

A RAPIDLY CONVERGING PHASE FIELD MODEL

XINFU CHEN AND GUNDUZ CAGINALP

Department of Mathematics
University of Pittsburgh, Pittsburgh, PA 15260

CHRISTOF ECK

Institute of Applied Mathematics
University Erlangen-Nuremberg 91058 Erlangen, Germany

ABSTRACT. We propose a phase field model that approximates its limiting sharp interface model (free boundary problem) up to second order in interface thickness. A broad range of double-well potentials can be utilized so long as the dynamical coefficient in the phase equation is adjusted appropriately. This model thereby assures that computation with particular value of interface thickness ε , will differ at most by $O(\varepsilon^2)$ from the limiting sharp interface problem. As an illustration, the speed of a traveling wave of the phase field model is asymptotically expanded to demonstrate that it differs from the speed of the traveling wave of the limit problem by $O(\varepsilon^2)$.

1. Introduction. Interface problems arising from solidification have been studied extensively in mathematics and physics for more than a century [29]. The mathematical study began with Lamè and Clapeyron [23] in 1831 who modeled the freezing of the ground using the heat equation, latent heat across the interface, and the condition that the temperature at the interface remains at the equilibrium freezing temperature. Reformulated in 1889, this problem became known as the classical Stefan model [31], and can be stated as follows. Determine the temperature, $T(x, t)$, and the interface, $\Gamma(t)$, satisfying the system of equations,

$$\begin{aligned} \rho c T_t &= K \Delta T && \text{in } \Omega \setminus \Gamma(t), \\ \rho \ell v_n &= K \llbracket \nabla T \cdot N \rrbracket_+^-, && T(x, t) = T_E \quad \text{on } \Gamma(t), \end{aligned}$$

with ℓ , c , as the latent heat and heat capacity per unit mass, K the diffusivity, ρ the density and T_E the equilibrium freezing temperature. The unit normal and velocity at the interface are given by N and v_n , and $\llbracket \cdot \cdot \rrbracket_+^+$ denotes the difference in the limits from the two sides of the interface. The classical Stefan model has the appealing mathematical feature that the temperature, $T(x, t)$, determines the phase at each point (x, t) . By definition, $T(x, t) > T_E$ implies the material is liquid at that point (or, more generally, in the phase with the higher internal energy), while $T(x, t) < T_E$ means it is solid, while $T(x, t) = T_E$ defines the interface $\Gamma(t)$. Thus, the condition that $T(x, t) = T_E$ at the interface appears to be mathematically convenient. The mathematical study of the classical Stefan model posed difficult challenges that

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continue to present day. Existence of solutions in two spatial dimensions was proven by Meirmanov [27].

Parallel to this development, however, was the realization in the materials science community that the temperature on the interface differed from the equilibrium value by an amount proportional to the sum of the principal curvatures at that point, denoted $\kappa(x, t)$. In the late 19th century, Gibbs [18] demonstrated in a related problem (involving pressure) that the proportionality constant involved the surface tension, σ , which is a material constant depending on the two phases in consideration. This equilibrium condition is often called the Gibbs-Thomson condition. In the 20th century, materials scientists began to argue [16] that an additional correction to the temperature at the interface was due to kinetic undercooling, or the motion of the interface, although there was not complete agreement on the precise form of the velocity dependence. From the phase field approach (as we will see in detail below) these two effects can be derived [6] as:

$$T(x, t) = T_E - \frac{\sigma}{[s]_E} \{ \kappa(x, t) + \alpha v_n(x, t) \}.$$

It is important to note that this condition (even the equilibrium condition in which $\alpha = 0$) alters the problem dramatically. First, it is no longer possible for temperature to retain its dual role in determining the phase as well. It is possible (as experiments show [16]) to have water, for example, well below the freezing temperature. This necessitates another means for distinguishing the interface. For example, one could track the interface in time. Mathematically, this does not present a problem until there is a self-intersection of the interface. Proving the existence of solutions for the system of equations {heat equation, latent heat condition, and the Gibbs-Thomson condition} poses a difficult mathematical problem that was accomplished by Chen and Reitich [15] for short times and Luckhaus [26] for global in time. Second, the computation of the interface is complicated by self-intersections, and the difficulty of tracking a moving interface. In fact, a complete problem would need to stipulate the conditions for a large number of types of intersecting interfaces. While front tracking has been used successfully in tracking interfaces in related problems, providing a very accurate description of the interface, it is generally considered a difficult computational method.

