

$$\varepsilon\frac{\partial\phi}{\partial n} + \frac{\partial\nu}{\partial\phi} = 0 \qquad \text{on} \quad \partial\Omega. \tag{4}$$

Young's equation (1) can be derived from the boundary condition (3) in the sharp interface limit (see for example [20]). A special case of (3) $\partial_n\phi = 0$ corresponds to the 90^{o} contact angle when ν is a constant function.

The dynamics of a two phase system on a solid surface can be modeled by the Cahn–Hilliard equation

$$\begin{cases} \phi_t = \Delta v, \qquad v = -\varepsilon\Delta\phi + \frac{1}{\varepsilon}F'(\phi) & \text{in } \ \Omega\times(0,\infty), \\ \phi_t + \alpha\left(\varepsilon\partial_n\phi + \nu'(\phi, x)\right) = 0 & \text{on } \ \partial\Omega\times(0,\infty), \\ \partial_n v = 0 & \text{on } \ \partial\Omega\times(0,\infty), \\ \phi(\cdot, t) = \phi_0(\cdot) & \text{on } \ \Omega\times\{0\} \end{cases} \tag{5}$$

where $' = \partial/\partial\phi$, $\partial_n = n\cdot\nabla$, and n is the unit exterior normal to the boundary $\partial\Omega$ of a smooth bounded domain Ω, v is the chemical potential in the bulk. The above system is a special case of a more general diffusive interface model for the two phase flow consisting of a coupled Cahn–Hilliard–Navier–Stokes system with the Generalized Navier Boundary Conditions (GNBC) introduced in [17–19] to model the moving contact line problem. In the slow dynamics, one can neglect the effect of the flow and the system is reduced to the Cahn–Hilliard equation with a relaxation boundary condition (5) which enables us to study the evolution of the interface along the solid boundary and the dynamic contact angle.

The system is a gradient flow of an energy functional (2) (see Section 2). We note that the Cahn–Hilliard equation with the standard boundary conditions $\partial_n v = 0$ and $\partial_n \phi = 0$ has been well-studied, see [3,7–9,16] and the references therein. However, there seems to be no standard theory in the literature that can be applied to obtain the well-posedness of the problem (5).

This paper consists of two objectives: a rigorous mathematical analysis for the well-posedness of the problem (5), and a formal derivation for dynamics of contact angle in the $\varepsilon \searrow 0$ limit. The former part shows that (5) is a mathematically sound formulation and the latter part shows its potential application, thereby supporting the conclusion that (5) is a reasonable model for the underlying physics.

We shall establish the global-in-time existence of a classical solution of (5). We first propose a new regularization scheme for the system (5) and prove the local-in-time existence of the solution by a standard fix-point approach for semi-linear problems. Clearly, the key for the global existence of a classical solution is the L^∞ estimate. For this, we utilize a technique that is quite different from that of Caffarelli–Muller [7]. In [7], the non-linear function f is assumed to be of linear growth, so potential theory for the linear part and Sobolev imbedding for the non-linear part cooperates in harmony. In general for semi-linear problems, even for gradient flow such as Navier–Stokes equations, one can only establish the global existence of a classical solution for low space dimensions. Nevertheless, bearing in mind that (5) is a gradient flow with a unique structure here, we imposed a condition that is opposite from [7]. We assume that f has a physically meaningful super-linear growth:

$$u f(u) \geqslant u^3 \text{ if } |u| \geqslant 2. \tag{6}$$

Such conditions work very well for second order parabolic equations (such as the Allen–Chan equation [1]), due to the celebrated tool of the maximum principle. Here we introduce a novel yet quite simple technique (Sections 3.2, 4.4) that enables us to use the idea of the maximum principle to show that the non-linear term is indeed a good term that forbids the solution from blow-up, thus being in agreement with the modeling of physics. As far as we know, our method of utilizing the non-linearity (6) to show the L^∞ bound for the fourth order Cahn–Hilliard equation and the phase field model is new. In essence, our technique can be classified as an *invariant region method*.

The Cahn–Hilliard equation is a phase field model used to describe interfacial dynamics. Clearly we would like to know what and how the macroscopic phenomena, that is law of motion of sharp interface ($\varepsilon \searrow 0$ limit of the zero level set of ϕ) are enforced by the Cahn–Hilliard equation. In this direction, the leading work is that by Pego [16] who derived the law of motion of interface. Rigorous verification of Pego's derivation is carried out in [2,9]. However, Pego's work did not touch the important issue of how the interface interacts with the boundary. Here we carry out, only on a formal level, a multi-scale expansion for the system. We demonstrate, in the case of a droplet spreading along a flat surface, that the Cahn–Hilliard system (5) models at the tip of interface the following dynamic contact angle law:

$$\frac{\mathrm{d}}{\mathrm{d}s}\beta(s) = \frac{\alpha}{\sqrt{A}}\frac{(\beta - \sin\beta\cos\beta)^{3/2}[\cos\beta - \sigma(p(s))]}{\sin\beta[\sin\beta - \beta\cos\beta]}.$$

Here $s = \varepsilon t$, A is the volume of the phase domain, $p(s)$ and $\beta(s)$ are, respectively, the contact point and contact angle of interface with the boundary $\partial\Omega$ (in the limit as $\varepsilon \to 0$ of zero level set of ϕ).

The paper is organized as follows. Sections 2–4 are rigorous mathematical analysis whereas Sections 5–6 are only in a formal level. In Section 2, we show some basic properties of the Cahn–Hilliard equation (5), mainly its gradient flow structure of a energy functional with a boundary energy term. In Section 3, we construct a regularized system for the equation and study its well-posedness. In Section 4, the well-posedness of (5) is studied. We prove the existence, uniqueness and regularity of the solution of the equation. In Section 5, we briefly go over Pego's conclusion [16] regarding the law of motion of interface. In the last section, we study the fast time behavior for (5) by asymptotic analysis, to derive the dynamics of the contact angle. In the regular time scale, the contact angle is seen as a constant, the equilibrium angle of Young's equation.

2. The gradient flow structure of (5)

We assume the explicit dependence of the surface energy density ν on the surface location x in the form of $\nu(\phi, x) = \sigma(x)\ell(\phi)$. We also assume that

$$\sigma, \ell, F, \partial\Omega \in C^\infty; \quad \ell'(u) = 0,\ F''(u) > 0,\ uF'(u) \geqslant |u|^3 \text{ when } |u| \geqslant 2. \tag{7}$$

The energy functional $\mathbf{E}$ associated with the Cahn–Hilliard equation (5) is defined by

$$\mathbf{E}[\phi] := \int_\Omega \left(\frac{\varepsilon}{2}|\nabla\phi|^2 + \frac{1}{\varepsilon}F(\phi)\right)\mathrm{d}x + \int_{\partial\Omega}\sigma(x)\ell(\phi)\mathcal{H}^{N-1}(\mathrm{d}x). \tag{8}$$

The first variation of energy in the direction ζ can be calculated as

$$\begin{aligned}\left\langle\frac{\delta\mathbf{E}[\phi]}{\delta\phi}, \zeta\right\rangle &:= \frac{\mathrm{d}}{\mathrm{d}s}\mathbf{E}[\phi + s\zeta]\Big|_{s=0}\\ &= \int_\Omega\left(\varepsilon\nabla\phi\cdot\nabla\zeta + \varepsilon^{-1}F'(\phi)\zeta\right) + \int_\Omega \sigma(x)\ell'(\phi)\zeta\\ &= \int_\Omega\left(-\varepsilon\Delta\phi + \varepsilon^{-1}F'(\phi)\right)\zeta + \int_{\partial\Omega}\left(\varepsilon\partial_n\phi + \sigma(x)\ell'(\phi)\right)\zeta.\end{aligned}$$

Note that

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{E}[\phi(\cdot,t)] = \left\langle \frac{\delta \mathbf{E}[\phi]}{\delta\phi}, \phi_t \right\rangle .$$

Hence, the Cahn–Hilliard dynamics is a **gradient flow** with dissipation rate

$$\begin{aligned}\mathbf{D}[v,\phi_t] &:= \int_\Omega |\nabla v|^2 + \frac{1}{\alpha}\int_{\partial\Omega}\phi_t^2 \\ &= \int_\Omega \left|\nabla(\varepsilon\Delta\phi - \varepsilon^{-1}F'(\phi))\right|^2 + \alpha\int_{\partial\Omega}\left|\varepsilon\partial_n\phi + \sigma(x)\ell'(\phi)\right|^2 . \end{aligned} \tag{9}$$

The second variation of $\mathbf{E}$ in the direction (ζ,ζ) can be calculated as

$$\begin{aligned}\mathbf{E}_2[\phi,\zeta] &:= \left\langle \frac{\delta^2\mathbf{E}[\phi]}{(\delta\phi)^2}, (\zeta,\zeta)\right\rangle := \frac{\mathrm{d}^2}{\mathrm{d}s^2}\mathbf{E}[\phi + s\zeta]\Big|_{s=0} \\ &= \int_\Omega \left(\varepsilon|\nabla\zeta|^2 + \varepsilon^{-1}F''(\phi)\zeta^2\right) + \int_\Omega \sigma(x)\ell''(\phi)\zeta^2. \end{aligned}\tag{10}$$

This gives

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{E}[\phi] = -\mathbf{D}[v,\phi_t], \qquad \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{D}[v,\phi_t] = -\mathbf{E}_2[\phi,\phi_t].$$

The gradient flow structure of the Cahn–Hilliard equation implies that a long time decay of its solution to a stationary one. This implies that a Gronwall-type argument can be applied to give the uniqueness of solutions (see Theorem 2 in Section 4). It will be proved in the following two sections. It is easy to see that solution of equation (5) also preserves the mass:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \phi\,\mathrm{d}x = \int_\Omega \phi_t\,\mathrm{d}x = \int_\Omega \Delta v\,\mathrm{d}x = \int_{\partial\Omega}\partial_n v\,\mathcal{H}^{N-1}(\mathrm{d}x) = 0.$$

3. Well-Posedness of a Regularized Problem

To establish the existence of a solution of (5), we start with the following regularization

$$\begin{cases} \delta\phi_t - \varepsilon\Delta\phi + \varepsilon^{-1}F'(\phi) = v, \quad \delta v_t - \Delta v = -\phi_t & \text{in } \Omega\times(0,\infty), \\ \phi_t - \delta\Delta_{\partial\Omega}\phi = -\alpha(\partial_n\phi + \sigma\ell'(\phi)), \quad \partial_n v = 0 & \text{on } \partial\Omega\times(0,\infty), \\ \phi(\cdot,0) = \phi_0, \quad v(\cdot,0) = v_0 & \text{on } \bar{\Omega}\times\{0\} \end{cases}\tag{11}$$

where $\delta \in (0,1]$ is a parameter and $\Delta_{\partial\Omega}$ is the surface Laplacian of the manifold $\partial\Omega$. Note that except for the boundary condition, this is the well-studied phase field model [5] in which ϕ is a phase order parameter and v is the temperature.

The main result in this section is the following theorem.

Theorem 1. *Assume (7) and $(\phi_0, v_0) \in C^2(\bar{\Omega})\times C^1(\bar{\Omega})$. Then problem (11) admits a unique solution and the solution is smooth on $\bar{\Omega}\times(0,\infty)$.*

The proof is given in two steps (see in Sections 3.1 and 3.2, respectively). In the first step, we prove a local in time existence. In the second step, we establish an L^∞ bound so the local solution can be extended step by step to $\bar{\Omega}\times[0,\infty)$.

3.1. Local in Time Existence

First we establish the existence of a solution on $\bar{\Omega}_T := \bar{\Omega} \times [0, T]$ where T is a small positive constant. In the sequel, $\eta \in (0, 1)$ is a fixed Hölder exponent and C is a generic constant that depends only on $\eta, \varepsilon, \alpha, \delta, \Omega, \sigma(\cdot), \ell(\cdot)$, and $F(\cdot)$, but not on T. We denote

$$c_0 := \frac{1}{|\Omega|} \int_\Omega (\delta v_0 + \phi_0)\, \mathrm{d}x, \qquad M_0 := \max\left\{1,\ \|v_0\|_{C^1(\bar{\Omega})},\ \|\phi_0\|_{C^2(\bar{\Omega})}\right\}.$$

We shall prove the local existence via the fixed point of a certain operator in the function space

$$\mathbf{X}_{M,T} := \left\{\phi \in C^{1,1/2}(\bar{\Omega}_T) \mid \|\phi\|_{C^{1,1/2}(\bar{\Omega}_T)} \leqslant M,\ \phi(\cdot, 0) = \phi_0\right\}$$

where $M \geqslant M_0$ is a positive constant to be chosen later. Here the index $(1, 1/2)$ in $C^{1,1/2}$ are corresponding to x and t respectively.

1. Fix an arbitrary $\phi \in \mathbf{X}_{M,T}$. Let V be the solution of the linear parabolic equation

$$\delta V_t - \Delta V = c_0 - \phi \ \text{ in } \ \Omega_T, \quad \partial_n V = 0 \ \text{ on } \ \partial\Omega_T, \quad V(\cdot, 0) = V_0 \tag{12}$$

where $V_0 \in C^2(\bar{\Omega})$ is defined by

$$-\Delta V_0 = c_0 - \delta v_0 - \phi_0 \text{ in } \ \Omega, \qquad \partial_n V_0 = 0 \ \text{ on } \ \partial\Omega, \qquad \textstyle\int_\Omega V_0 = 0.$$

By the classical elliptic estimate [11,13],

$$\|V_0\|_{C^{2+\eta}(\bar{\Omega})} \leqslant C\|\delta v_0 + \phi_0\|_{C^1(\bar{\Omega})} \leqslant C M_0.$$

Comparing V with a linear function of t, we find that

$$\|V\|_{L^\infty(\Omega_T)} \leqslant \|V_0\|_{L^\infty(\Omega)} + \delta^{-1}\|c_0 - \phi\|_{L^\infty(\Omega_T)} T.$$

Hence, applying Schauder regularity theory [14] for the parabolic equation (12) we have

$$\begin{aligned} \|V\|_{C^{2+\eta,1+\eta/2}(\bar{\Omega}_T)} &\leqslant C\{\|V\|_{L^\infty(\Omega_T)} + \|V_0\|_{C^{2+\eta}(\bar{\Omega})} + \|c_0 - \phi\|_{C^{1,1/2}(\bar{\Omega}_T)}\} \\ &\leqslant C M\{1 + T\}. \end{aligned} \tag{13}$$

Setting $v = V_t$ we see that v is the unique solution (in a distribution sense) of

$$\delta v_t - \Delta v = -\phi_t \ \text{ in } \ \Omega_T, \qquad \partial_n v = 0 \ \text{ on } \ \partial\Omega_T, \qquad v = v_0 \ \text{ on } \ \bar{\Omega} \times \{0\}.$$

2. Next, we define the boundary value $\hat{\phi}$ as the solution of

$$\hat{\phi}_t - \delta \Delta_{\partial\Omega} \hat{\phi} = -\alpha(\partial_n \phi + \sigma \ell'(\phi)) \text{ in } \partial\Omega_T, \qquad \hat{\phi} = \phi_0 \text{ on } \partial\Omega \times \{0\}. \tag{14}$$

Then by parabolic estimate [14],

$$\begin{aligned} \|\hat{\phi}\|_{C^{1+\eta,(1+\eta)/2}(\partial\Omega_T)} &\leqslant C\left\{\|\phi_0\|_{C^2(\partial\Omega)} + (1 + T)\|\partial_n \phi + \sigma \ell'(\phi)\|_{C(\partial\Omega_T)}\right\} \\ &\leqslant \tilde{C} M\{1 + T\}. \end{aligned} \tag{15}$$

Finally, we define ψ as the solution of

$$\begin{aligned}&\delta\psi_t - \varepsilon\Delta\psi + \varepsilon^{-1}F'(\psi) = V_t \ \text{ in } \ \Omega_T, \quad \psi = \hat{\phi} \text{ on } \partial\Omega_T,\\ &\psi = \phi_0 \text{ on } \Omega\times\{0\}.\end{aligned} \tag{16}$$

Note that $\varepsilon^{-1}F'(\psi) \leqslant V_t$ at any interior point of local maximum of ψ and $\varepsilon^{-1}F'(\psi) \geqslant V_t$ at any interior point of local minimum. Hence, we can use (7) to derive that

$$\|\psi\|_{L^\infty(\Omega_T)} \leqslant \max\left\{\|\hat{\phi}\|_{C(\bar{\Omega}_T)}, \|\phi_0\|_{C(\bar{\Omega})}, 2, \sqrt{\varepsilon\|V_t\|_{L^\infty(\bar{\Omega}_T)}}\right\} \leqslant CM\{1+T\}.$$

It then follows by parabolic estimate [14] that

$$\begin{aligned}&\|\psi\|_{C^{1+\eta,(1+\eta)/2}(\bar{\Omega}_T)}\\ &\leqslant C\left\{\|\phi_0\|_{C^2(\bar{\Omega})} + \|\hat{\phi}\|_{C^{1+\eta,(1+\eta)/2}(\partial\Omega_T)} + \|\varepsilon^{-1}F'(\psi) - V_t\|_{L^\infty(\Omega_T)}(1+T)\right\}\\ &\leqslant C\left\{M + |F'(CM[1+T])| + |F'(-CM[1+T])|\right\}(1+T).\end{aligned}$$

Finally, by the definition of the Hölder norm, we can derive that

$$\|\psi - \phi_0\|_{C^{1,1/2}(\bar{\Omega}_T)} \leqslant \|\psi\|_{C^{1+\eta,(1+\eta)/2}(\bar{\Omega}_T)} T^{\eta/2}.$$

3. Fix $M = 2M_0$. One can check that if $T > 0$ is sufficiently small, the map $\phi \to \psi$ maps $\mathbf{X}_{M,T}$ to itself and is a contraction, and therefore admits a unique fixed point. The unique fixed point provides a unique solution of (11) on $\bar{\Omega}_T$. In addition, by a bootstrap argument and standard parabolic regularity theory [14], (ϕ, v) is smooth in $\bar{\Omega}\times(0, T]$. We omit the details.

3.2. Global Existence

Let (ϕ, v) be a solution of (11) in $\bar{\Omega}\times[0, T)$. Suppose we can show that $\|\phi\|_{L^\infty(\Omega_T)}$ is bounded. Then from the equation for V in (12) and the parabolic L^p estimate, $v = V_t$ is bounded in $L^p(\Omega_T)$ for any $p > 1$. Consequently, from the equation for ϕ, we see that ϕ is bounded in $W_p^{2,1}(\Omega_T)$ for any $p > 1$, which implies that ϕ is bounded in $C^{1+\eta,(1+\eta)/2}(\bar{\Omega}_T)$; see the derivation from (19) (with $L^\infty(\Omega_T)$ replaced by $L^p(\Omega_T)$ for $p \gg 1$) to (20) below. A bootstrap argument then shows that $(\phi, v) \in C^\infty(\bar{\Omega}\times(0, T])$. Hence, the solution can be extended beyond T. Therefore, to establish the global in time existence, we need only establish an L^∞ bound of ϕ. For this, assume that (ϕ, v) is a solution in $\bar{\Omega}\times[0, T]$ and define

$$M_1 = \max_{\bar{\Omega}_T}|\phi|, \quad M_2 = \max_{\bar{\Omega}_T}|v| = \max_{\bar{\Omega}_T}|V_t|.$$

As we are establishing the upper bound of M_1, we need only consider the case $M_1 > 2M_0$.