Since the possibility of undercooling makes it impossible for temperature to distinguish the phases, it is natural to seek a different function that defines the phase. Prior to the development of the phase field approach, the closest analogy that was available in physics appeared to be the order parameter approach of Landau theory [24] that was used chiefly for studying the critical point. This involves high temperatures at which liquid and vapor cease to be distinct phases. The order parameter approach was used to calculate the critical exponents whereby thermodynamic functions diverged. But unfortunately, these exponents were shown to be incorrect (though they were in the right order of magnitude) once exact calculations were performed on the Ising model. Thus the order parameter approach, to some extent, was a disappointment. Another hurdle in attempting to apply this idea was the fact that Landau's rationale for the order parameter lay in the fact that the correlation length (distance at which there is a probabilistic correlation between spins or atoms) diverges to infinity near the critical point. For an ordinary phase transition, one has the opposite extreme, namely, the correlation length is a few atomic lengths (or Angstroms). Another issue was the fact that universality was intrinsic to critical phenomena. In other words, minor changes in a model (e.g., the

precise nature of the interactions between spins or atoms) did not alter the exponents. In any meaningful application of the order parameter idea for a solid-liquid transition, the solutions to the equations (temperature and interface position) must be precisely the correct ones, and one cannot “hide behind universality.” Consequently, the order parameter idea applied to ordinary phase boundaries needed to be valid in a different regime than one for which the theory was originally intended, even though it was not completely valid even in that region. Furthermore, it needed to have this additional level of precision due to the lack of universality.

In the 1970’s a review article by Hohenberg and Halperin [20] discussed the dynamics of order parameter in the context of critical phenomena. Similar ideas were utilized for spinodal decomposition (Cahn and Hilliard [14]), grain boundaries (Allen and Cahn [4]) in which there is no difference in internal energy between the two “phases,” and some equilibrium problems [25]. The possibility that an order parameter could be used in the context of a system of equations was explored from a physical and mathematical perspective in the 1980’s (Caginalp [7, 8, 6, 5]). In particular, the coupling between the temperature and order parameter, ϕ , can be written in a form (see Caginalp and Chen [10, 9])

$$\begin{cases} \varepsilon^2(\alpha_\varepsilon\varphi_t - \Delta\varphi) + W'(\varphi) &= \varepsilon G'(\varphi)(T - T_E) \\ \rho c T_t + \frac{\rho\ell}{2}\varphi_t &= K \Delta T \end{cases}$$

where φ takes on values between -1 and $+1$, with the liquid (or higher energy phase) defined by $+1$, and the solid defined by -1 . Here, G is a smooth function such that $G(1)$ exceeds $G(-1)$, and W is a smooth double-well function. With the equations appropriately scaled, the parameter ε is a measure of the interface thickness. The interface, $\Gamma_\varepsilon(t)$, is now defined as the set of points for which φ vanishes. For any meaningful physical or engineering applications, a rigorous study of the coupled system was crucial. In particular, a theory could be reasonable only if T and φ make the appropriate transitions near the interface, and satisfy a number of other conditions, such as boundedness. Beyond these issues is the key question of whether the solutions of the phase field equations converge to the sharp interface problem in the mathematical limit as ε approaches zero. This was resolved in stages, as the formal asymptotic analysis [6] was confirmed by rigorous results first in particular situations or symmetry [11, 10] and then in the general case (see [9] and Soner [30]). In particular, Caginalp and Chen [9] proved that in the distinguished limit $\varepsilon \rightarrow 0$, with all other parameters held constant, solutions of the phase field equations approach those of the sharp interface problems derived in [6] whenever the latter have a classical solution.