Let $(x^*, t^*) \in \bar{\Omega}_T$ be a point such that $M_1 = |\phi(x^*, t^*)|$. Without loss of generality, we assume that $\phi(x^*, t^*) > 0$. As $M_1 \geqslant 2M_0$, we have $t^* > 0$. If $x^* \in \partial\Omega$, then $\partial_n\phi(x^*, t^*) > 0$, $\partial_t\phi(x^*, t^*) > 0$, and $\Delta_{\partial\Omega}\phi(x^*, t^*) \leqslant 0$, so the boundary condition for ϕ implies that $\sigma(x^*)\ell'(\phi(x^*, t^*)) < 0$. By (7), this implies that $\phi(x^*,t^*) \leqslant 2$, contradicting the assumption $\phi(x^*,t^*) = M_1 > 2M_0 \geqslant 2$. Hence, $x^* \in \Omega$ and $t^* > 0$. Consequently, $\Delta\phi(x^*,t^*) \leqslant 0$, $\phi_t(x^*,t^*) \geqslant 0$, so $\varepsilon^{-1}F'(\phi(x^*,t^*)) \leqslant v(x^*,t^*)$. This implies that, by (7),

$$(M_1)^2 \leqslant F'(\phi(x^*,t^*)) \leqslant \varepsilon v(x^*,t^*) \leqslant \varepsilon M_2. \tag{17}$$

Similarly, if $\phi(x_*,t_*)$ is a global minimum of ϕ then either $\phi(x_*,t_*) \geqslant -2M_0$ or $F'(\phi(x_*,t_*)) \geqslant -\varepsilon M_2$. Without loss of generality, we can assume that $M_2 \geqslant 1$. Then,

$$\begin{aligned}\|F'(\phi)\|_{C(\bar\Omega_T)} &\leqslant \max\left\{\max_{u\in[-2,2]}|F'(u)|,\ |F'(\phi(x^*,t^*))|, |F'(\phi(x_*,t_*))|\right\}\\ &\leqslant CM_2. \end{aligned}\tag{18}$$

Applying the parabolic estimates first for $\hat\phi$ and then for ϕ we derive that

$$\begin{aligned}&\|\phi\|_{C^{1+\eta,(1+\eta)/2}(\bar\Omega_T)} \leqslant C\{1+T\}\{M_0 + \|\varepsilon^{-1}F'(\phi) - v\|_{L^\infty(\Omega_T)}\\ &\quad +\|\partial_n\phi\|_{C(\partial\Omega_T)} + 1\}.\end{aligned}\tag{19}$$

The quantity $\|\partial_n\phi\|_{C(\partial\Omega_T)}$ on the right-hand side can be control by the left-hand side via the interpolation: there exists a positive constant $C = C(\Omega,\eta)$ such that for any $\hat\delta \in (0,1]$,

$$\|\nabla\phi\|_{C(\bar\Omega_T)} \leqslant C\hat\delta^{-1/\eta}\|\phi\|_{C(\bar\Omega_T)} + \hat\delta\|\phi\|_{C^{1+\eta,(1+\eta)/2}(\bar\Omega_T)}.$$

Setting $\hat\delta = 1/[2C(1+T)]$ we then derive from (19) and (18) that

$$\begin{aligned}\|\phi\|_{C^{1+\eta,(1+\eta)/2}(\bar\Omega_T)} &\leqslant C\{1+T\}^{1/\eta+1}\{M_1 + \|\varepsilon^{-1}F' - v\|_{L^\infty(\Omega_T)}\}\\ &\leqslant \tilde C\{1+T\}^{1/\eta+1}M_2.\end{aligned}\tag{20}$$

Now we use the parabolic estimate for (12) to obtain

$$\begin{aligned}\|V\|_{L^\infty(\Omega_T)} &\leqslant C\{\|V_0\|_{L^\infty(\Omega)} + \|c_0-\phi\|_{L^\infty(\Omega_T)}T\} \leqslant C[1+T]M_1,\\ \|V\|_{C^{2+\eta,1+\eta/2}(\bar\Omega_T)} &\leqslant C\{\|V_0\|_{C^{2+\eta}(\bar\Omega)} + \|c_0-\phi\|_{C^{1,1/2}(\bar\Omega_T)}(1+T)\}\\ &\leqslant C[1+T]^{1/\eta+2}M_2\end{aligned}$$

by (20). Finally, using $v = V_t$ and the interpolation with $\theta = \eta/(1+\eta)$ we obtain

$$M_2 \leqslant \|V\|_{C^{2,1}(\bar\Omega_T)} \leqslant 2\|V\|^{\theta}_{L^\infty(\Omega_T)}\|V\|^{1-\theta}_{C^{2+\eta,1+\eta/2}(\bar\Omega_T)} \leqslant \tilde C[1+T]^{1/\eta+1}M_1^\theta M_2^{1-\theta}.$$

Upon using $M_1 \leqslant \sqrt{\varepsilon M_2}$ we derive that

$$M_2 \leqslant C(1+T)^{1/\eta+1}M_2^{\theta/2}M_2^{1-\theta}$$

so that

$$M_2 \leqslant C[1+T]^{2(1/\eta+1)/\theta}, \qquad M_1 \leqslant C[1+T]^{(1/\eta+1)/\theta}.$$

This completes the proof of Theorem 1. □

3.3. Energy Estimates

The a priori estimates in the preceding subsection depend on δ. In order to pass to the limit $\delta \searrow 0$, we need estimates that do not depend on δ. For this, we employ energy estimates.

1. For each $t > 0$, integrating $\delta v_t - \Delta v + \phi_t = 0$ multiplied by $v = \delta\phi_t - \varepsilon\Delta\phi + \varepsilon^{-1}F'(\phi)$ over Ω, using integrating by parts with the substitution $\partial_n v = 0$ and $-\varepsilon\partial_n\phi = [\phi_t - \delta\Delta_{\partial\Omega}\phi + \alpha\sigma\ell'(\phi)]/\alpha$ on $\partial\Omega$ we obtain

$$\begin{aligned}
0 &= \int_\Omega v(\delta v_t - \Delta v + \phi_t) = \int_\Omega \Big(\delta v v_t - v\Delta v + [\delta\phi_t - \varepsilon\Delta\phi + \varepsilon^{-1}F'(\phi)]\phi_t\Big) \\
&= \int_\Omega \left(\delta v v_t + |\nabla v|^2 + \delta\phi_t^2 + \varepsilon\nabla\phi\cdot\nabla\phi_t + \frac{F'(\phi)\phi_t}{\varepsilon}\right) \\
&\quad + \int_{\partial\Omega} \frac{\phi_t - \delta\Delta_{\partial\Omega}\phi + \alpha\sigma\ell'(\phi)]}{\alpha}\phi_t \\
&= \frac{\mathrm{d}}{\mathrm{d}t}\left\{\int_\Omega\left(\frac{\delta v^2}{2} + \frac{\varepsilon|\nabla\phi|^2}{2} + \frac{F(\phi)}{\varepsilon}\right) + \int_{\partial\Omega}\left(\frac{\delta|\nabla_{\partial\Omega}\phi|^2}{2\alpha} + \sigma\ell(\phi)\right)\right\} \\
&\quad + \int_\Omega\Big(|\nabla v|^2 + \delta\phi_t^2\Big) + \int_{\partial\Omega}\frac{\phi_t^2}{\alpha}.
\end{aligned}$$

Similarly, using $-\varepsilon\partial_n\phi_t = -(\varepsilon\partial_n\phi)_t = [\phi_{tt} - \delta\Delta_{\partial\Omega}\phi_t + \sigma\ell''(\phi)\phi_t]/\alpha$ on $\partial\Omega$, we derive that

$$\begin{aligned}
0 &= \int_\Omega v_t\,(\delta v_t - \Delta v + \phi_t) = \int_\Omega\Big(\delta v_t^2 - v_t\Delta v + [\delta\phi_{tt} - \varepsilon\Delta\phi_t + \varepsilon^{-1}F''(\phi)\phi_t]\phi_t\Big) \\
&= \frac{\mathrm{d}}{\mathrm{d}t}\left\{\int_\Omega\left(\frac{|\nabla v|^2}{2} + \frac{\delta\phi_t^2}{2}\right) + \int_{\partial\Omega}\frac{\phi_t^2}{2\alpha}\right\} \\
&\quad + \int_\Omega\left(\delta v_t^2 + \varepsilon|\nabla\phi_t|^2 + \frac{F''(\phi)\phi_t^2}{\varepsilon}\right) + \int_{\partial\Omega}\left(\frac{\delta|\nabla_{\partial\Omega}\phi_t|^2}{\alpha} + \sigma\ell''(\phi)\phi_t^2\right).
\end{aligned}$$

Since both F'' and ℓ'' have lower bounds, these two energy estimates will provide norm bounds that do not depend on the non-linearity of F.

2. Non-linearity may mess up the usefulness of higher order energy estimates. We write two of them:

$$\begin{aligned}
0 &= \int_\Omega v_t\,(\delta v_t - \Delta v + \phi_t)_t \\
&= \int_\Omega\Big(\delta v_t v_{tt} - v_t\Delta v_t + [\delta\phi_{tt} - \varepsilon\Delta\phi_t + \varepsilon^{-1}F''(\phi)\phi_t]\phi_{tt}\Big) \\
&= \frac{\mathrm{d}}{\mathrm{d}t}\left\{\int_\Omega\left(\frac{\delta v_t^2}{2} + \frac{\varepsilon|\nabla\phi_t|^2}{2} + \frac{F''(\phi)\phi_t^2}{2\varepsilon}\right) + \int_{\partial\Omega}\frac{\delta|\nabla_{\partial\Omega}\phi_t|^2}{2\alpha}\right\} \\
&\quad + \int_\Omega\left(|\nabla v_t|^2 + \delta\phi_{tt}^2 - \frac{F'''(\phi)\phi_t^3}{2\varepsilon}\right) + \int_{\partial\Omega}\left(\frac{\phi_{tt}^2}{\alpha} + \frac{\sigma\ell'''(\phi)\phi_t\phi_{tt}}{2}\right),
\end{aligned}$$

$$
\begin{aligned}
0 &= \int_\Omega v_{tt}\,(\delta v_t - \Delta v + \phi_t)_t \\
&= \int_\Omega (\delta v_{tt}^2 - v_{tt}\Delta v_t) + [\delta\phi_{ttt} - \varepsilon\Delta\phi_{tt} + \varepsilon^{-1}F''(\phi)\phi_{tt} + \varepsilon^{-1}F'''(\phi)\phi_t^2]\phi_{tt} \\
&= \frac{\mathrm{d}}{\mathrm{d}t}\left\{\int_\Omega \left(\frac{|\nabla v_t|^2}{2} + \frac{\delta\phi_{tt}^2}{2}\right) + \int_{\partial\Omega}\frac{\phi_{tt}^2}{2\alpha}\right\} \\
&\qquad + \int_{\partial\Omega}\left(\frac{\delta|\nabla_{\partial\Omega}\phi_{tt}|^2}{\alpha} + \sigma\ell''(\phi)\phi_{tt}^2 + \sigma\ell'''(\phi)\phi_t^2\phi_{tt}\right) \\
&\qquad + \int_\Omega \left(\delta v_{tt}^2 + \varepsilon|\nabla\phi_{tt}|^2 + \frac{F''(\phi)\phi_{tt}^2 + F'''(\phi)\phi_t^2\phi_{tt}}{\varepsilon}\right).
\end{aligned}
$$

We summarize the estimates as follows. Introduce

$$
\begin{aligned}
\mathbf{E}[\phi] &= \int_\Omega \left(\frac{\varepsilon|\nabla\phi|^2}{2} + \frac{F(\phi)}{\varepsilon}\right) + \int_{\partial\Omega}\sigma\ell(\phi), \\
\mathbf{D}[v,\zeta] &= \int_\Omega |\nabla v|^2 + \int_{\partial\Omega}\frac{\zeta^2}{\alpha}, \\
\mathbf{E}_2[\phi,\zeta] &= \int_\Omega \left(\varepsilon|\nabla\zeta|^2 + \frac{F''(\phi)\zeta^2}{\varepsilon}\right) + \int_{\partial\Omega}\sigma\ell''(\phi)\zeta^2.
\end{aligned}
$$

Then we have the fundamental energy identities

$$
\begin{aligned}
0 &= \frac{\mathrm{d}}{\mathrm{d}t}\left(\mathbf{E}[\phi] + \frac{\delta}{2}\left[\|v\|_{L^2(\Omega)}^2 + \alpha^{-1}\|\nabla_{\partial\Omega}\phi\|_{L^2(\partial\Omega)}^2\right]\right) + \mathbf{D}[v,\phi_t] + \delta\|\phi_t\|_{L^2(\Omega)}^2, \\
0 &= \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left(\mathbf{D}[v,\phi_t] + \delta\|\phi_t\|_{L^2(\Omega)}^2\right) + \mathbf{E}_2[\phi,\phi_t] + \delta[\|v_t\|_{L^2(\Omega)}^2 \\
&\quad + \alpha^{-1}\|\nabla_{\partial\Omega}\phi_t\|_{L^2(\partial\Omega)}^2].
\end{aligned}
$$

Higher order energy identities can be derived by direct differentiation: for any positive integer k,

$$
\begin{aligned}
\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\,\mathbf{E}_2^\delta[\phi,\partial_t^k\phi,\partial_t^k v] + \mathbf{D}^\delta[\partial_t^k v,\partial_t^{k+1}\phi] &= N_{2k+1}, \\
\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\,\mathbf{D}^\delta[\partial_t^k v,\partial_t^{k+1}\phi] + \mathbf{E}^\delta[\phi,\partial_t^{k+1}\phi,\partial^{k+1}v] &= N_{2k+2}
\end{aligned}
$$

where $\partial_t^k = \frac{\partial^k}{\partial t^k}$ and

$$
\begin{aligned}
\mathbf{E}_2^\delta[\phi,\partial_t^k\phi,\partial_t^k v] &:= \int_\Omega \left(\varepsilon|\nabla\partial_t^k\phi|^2 + \frac{F''(\phi)|\partial_t^k\phi|^2}{\varepsilon} + \delta|\partial_t^k v|^2\right) + \int_{\partial\Omega}\frac{\delta|\nabla_{\partial\Omega}\partial_t^k\phi|^2}{\alpha}, \\
\mathbf{D}^\delta[\partial_t^k v,\partial_t^{k+1}\phi] &:= \|\nabla\partial_t^k v\|_{L^2(\Omega)}^2 + \alpha^{-1}\|\partial_t^{k+1}\phi\|_{L^2(\partial\Omega)}^2 + \delta\|\partial_t^{k+1}\phi\|_{L^2(\Omega)}^2, \\
N_{2k+1} &:= \frac{1}{\varepsilon}\int_\Omega \left(\partial_t^{k+1}\phi\left[\partial_t^k F'(\phi) - F''(\phi)\partial_t^k\phi\right] - \frac{F'''(\phi)\phi_t(\partial_t^k\phi)^2}{2}\right) \\
&\quad + \int_{\partial\Omega}\sigma\partial_t^{k+1}\phi\,\partial_t^k\ell'(\phi), \\
N_{2k+2} &:= \frac{1}{\varepsilon}\int_\Omega \partial_t^{k+1}\phi\left[\partial_t^{k+1}F'(\phi) - F''(\phi)\partial_t^{k+1}\phi\right] + \int_{\partial\Omega}\sigma\partial_t^{k+1}\phi\,\partial_t^{k+1}\ell'(\phi).
\end{aligned}
$$

3. Using cut-off functions, one can establish estimates for arbitrary higher order derivatives. For interior estimates, suppose $\zeta = \zeta(x)$ is smooth and $\zeta = 0$ on $\partial\Omega$. Then for any integer index $\beta = (\beta_1, \ldots, \beta_{N+1})$, denoting $\partial^\beta = \frac{\partial^{|\beta|}}{\partial x_1^{\beta_1} \cdots \partial x_N^{\beta_N} \partial t^{\beta_{N+1}}}$ we have

$$\begin{aligned}
0 &= \int_\Omega \zeta \partial^\beta v \partial^\beta [\delta v_t - \Delta v + \phi_t] \\
&= \int_\Omega \zeta \left\{ \delta \partial^\beta v \partial^\beta v_t - \partial^\beta v \Delta \partial^\beta v + \partial^\beta [\delta \phi_t - \varepsilon \Delta \phi + F'(\phi)] \partial^\beta \phi_t \right\} \\
&= \frac{1}{2} \frac{\mathrm{d}}{\mathrm{d}t} \int_\Omega \left(\delta |\partial^\beta v|^2 + \varepsilon |\nabla \partial^\beta \phi|^2 + \frac{F''(\phi)}{\varepsilon} |\partial^\beta \phi|^2 \right) \zeta \\
&\quad + \int_\Omega \left(|\nabla \partial^\beta v|^2 + \delta |\partial^\beta \phi_t|^2 \right) \zeta + \cdots
\end{aligned}$$

where $\cdots$ are lower order terms.

Near the boundary, one can begin with estimating tangential derivatives, $\nabla_{\partial\Omega} := \nabla - n(n \cdot \nabla)$ where n is a smooth vector function in $\bar{\Omega}$ such that n is the unit exterior normal to $\partial\Omega$. For example, suppose $p \in \partial\Omega$ and ζ is a smooth function in $\mathbb{R}^N$ vanishing outside of a small neighborhood of p. Then

$$\begin{aligned}
0 &= \int_\Omega \zeta \nabla_{\partial\Omega} v \cdot \nabla_{\partial\Omega} [\delta v_t - \Delta v + \phi_t] \\
&= \int_\Omega \zeta \left\{ \delta \nabla_{\partial\Omega} v \cdot \nabla_{\partial\Omega} v_t - \nabla_{\partial\Omega} v \cdot \nabla_{\partial\Omega} \Delta v + \nabla_{\partial\Omega} [\delta \phi_t - \varepsilon \Delta \phi + F'(\phi)] \cdot \nabla_{\partial\Omega} \phi_t \right) \\
&= \frac{1}{2} \frac{d}{dt} \left(\int_\Omega \left(\delta |\nabla_{\partial\Omega} v|^2 + \varepsilon |\nabla \nabla_{\partial\Omega} \phi|^2 + \frac{F''(\phi)}{\varepsilon} |\nabla_{\partial\Omega} \phi|^2 \right) \zeta + \int_{\partial\Omega} \frac{\delta |\nabla^2_{\partial\Omega} \phi|^2}{2\alpha} \zeta \right) \\
&\quad + \int_\Omega \left(|\nabla \nabla_{\partial\Omega} v|^2 + \delta |\nabla_{\partial\Omega} \phi_t|^2 \right) \zeta + \int_{\partial\Omega} \frac{\delta |\nabla_{\partial\Omega} \phi_t|^2}{\alpha} \zeta + \cdots
\end{aligned}$$

Here we use the fact that the boundary condition equations $\partial_n v = 0$ and $\partial_t \phi + \alpha(\varepsilon \partial_n + \sigma \ell'(\phi)) = 0$ can be differentiated in t and in any tangential directions.

Finally, any other derivatives involving differentiation in the normal direction can be estimated by using the differential equation and the boundary condition equation. We omit the details.

4. Well-posedness of (5)

In this section, we establish the well-posedness of (5). We show the uniqueness of the weak solution of (5) in Theorem 2 and the existence and regularity of the solution in Theorem 3. The proof of Theorem 3 is based on a L^∞ estimate which is shown in Section 4.4. In the last subsection, we derive formally the sharp-interface limit of the Cahn–Hilliard equation.

4.1. Weak Solution and Uniqueness

For completeness, we begin with the definition of a weak solution and its uniqueness.

Definition 1. A pair (ϕ, v) is called a weak solution of (5) if for every $T > 0$,

$$\phi, \nabla\phi, v, \nabla v \in L^2(\Omega_T), \quad \phi F'(\phi) \in L^1(\Omega_T), \quad \phi_t, \sigma\ell'(\phi) \in L^2(\partial\Omega_T)$$

and for every smooth ζ, η with compact support in $\bar{\Omega} \times [0, \infty)$,

$$\int_0^\infty\int_\Omega v\zeta \,\mathrm{d}x\,\mathrm{d}t = \int_0^\infty\int_\Omega \left(\varepsilon\nabla\phi\cdot\nabla\zeta + \frac{F'(\phi)\zeta}{\varepsilon}\right) + \int_0^\infty\int_{\partial\Omega}\left(\frac{\phi_t\zeta}{\alpha} + \sigma\ell'(\phi)\zeta\right),$$
$$\int_0^\infty\int_\Omega \nabla v\cdot\nabla\eta \,\mathrm{d}x\,\mathrm{d}t = \int_0^\infty\int_\Omega \phi\eta_t + \int_\Omega \phi_0(\cdot)\eta(\cdot,0).$$

Theorem 2. *Assume that F, σ, ℓ are smooth and $F'' \geqslant -m$ and $|\ell''| \leqslant m$ for some $m \in (0,\infty)$. Then for every $\phi_0 \in L^2(\Omega)$, there exists at most one weak solution of* (5).

Proof. Let (ϕ_1, v_1) and (ϕ_2, v_2) be two weak solutions. Fix $T > 0$. Set $\zeta = \phi_1 - \phi_2$ and $\eta(\cdot, t) = \int_T^t (v_1(\cdot,\tau) - v_2(\cdot,\tau))\,\mathrm{d}\tau$ for $t \in [0, T]$ and set $\zeta = 0, \eta = 0$ for $t > T$. Since $F(u) + mu^2/2$ is a convex function we can derive that for every $u_1, u_2 \in \mathbb{R}$,

$$\max\{|u_2F'(u_1)|, |u_1F'(u_2)| \leqslant \max\{|u_1F'(u_1)|, |u_2F'(u_2)|\} + m[|u_1|^2 + |u_2|^2]\,.$$

This implies that both $\phi_1F'(\phi_2)$ and $\phi_2F'(\phi_1)$ are in $L^1(\Omega_T)$. Thus, by an approximation process, both ζ and η can be used as test functions. Taking the difference of the definition equations for (ϕ_1, v_1) and (ϕ_2, v_2) and using $\eta_t = v_1 - v_2$ we obtain

$$\int_0^T\int_\Omega \nabla(v_1 - v_2)\cdot\nabla\eta = \int_0^T\int_\Omega (\phi_1 - \phi_2)\eta_t = \int_0^\infty\int_\Omega (v_1 - v_2)\zeta$$
$$= \int_0^T\int_\Omega\left(\varepsilon|\nabla\zeta|^2 + \frac{(F'(\phi_1) - F'(\phi_2))\zeta}{\varepsilon}\right) + \int_0^T\int_{\partial\Omega}\left(\frac{\zeta_t\zeta}{\alpha} + \sigma[\ell'(\phi_1) - \ell'(\phi_2)]\zeta\right).$$

As $v_1 - v_2 = \eta_t$ the left-hand side equals

$$\int_0^T\int_\Omega \nabla(v_1 - v_2)\cdot\nabla\eta = \int_0^T\int_\Omega \nabla\eta_t\cdot\nabla\eta = -\frac{1}{2}\int_\Omega |\nabla\eta(\cdot,0)|^2.$$

Also, using $F'' \geqslant -m$ and $|\ell''| \leqslant m$ we have

$$(F'(\phi_1) - F'(\phi_2))\zeta \geqslant -m\zeta^2, \quad \sigma[\ell'(\phi_1) - \ell'(\phi_2)]\zeta \geqslant -m\|\sigma\|_{L^\infty}\zeta^2.$$

By Sobolev embedding there exists a constant $A = A(\varepsilon, m, \|\sigma\|_{L^\infty}, \Omega)$ such that

$$\frac{m}{\varepsilon}\int_\Omega \zeta^2 + m\|\sigma\|_{L^\infty}\int_{\partial\Omega}\zeta^2 \leqslant \frac{\varepsilon}{2}\int_\Omega |\nabla\zeta|^2 + A\int_{\partial\Omega}\zeta^2. \tag{21}$$

Thus we obtain

$$
\begin{aligned}
-\frac{1}{2}\int_{\Omega}|\nabla\eta(\cdot,0)|^2 &\geqslant \int_0^T\int_{\Omega}(\varepsilon|\nabla\zeta|^2-\frac{m\zeta^2}{\varepsilon})+\int_{\Omega}\frac{\zeta(\cdot,T)^2}{2\alpha}-m\|\sigma\|_{L^\infty}\int_0^T\int_{\partial\Omega}\zeta^2\\
&\geqslant \frac{\varepsilon}{2}\int_{\Omega}|\nabla\zeta|^2+\frac{1}{2\alpha}\int_{\partial\Omega}\zeta(\cdot,T)^2-A\int_0^T\int_{\partial\Omega}\zeta^2.
\end{aligned}
$$

In particular, setting $w(t)=\int_{\partial\Omega}[\phi_1(\cdot,t)-\phi_2(\cdot,t)]^2$ we find that $w(T)\leqslant 2\alpha A\int_0^T w(t)dt$. As $w(0)=0$ and $T>0$ is arbitrary, the Gronwall's inequality then implies that $w\equiv 0$, from which we derive that $\phi_1\equiv\phi_2$ and $v_1\equiv v_2$. This completes the proof. □

4.2. Existence of a Strong Solution

A weak solution is called a strong solution if it has more regularity than is needed in the definition. It is called a classical solution if all of the derivatives that appeared in (5) exist in a classical sense and the equations are satisfied pointwisely. We can now pass to the limit $\delta\searrow 0$ from the solution of (11) to obtain a strong solution of (5).

Theorem 3. *Assume* (7). *Let* $\phi_0\in C^\infty(\bar{\Omega}_T)$ *be given. Set* $v_0=\varepsilon^{-1}F'(\phi_0)-\varepsilon\Delta\phi_0$, $\phi_{0t}=\Delta v_0$ *and assume that the compatibility condition* $\phi_{0t}+\alpha(\partial_n\phi_0+\sigma\ell'(\phi_0))=0$ *on* $\partial\Omega$ *holds. Then problem* (5) *admits a unique weak solution. The solution satisfies the following estimates:*

$$
\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega}\phi\,\mathrm{d}x=0,\qquad \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{E}[\phi]=-\mathbf{D}[v,\phi_t],
$$
$$
\mathbf{D}[v,\phi_t]+2\int_0^t\mathbf{E}_2[\phi,\phi_t]\,\mathrm{d}\tau\leqslant\mathbf{D}[v_0,\phi_{0t}].
$$

In addition, if the space dimension $N\leqslant 3$, *then the solution is smooth in* $\bar{\Omega}\times(0,\infty)$.

Proof. Denote

$$
m=\max\left\{-\min_{u\in\mathbb{R}}F''(u),\max_{u\in\mathbb{R}}|\ell''(u)|\right\}.
$$

We derive from (21) that

$$
\mathbf{E}_2[\phi,\zeta]\geqslant\frac{\varepsilon}{2}\int_{\Omega}(|\nabla\zeta|^2+\zeta^2)-A\int_{\partial\Omega}\zeta^2\geqslant\frac{\varepsilon}{2}\|\zeta\|^2_{H^1(\Omega)}-A\alpha\,\mathbf{D}[v,\zeta]. \tag{22}
$$

Hence, for the solution of (11), integrating the first two energy identities we obtain

$$
\begin{aligned}
&\sup_{t>0}\left(\mathbf{E}[\phi]+\delta\|v\|^2_{L^2(\Omega)}+\frac{\delta\|\nabla_{\partial\Omega}\phi\|^2_{L^2(\partial\Omega)}}{\alpha}\right)\\
&\quad+\int_0^\infty\left(\mathbf{D}[v,\phi_t]+\delta\|\phi_t\|^2_{L^2(\Omega)}\right)\mathrm{d}t\leqslant C_0,
\end{aligned}
$$

$$\sup_{t\geqslant 0}\Big(\mathbf{D}[v,\phi_t]+\delta\|\phi_t\|^2_{L^2(\Omega)}\Big)+\int_0^\infty\left(\varepsilon\|\phi_t\|^2_{H^1(\Omega)}+\delta\|v_t\|^2_{L^2(\Omega)}+\frac{\delta\|\nabla_{\partial\Omega}\phi_t\|^2_{L^2(\partial\Omega)}}{\alpha}\right)\leqslant C_0$$

where C_0 is a constant that does not depend on $\delta\in(0,1]$.

It then follows from a standard procedure that along a sequence of $\delta\searrow 0$, the solution of (11) approaches a limit which is a strong solution of (5). As weak solutions are unique, the whole sequence of solutions of (11) converges to the weak solution of (5), as $\delta\searrow 0$.

Suppose $N\leqslant 3$ and we can show that solution of (5) is bounded, then we can use higher order energy identities to estimate $\mathbf{E}_2[\phi,\frac{\partial^k\phi}{\partial t^k}]$ and $\mathbf{D}[\frac{\partial^k v}{\partial t^k},\frac{\partial^{k+1}\phi}{\partial t^{k+1}}]$ for $k=2,3,\ldots$. Also one establishes energy estimates for spatial derivatives to derive that (ϕ,v) is smooth and is a classical solution.

Hence, to show that we have a classical solution, thereby completing the proof of Theorem 3, we need only establish an L^∞ estimate for the solution. This will be done in the next two subsections.

Suppose we can show that $\|\phi\|_{L^\infty(\Omega_T)}\leqslant K(T)$ for a classical solution. For weak solutions, we argue as follows: first we modify F' by zero in $(-\infty,-K(T)-1]\cup[K(T)+1,\infty)$ to obtain a classical solution. This classical solution will be bounded by $K(T)$ so it is the weak solution of the original problem. Hence, we need only work on classical solutions. □

4.3. The Principal Eigenvalue

We denote

$$\lambda_\varepsilon(t):=\inf_{\int_\Omega\zeta=0}\frac{\int_\Omega[\varepsilon|\nabla\zeta|^2+\varepsilon^{-1}F''(\phi)\zeta^2]+\int_{\partial\Omega}\sigma(x)\ell''(\phi)\zeta^2}{\frac{1}{\alpha}\int_{\partial\Omega}\zeta^2+\int_\Omega|\nabla\Delta_N^{-1}\zeta|^2},$$
$$\Lambda_\varepsilon:=\min\left\{\inf_{t\in[0,\infty)}\lambda_\varepsilon(t)\ ,\ 0\right\}$$

where Δ_N^{-1} is the inverse of the Laplace operator under the Neumann boundary condition, that is, $\hat\zeta=\Delta_N^{-1}\zeta$ is defined as the solution of

$$\Delta\hat\zeta=\zeta-\frac{1}{|\Omega|}\int_\Omega\zeta\ \text{in}\ \Omega,\qquad \partial_n\hat\zeta=0\ \text{on}\ \partial\Omega,\qquad \int_\Omega\hat\zeta\,\mathrm{d}x=0.$$

Note that $\Lambda_\varepsilon\geqslant -A\alpha$ where A is defined in (22). If the interface is well-developed, the eigenvalue is as that investigated in [10], with the conclusion that Λ_ε is bounded from below by a constant that does not depend on ε. Here we allow Λ_ε to depend on ε.

The energy identity implies that

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{D}[v,\phi_t]=-\mathbf{E}_2[\phi,\phi_t]\leqslant-\lambda_\varepsilon(t)\mathbf{D}[v,\phi_t]\leqslant\Lambda_\varepsilon\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{E}[\phi].$$

Set $D(t) = \mathbf{D}[v(\cdot,t), \phi_t(\cdot,t)]$ and $E(t) := \mathbf{E}[\phi(\cdot,t)]$. Integrating the above inequality in $[0,t]$ we obtain

$$D(t) \leqslant D(0) - 2\Lambda_\varepsilon[E(0) - E(t)] \leqslant D(0) + 2A\alpha E(0) =: C.$$

Thus, we have

$$\sup_{t\geqslant 0}\left(\int_\Omega |\nabla v|^2 + \frac{1}{\alpha}\int_{\partial\Omega}\phi_t^2\right) \leqslant C.$$

Using [9, Lemma 3.4] we have

$$\|v\|_{H^1(\Omega)} := \|\nabla v\|_{L^2(\Omega)} + \|v\|_{L^2(\Omega)} \leqslant C(\Omega, m)\left(\mathbf{E}[\phi] + \|\nabla v\|_{L^2(\Omega)}\right) \leqslant C_1.$$

Hence, by Sobolev's imbedding

$$\|v\|_{L^p(\Omega)} \leqslant C(p,\Omega)\|v\|_{H^1(\Omega)} \leqslant CC_1, \;\; p = \frac{2N}{N-2} \quad (\text{if } N \leqslant 2,\ p > 1 \text{ is arbitrary})\,.$$

4.4. The L^∞ Estimate

Assume $N \leqslant 3$. Then $p := 2N/(N-2) > N$.
Let a_ε be a constant defined in (23) below. We set

$$k = \alpha\left(5a_\varepsilon + \|\sigma\ell'\|_{L^\infty(\Omega\times\mathbb{R})}\right) + 1.$$

Let $(x^*, t^*) \in \bar{\Omega} \times [0, T]$ be a point such that

$$\phi(x^*, t^*) - kt^* = \max_{\bar{\Omega}\times[0,T]}(\phi(x,t) - kt).$$

Then $\max_{\bar{\Omega}_T}\phi \leqslant \phi(x^*, t^*) + kT$. We now estimate $\phi(x^*, t^*)$.

(i) If $t^* = 0$, we have $\phi(x^*, t^*) = \phi_0(x^*) \leqslant M_0$.
(ii) Suppose $t^* > 0$. Denote $\Phi(y,t) = \phi(x^* + \varepsilon y, t)$, $B = \{y \mid |y| < 1, x^* + \varepsilon y \in \Omega\}$. Then

$$\varepsilon v = -\Delta_y \Phi + F'(\Phi) \quad \text{in} \;\; B.$$

Let $\Psi(\cdot, t)$ be a solution of

$$-\Delta\Psi = \tilde{v}(y) := \varepsilon v(x^* + \varepsilon y, t) \text{ in } \; B, \quad \Psi = 0 \;\text{ on }\; \partial B.$$

Then, since $p > N$,

$$\begin{aligned}\|\nabla_y \Psi(\cdot,t)\|_{L^\infty(B)} + \|\Psi(\cdot,t)\|_{L^\infty(B)} &\leqslant C\|\tilde{v}\|_{L^p(B)} \leqslant C\varepsilon^{1-N/p}\|v\|_{L^p(\Omega)} \\ &\leqslant C\varepsilon^{2-N/2}\|v\|_{L^\infty(0,\infty;L^p(\Omega))} =: a_\varepsilon. \qquad (23)\end{aligned}$$

Denote $\tilde{\Psi} = \Psi - 2a_\varepsilon(1 - |y|^2)$ and $\tilde{\Phi} = \Phi - \tilde{\Psi}$. Then $\Phi = \tilde{\Phi} + \tilde{\Psi}$ and

$$-\Delta_y \tilde{\Phi} = -F'(\tilde{\Phi} + \tilde{\Psi}) + 4Na_\varepsilon \qquad \text{in} \;\; B.$$

Let $(\hat{y}, \hat{t}) \in \bar{B} \times [0, T]$ be a point of maximum of $\tilde{\Phi} - kt$ in $\bar{B} \times [0, T]$.

(1) The case $|\hat{y}| = 1$ is impossible, since we would have $\tilde{\Psi}(\hat{y}, \hat{t}) = 0$ so

$$\Phi(\hat{y}, \hat{t}) - k\hat{t} = \Phi(\hat{y}, \hat{t}) - k\hat{t} \leqslant \phi(x^*, t^*) - kt^* = \tilde{\Phi}(0, t^*) + \tilde{\Psi}(0, t^*) - kt^*$$
$$\leqslant \tilde{\Phi}(0, t^*) - kt^* - a_\varepsilon,$$

which contradicts the definition of $(\hat{y}, \hat{t})$.

(2) The case $\hat{x} := x^* + \varepsilon\hat{y} \in \partial\Omega$ is also impossible, since at $(\hat{x}, \hat{t})$, we would have $\phi_t = \tilde{\Phi}_t(\hat{y}, \hat{t}) \geqslant k$ (here we observe that $\tilde{\Psi}_t = 0$ on $\partial B \times [0, T]$) and $\varepsilon\partial_n\phi \geqslant -\|\nabla\tilde{\Psi}\|_{L^\infty} \geqslant -5a_\varepsilon$, contradicts the boundary condition $\phi_t + \alpha(\varepsilon\partial_n\phi + \sigma\ell'(\phi)) = 0$ and the definition of k.

(3) Hence, $\hat{y}$ must be an interior point of B. Then $-\Delta_y\tilde{\Phi}(\hat{y}, \hat{t}) \geqslant 0$, so we have $F'(\tilde{\Phi} + \tilde{\Psi}) \leqslant 4Na_\varepsilon$. This implies that $\tilde{\Phi}(\hat{y}, \hat{t}) + \tilde{\Psi}(\hat{y}, \hat{t}) \leqslant 2 + \sqrt{4Na_\varepsilon}$. Hence,

$$\phi(x^*, t^*) = \tilde{\Phi}(0, t^*) + \tilde{\Psi}(0, t^*) \leqslant \tilde{\Phi}(\hat{y}, \hat{t}) + k(t^* - \hat{t}) + \tilde{\Psi}(0, t^*)$$
$$\leqslant 2 + \sqrt{4Na_\varepsilon} - \tilde{\Psi}(\hat{y}, \hat{t}) + k(t^* - \hat{t}) + \tilde{\Psi}(0, t^*)$$
$$\leqslant 2 + \sqrt{4Na_\varepsilon} + kT + 3a_\varepsilon.$$

Similarly, we can establish a lower bound of ϕ. Hence, we have

$$K(T) := \max_{\bar{\Omega}\times[0,T]} |\phi| \leqslant M_0 + 2kT + 3a_\varepsilon + \sqrt{4Na_\varepsilon}.$$

This completes the proof of Theorem 3.

5. Formal Asymptotic Limit as $\varepsilon \searrow 0$

Assume that F is a double equal-well potential: $F(u) > F(\pm 1) = 0$ for all $u \neq \pm 1$. Also assume that the initial data $\phi_0 = \phi_0^\varepsilon$ depends on ε and satisfies

$$\frac{1}{|\Omega|}\int_\Omega \phi_0^\varepsilon(x)\,\mathrm{d}x = m, \qquad \mathbf{E}[\phi_0^\varepsilon] \leqslant e_0$$

where $m \in (-1, 1)$ and e_0 are positive constants that do not depend on ε. Denote the solution of (5) by $(\phi_\varepsilon, v_\varepsilon)$. Then one can show that along a sequence $\varepsilon \searrow 0$, $(\phi_\varepsilon, v_\varepsilon)$ approaches a limit (ϕ^*, v^*) having the property $|\phi^*| = 1$ almost everywhere; see, for example [9]. Also, denote

$$\Omega_t^\pm = \left\{ x \in \bar{\Omega} \;\middle|\; \underline{\lim}_{r\searrow 0}\, \underline{\lim}_{\varepsilon\searrow 0} \min_{y\in\bar{\Omega}, |y-x|\leqslant r} \{\pm\phi_\varepsilon(y, t)\} \geqslant 1 \right\},$$
$$\Gamma_t = \partial\Omega_t^+ \cap \partial\Omega_t^-, \qquad \Gamma = \cup_{t\geqslant 0}\Gamma_t \times \{t\},$$

It is formally derived by Pego [16] and then rigorously verified by Alikakos, Bates and Chen [2,9] for the classical Cahn–Hilliard system that v^* solves

$$\Delta v^* = 0 \ \text{ in } \ \Omega\backslash\Gamma_t, \qquad v^* = \sigma_0(N-1)\mathcal{K}_{\Gamma_t}, \quad [n_{\Gamma_t}\cdot\nabla v^*]\Big|_{\Gamma_t} = 2V_{\Gamma_t} \ \text{ on } \ \Gamma_t,$$

where $\sigma_0 = \int_{-1}^{1} \sqrt{F(s)/2}\, \mathrm{d}s$, $[\cdot]|_{\Gamma_t}$ is the jump across Γ_t, n_{Γ_t} is the normal of $\partial\Omega_t^+$ at Γ_t, κ_{Γ_t} and V_t are the mean curvature and advancing speed of the front Γ_t of Ω_t^+. Together with the boundary condition $\partial_n v^* = 0$ on $\partial\Omega$, the limit free boundary problem for (v^*, Γ) is well-posed provided we know the dynamics of the intersection $\Gamma_t \cap \partial\Omega$.

Here we provide a formal argument showing that the intersection of interface Γ_t with $\partial\Omega$ does not change in time:

$$\Gamma_\tau \cap \partial\Omega \subset \Gamma_t \cap \partial\Omega \quad \forall\, 0 \leqslant \tau < t\ .$$

For this assume $N = 2$ and $[-1, 1] \times \{0\}$ is part of the boundary of $\partial\Omega$. Assume that one of the intersection points is $(x_\varepsilon(t), 0)$, and that from $t = 0$ to $t = T$, the intersection point moves from $x_\varepsilon(0) = 0$ to $x_\varepsilon(T) = b > 0$. For each $x_1 \in (0, b)$, denote by $t_\varepsilon^\pm(x_1)$ the time at which $\phi_\varepsilon(x_1, 0, t_\varepsilon^\pm(x_1)) = \pm 1/2$. Then

$$\begin{aligned}
b &= \lim_{\varepsilon \searrow 0} \int_0^b [\phi_\varepsilon(x_1, 0, t_\varepsilon^+(x_1)) - \phi(x_1, 0, t_\varepsilon^-(x_1))]\, \mathrm{d}x_1 \\
&= \lim_{\varepsilon \searrow 0} \int_0^b \int_{t_\varepsilon^-(x_1)}^{t_\varepsilon^+(x_1)} \phi_{\varepsilon,t}(x_1, 0, t)\, \mathrm{d}t\, \mathrm{d}x_1 \\
&\leqslant \overline{\lim_{\varepsilon \searrow 0}} \sqrt{\int_0^\infty \int_{\partial\Omega} \phi_{\varepsilon,t}^2}\, \sqrt{|D_\varepsilon|} \leqslant C_0\, \overline{\lim_{\varepsilon \searrow 0}} \sqrt{|D_\varepsilon|}
\end{aligned}$$

where $|D_\varepsilon|$ is the area of the region $D_\varepsilon := \{(x, t) \mid x \in \partial\Omega, 0 \leqslant t \leqslant T, |\phi_\varepsilon(x, t)| \leqslant 1/2\}$. Formally, D_ε has thickness $O(\varepsilon)$ so $\lim_{\varepsilon \searrow 0} |D_\varepsilon| = 0$. Thus $b = 0$. Hence, formally, in the limit $\varepsilon \searrow 0$, intersection points of Γ_t with $\partial\Omega$ do not move.

6. Fast Time Motion

Assume that $N = 2$ and Γ_t has only one component. When $1 \ll t \ll 1/\varepsilon$, the interface is almost circular whereas its intersection with $\partial\Omega$ does not show noticeable motion. Hence we assume that initially the interface is circular and use fast time $s = \varepsilon t$. Note that $s \in [0, 1]$ is equivalent to $t \in [0, 1/\varepsilon]$.

To derive the dynamic laws for the interface, contact angle and the contact points under the fast time s, we use the techniques of the matched asymptotic expansions. We shall first perform the standard matched asymptotic expansion away from the solid boundary which follows the steps given in [16]. For simplicity, we only summarize the results from the outer and inner expansions. We then focus our attention on the near contact point expansion to derive the dynamics of the contact angle and the intersection points.

The initial-boundary value problem of the Cahn–Hilliard equation becomes

$$\begin{cases}
F'(\phi) - \varepsilon^2 \Delta\phi = \varepsilon v, & \Delta v = \varepsilon \phi_s \quad \text{in } \Omega \times (0, \infty), \\
\varepsilon \phi_s = -\alpha[\varepsilon \partial_n \phi + \sigma(x) \ell'(\phi)], & \partial_n v = 0, \quad \text{on } \partial\Omega \times (0, \infty) \\
\phi = \phi_0 & \quad \text{on } \bar{\Omega} \times \{0\}.
\end{cases} \tag{24}$$

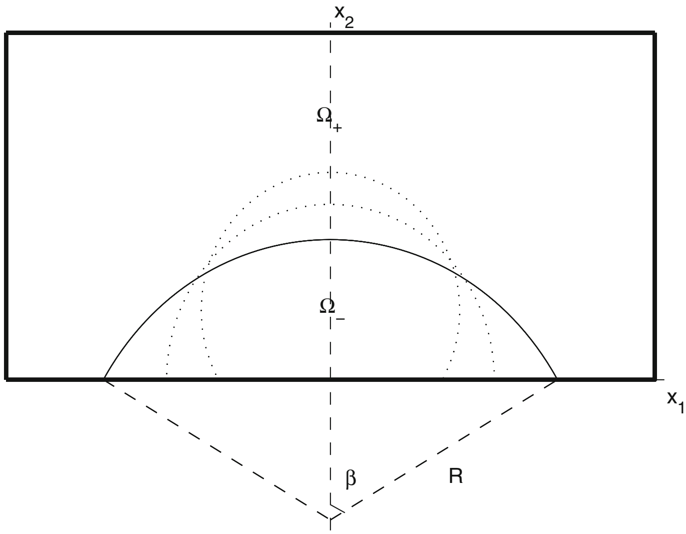

Fig. 2. Region Ω, Ω^+, Ω^-

The energy identity implies that

$$\int_0^\infty \left(\int_\Omega |\nabla v|^2 + \alpha \int_{\partial\Omega} [\varepsilon \partial_n \phi + \sigma(x)\ell'(\phi)]^2 \right) \leqslant \varepsilon \mathbf{E}[\phi_0].$$

Hence as $\varepsilon \searrow 0$, $v(\cdot, s)$ approaches a constant, which indicates that the interface is circular.

We consider a simple case (see Fig. 2) where $\Omega = (-1, 1) \times (0, 1)$ and the initial interface is a circular arc:

$$\Gamma_0 = \{\langle 0, -h(0)\rangle + R(0)\langle \sin\theta, \cos\theta\rangle \mid |\theta| \leqslant \beta(0)\},$$
$$\Omega_0^- = \{(x_1, x_2) \mid x_2 > 0, x_1^2 + (x_2 + h(0))^2 < R(0)^2\}$$

where $h(0) = R(0)\cos\beta(0)$ and $\beta(0) \in (0, \pi)$ and $R(0) > 0$. The area of the region Ω_0^- is

$$A = |\Omega_0^-| = R(0)^2 \left(\beta(0) - \sin\beta(0)\cos\beta(0)\right).$$

6.1. The Outer Expansion

Away from the interface in the phase region $\Omega_s^\pm$, we have the outer expansions

$$v \sim v^\pm \sim v_0^\pm + \textstyle\sum_{i\geqslant 1} \varepsilon^i v_i^\pm, \qquad \Delta v^\pm = \varepsilon \phi_s^\pm,$$
$$\phi \sim \phi^\pm \sim \phi_0^\pm + \textstyle\sum_{i\geqslant 1} \varepsilon^i \phi_i^\pm, \qquad F'(\phi^\pm) = \varepsilon v^\pm + \varepsilon^2 \Delta\phi^\pm.$$

It is easy to show that the leading order solutions are $\phi_0^\pm = \pm 1$ and $v_0^\pm$ satisfy

$$\Delta v_0^\pm = 0$$

with boundary condition

$$\partial_n v_0^{\pm} = 0 \qquad \text{on } \partial\Omega \cap \partial\Omega_s^{\pm}. \tag{25}$$

Since the outer expansion equations for $\phi_j^{\pm}$ do not allow the imposition of any boundary conditions, boundary layers are expected.

6.2. The Inner Expansion

For $s > 0$, we expect the limit interface ($\varepsilon \to 0$) be a circular arc centered at $(0, -h(s))$ with radius $R(s)$:

$$\Gamma_s = \left\{ \langle 0, -h(s)\rangle + R(s)\langle \sin\theta, \cos\theta\rangle \;\middle|\; |\theta| \leqslant \beta(s) \right\}, \qquad h(s) = R(s)\cos\beta(s).$$

We assume that the zero level set, Γ_s^{ε} of ϕ can be written as

$$\Gamma_s^{\varepsilon} = \left\{ \langle 0, -h(s)\rangle + R^{\varepsilon}(\theta, t)\langle \sin\theta, \cos\theta\rangle \;\middle|\; |\theta| \leqslant \beta^{\varepsilon}(s) \right\}.$$

We use the expansion

$$R^{\varepsilon}(\theta, s) \sim R(s) + \sum_{i\geqslant 1} \varepsilon^i R_i(\theta, s) = R(s) + \varepsilon \hat{R}^{\varepsilon}(\theta, s), \qquad \hat{R} \sim \sum_{i\geqslant 1} \varepsilon^{i-1} R_i.$$

It is convenient to use the polar coordinates (r, θ) centered at $(0, -h(s))$:

$$x = \langle 0, -h(s)\rangle + r\langle \sin\theta, \cos\theta\rangle,\ r := |x - \langle 0, -h(t)\rangle|,\ \theta = \operatorname{Arctan} \frac{x_1}{x_2 + h(s)}.$$

We now consider the change of variable $(x, s) \to (z, \theta, s)$ where z, a special version of the **stretched variable**, is defined by[1]

$$z = \frac{r - R^{\varepsilon}(\theta, s)}{\varepsilon} = \frac{|x - \langle 0, -h(s)\rangle| - R(s) - \varepsilon \hat{R}^{\varepsilon}(\theta, s)}{\varepsilon}.$$

Near the interface, we use the expansion

$$\phi(x, s) \sim \sum_{i\geqslant 0} \varepsilon^i \phi_i(z, \theta, s), \qquad v(x, t) \sim \sum_{i\geqslant 0} \varepsilon^i v_i(z, \theta, s). \tag{26}$$

Denote

$$X(\theta, s) := \langle 0, -h(s)\rangle + R(s)N(\theta), \quad N(\theta) = \langle \sin\theta, \cos\theta\rangle.$$

One can derive the following matching conditions, as $z \to \pm\infty$:

$$\begin{aligned} v_0(z, \theta, s) &\sim v_0^{\pm}(X(\theta, s), s), \\ v_1(z, \theta, s) &\sim v_1^{\pm}(X(\theta, s), s) + (R_1(\theta, s) + z)v_{0,r}(X(\theta, s), s), \\ &\quad \cdots\cdots\cdots \end{aligned}$$

Similarly, we can also derive matching conditions for ϕ.

---

[1] Typically the stretched variable is defined as $z = d(x, \Gamma_s^{\varepsilon})/\varepsilon$ where $d(x, \Gamma_s^{\varepsilon})$ is the signed distance from x to Γ_s^{ε}.

Substituting the expansions (26) into the Cahn–Hilliard equations (24), we can easily derive the leading order solution $\phi_0(z, \theta, s)$,

$$\phi_0(z, \theta, s) = Q(z)$$

where Q is the unique solution of

$$Q_{zz} - F'(Q) = 0 \text{ on } \mathbb{R}, \qquad Q(\pm\infty) = \pm 1, \quad Q(0) = 0. \tag{27}$$

This implies that

$$Q_z(z) = \sqrt{2F(Q(z))}, \qquad \int_0^{Q(z)} \frac{\mathrm{d}u}{\sqrt{2F(u)}} = z \quad \forall\, z \in \mathbb{R}.$$

For the leading order v_0, we have

$$v_0(z, \theta, s) = -\frac{\sigma_0}{R(s)},$$

where

$$\sigma_0 := \frac{1}{2}\int_{\mathbb{R}} Q_z^2(z)\,\mathrm{d}z = \frac{1}{\sqrt{2}}\int_{-1}^{1}\sqrt{F(u)}\mathrm{d}u. \tag{28}$$

The solvability condition for the higher order solutions then shows that the interface dynamics preserve the area of Ω_s^-, that is

$$|\Omega_s^-| = R^2[\beta - \sin\beta\cos\beta] = |\Omega_0^-| = A.$$

6.3. Expansion Near Contact Point

Assume for simplicity that the solution is symmetric with respect to the x_2-axis. Near the right intersection $p_\varepsilon = \langle R^\varepsilon(\theta, s)\sin\theta, 0\rangle|_{\theta=\beta^\varepsilon(s)}$, we use the stretched variable (y, z) defined by

$$y = \frac{x_2}{\varepsilon}, \quad z = \frac{r - R^\varepsilon(\theta, s)}{\varepsilon} \quad \left(r = \sqrt{x_1^2 + (x_2 + h(s))^2}, \quad \theta = \text{Arctan}\,\frac{x_1}{x_2 + h(s)}\right).$$

Expand $\phi \sim \sum_{i\geqslant 0}\varepsilon^i \Phi^i(z, y, s)$, $v \sim \sum_{i\geqslant 0}\varepsilon^i V^i(z, y, s)$, and $\beta_\varepsilon(s) \sim \beta(s) + \sum_{i\geqslant 0}\varepsilon^i\beta^i(s)$. The leading order expansion becomes

$$\begin{cases} \Phi^0_{zz} + 2\cos\beta\;\Phi^0_{yz} + \Phi^0_{yy} - F(\Phi^0) = 0 & \forall\, z \in \mathbb{R},\ y > 0,\ s > 0, \\ \Phi^0(z, \infty, s) = Q(z), & \forall\, z \in \mathbb{R},\ s > 0, \\ (h_s\cos\beta - R_s - \alpha\cos\beta)\Phi^0_z & \\ \quad = \alpha[\Phi^0_y - \sigma(R\sin\beta, 0)\ell'(\Phi^0)] & \forall z \in \mathbb{R},\ y = 0,\ s > 0. \end{cases} \tag{29}$$

In general it is very hard to find an explicit solution for this problem. Nevertheless, we can assume, for simplicity, that

$$\ell'(u) = \sqrt{2F(u)}$$

so that we have

$$\ell'(Q) = Q_z.$$

This choice of $\ell(u)$ is in fact preferred as argued in [20]. Then, we have an explicit solution $\Phi_0(z, y, s) = Q(z)$, subject to the compatibility condition

$$h_s \cos\beta - R_s = \alpha\left(\cos\beta - \sigma(R\sin\beta, 0)\right).$$

Using the relations

$$R = \frac{\sqrt{A}}{\sqrt{\beta - \sin\beta\cos\beta}}, \quad h = R\cos\beta = \frac{\sqrt{A}\cos\beta}{\sqrt{\beta - \sin\beta\cos\beta}} \tag{30}$$

we then derive the dynamics

$$\frac{\mathrm{d}}{\mathrm{d}s}\beta(s) = \frac{\alpha}{\sqrt{A}} \frac{(\beta - \sin\beta\cos\beta)^{3/2}[\cos\beta - \sigma(\frac{\sqrt{A}\sin\beta}{\sqrt{\beta - \sin\beta\cos\beta}}, 0)]}{\sin\beta[\sin\beta - \beta\cos\beta]}. \tag{31}$$

Once the contact angle $\beta(s)$ is solved from (31), the evolution of the drop radius $R(s)$ and the position of the contact point $x(s) = R(s)\sin(\beta(s))$ can then determined by using (30).

6.4. A Traveling Wave Problem

For general ℓ, the dynamics can be obtained as follows. First we solve a non-linear eigenvalue problem: for $p \in \partial\Omega$ and $\theta \in (0, \pi)$, find $\lambda = \lambda(p, \theta)$ and $\Phi(\cdot) = \Phi(p, \theta; \cdot)$ on $\mathbb{R} \times [0, \infty)$ such that

$$\begin{cases} \Phi_{zz} + 2\cos\theta\,\Phi_{yz} + \Phi_{yy} - F'(\Phi) = 0 & \text{on } \mathbb{R} \times (0, \infty), \\ \Phi(\cdot, \infty) = Q(\cdot), & \text{on } \mathbb{R} \times \{\infty\}, \\ \Phi_y = \sigma(p)\ell'(\Phi) - \lambda\Phi_z & \text{on } \mathbb{R} \times \{0\}. \end{cases} \tag{32}$$

Then the dynamics becomes

$$h_s \cos\beta - R_s = \alpha[\cos\beta - \lambda(p, \beta)], \quad h = R\cos\beta,\ p = \langle R\sin\beta, 0\rangle.$$

Note that from a solution of (32), we have a traveling wave of the form $u(z, y, s) = \Phi(z - \lambda s, y)$ where u solves

$$\begin{aligned} &u_{zz} + 2\cos\theta\, u_{zy} + u_{yy} = F'(u) && \text{on } \mathbb{R} \times (0, \infty) \times \mathbb{R}, \\ &u_s = u_y - \sigma(p)\ell'(u) && \text{on } \mathbb{R} \times \{0\} \times \mathbb{R}. \end{aligned}$$

It is still open to show that the non-linear eigenvalue problem (32) admits a unique solution for general monotonic $\ell(\cdot)$ satisfying $\ell'(\pm 1) = 0$.

To have a basic estimate of λ, note that

$$\frac{\partial}{\partial z}\left(\frac{1}{2}\Phi_z^2 - \frac{1}{2}\Phi_y^2 - F(\Phi)\right) + \frac{\partial}{\partial y}\left(\Phi_y\Phi_z + \cos\theta\,\Phi_z^2\right) = 0.$$

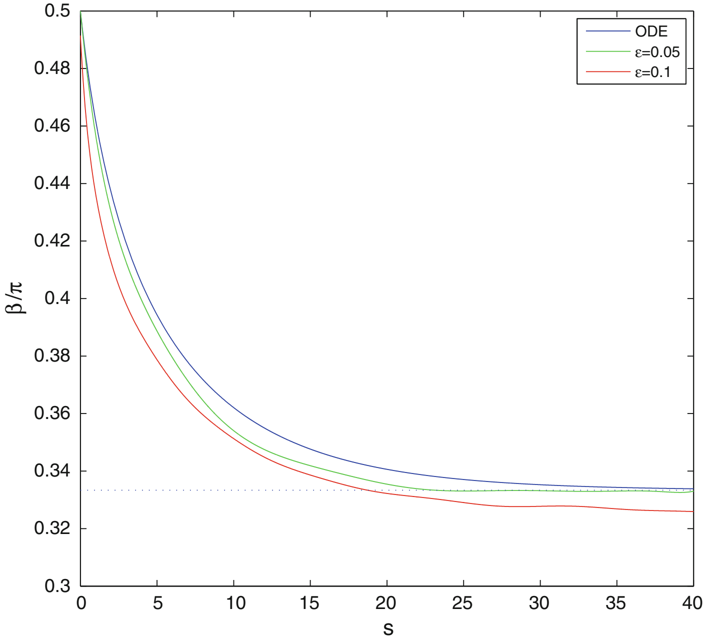

Fig. 3. Contact angle dynamics—the function $\beta = \beta^{\varepsilon}(s)$. *Top curve* is the solution of (31); *middle* and *bottom curves* correspond to the solution of the Cahn–Hilliard equation with $\varepsilon = 0.05$ and $\varepsilon = 0.1$, respectively. The *dotted line* corresponds to the equilibrium contact angle $\pi/3$

Integrating over $z \in \mathbb{R}$ we then derive that

$$\frac{\mathrm{d}}{\mathrm{d}y}\int_{\mathbb{R}}\left(\Phi_z\Phi_y + \cos\theta\,\Phi_z^2\right)\mathrm{d}z = 0 \quad \forall\, y > 0.$$

This implies that

$$\int_{\mathbb{R}}\Phi_y(z,0)\Phi_z(z,0)\,\mathrm{d}z = \cos\theta\int_{\mathbb{R}}[Q_z^2(z) - \Phi_z^2(z,0)]\,\mathrm{d}z.$$

Thus, integrating $\Phi_y(z,0) = \sigma(p)\ell'(\Phi) - \lambda\Phi_z$ multiplied by Φ_z over $z \in \mathbb{R}$ we derive that

$$\lambda = \sigma(p)\frac{\ell(1) - \ell(-1)}{\int_{\mathbb{R}}\Phi_z^2(z,0)\,\mathrm{d}z} \;+\; \cos\theta\,\frac{\int_{\mathbb{R}}[\Phi_z^2(z,0) - Q_z^2(z)]\,\mathrm{d}z}{\int_{\mathbb{R}}\Phi_z^2(z,0)\,\mathrm{d}z};$$

here, of course, Φ depends on p and θ.

6.5. Numerical Verification of the Contact Angle Evolution Law (31).

Here we numerically verify (31) by (i) numerically solving the Cahn–Hilliard equation (24) with small ε, (ii) finding the evolution of the contact angle from the resulting numerical solution, and (iii) comparing the dynamics of the contact angle with the solution of (31).

We set $\sigma(\cdot) \equiv \cos(\pi/3) = 1/2$ and $\alpha = 1$ and choose $\Omega = (-1, 1) \times (0, 1)$ and initial drop as a half disk with radius $R^\varepsilon(0)= \sqrt{0.8/\pi} \approx 0.5046$, contact angle $\beta^\varepsilon(0) = \pi/2$, and volume $A = \pi R^\varepsilon(0)^2/2 = 0.4$.

The solution $\beta = \beta(t)$ of the equation (31) is plotted in Fig. 3. It is clear that when $t \to \infty$, $\beta(t)$ approaches the equilibrium contact angle $\beta(\infty) = \arccos\sigma = \pi/3$.

Numerically solving the Cahn–Hilliard equation with small ε is very difficult. We use a numerical scheme recently developed by Gao and Wang in [22]. From the numerical solution, we compute the dynamics of the point and angle of contact by following the evolution of the intersection of the zero contour line of $\phi_\varepsilon(x, t)$ with the boundary. The evolutions of the computed contact angles, for $\varepsilon = 0.1$ and $\varepsilon = 0.05$, are shown in Fig. 3. The results not only illustrate a good convergence to the dynamic law (31) as $\varepsilon \to 0$, but also demonstrate the excellent performance of the numerical scheme developed in [22].

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Department of Mathematics
University of Pittsburgh
Pittsburgh PA 15260, USA
e-mail: xfc@math.pitt.edu

and

Department of Mathematics
The Hong Kong University of Science and Technology
Clear Water Bay
Kowloon, Hong Kong, China
e-mail: mawang@ust.hk

and

Institute of Computational Mathematics and Scientific/Engineering Computing
Chinese Academy of Sciences
Beijing 100080, China
e-mail: xmxu@lsec.cc.ac.cn

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