While these works resolved many of the mathematical issues, the application of phase field equations to practical computations led to other interesting questions on the nature of this convergence. From the computational perspective, one can view the phase field approach as a methodology for computation of sharp interface models. Since the interface thickness is only a few atomic lengths, this perspective is very reasonable from a physical point of view. The practical issue can be stated as follows in terms of the value of ε . The physical value of ε is on the order of 10^{-8} centimeters (cm) and the sharp interface limits corresponds to $\varepsilon = 0$. However, in order to compute the surface tension properly (see below) one needs to have a number of grid points in the interfacial region. This requires a grid spacing to be smaller than ε . Thus, computations, even on supercomputers, in three-dimensional space are limited to $\varepsilon \geq 10^{-4}$ cm (for an overall size of the domain that is typically

1 cm). In other words, if one is to use the phase field equations for realistic computations the interface motion for the system with $\varepsilon = 10^{-4}$ and $\varepsilon = 10^{-8}$ must be nearly identical. This physical ansatz that the interface thickness could be stretched out by a factor of ten thousand without significantly altering the motion of the interface was suggested and confirmed numerically in [13]. Since then, phase field equations have been used for a number of applications, and appear to be one of the most viable methods for computing interface motion. With these results and increased computer speeds, it has become possible to perform computations using realistic parameters (with ε as a “free parameter” that can be chosen for computational convenience). See for example, [3, 22, 19, 21, 28] and references contained therein. In particular, the physical value of the capillarity length d_0 that arises from the surface tension, is often about 10^{-7} cm, while the radius of curvature of the (dendritic) tips of the interface are often about 10^{-5} cm or smaller. If the true velocity of the interface for the sharp interface problem is given by v^{sharp} and the phase field approximation is v^ε , then the rigorous asymptotic analysis to date suggests that the difference is, at best,

$$|v^\varepsilon - v^{sharp}| \leq C\varepsilon,$$

and similarly for the interface position. As noted above, the value of ε must be at least 10^{-4} while the interface to be resolved is of the scale (radius of curvature, for example) 10^{-3} or 10^{-4} . Consequently, if we could define a new phase field model, along with a proof that

$$|v^\varepsilon - v^{sharp}| \leq C\varepsilon^2,$$

then there would be tremendous computational advantage, namely from $\varepsilon = 10^{-4}$ to $\varepsilon^2 = 10^{-8}$. From a physical perspective, the difference in error is reduced from mid-branch width to atomic width.

In this paper, we propose a new phase field model, by redefining W , G and α_ε , such that for any limiting sharp interface problem with any material parameters, the solutions of our phase field equations differ from the sharp interface problem by $O(\varepsilon^2)$ in the manner indicated above. In addition, we use a different perspective in differential geometry that simplifies the asymptotic analysis and the proofs of convergence.

To be specific, we write the dimensionless phase field model under consideration as

$$\begin{cases} \varepsilon^2(\alpha_\varepsilon\varphi_{\varepsilon t} - \Delta\varphi_\varepsilon) + W'(\varphi_\varepsilon) = \varepsilon m G'(\varphi_\varepsilon)u_\varepsilon & \text{in } \Omega \times (0, \infty), \\ (u_\varepsilon + \frac{1}{2}\ell\varphi_\varepsilon)_t = \Delta u_\varepsilon & \text{in } \Omega \times (0, \infty), \end{cases} \quad (1.1)$$

where the unknowns $u_\varepsilon(x, t)$ and $\varphi_\varepsilon(x, t)$ are respectively the temperature and the phase indicator ($\varphi_\varepsilon = 1$ for liquid and -1 for solid), ε is a small positive parameter representing the interface thickness, Ω is a bounded domain in \mathbb{R}^n with smooth boundary $\partial\Omega$, $W(\cdot)$ is a smooth double-well potential and G a smooth function satisfying

$$\begin{aligned} W(\pm 1) = 0 < W(s) \quad \forall s \neq \pm 1, \quad W''(\pm 1) > 0, \\ G'(\pm 1) = 0, \quad G(1) - G(-1) = \int_{-1}^1 \sqrt{2W(s)} ds. \end{aligned} \quad (1.2)$$

Here, m and ℓ are non-negative constants and

$$\alpha_\varepsilon = \alpha + \varepsilon\alpha_1 \geq 0, \quad \text{where } \alpha, \alpha_1 \text{ are constants independent of } \varepsilon. \quad (1.3)$$

It is shown in [10] that as $\varepsilon \searrow 0$, solutions to (1.1) under appropriate initial and boundary conditions converge to solutions to the following limit free boundary problem: Find phase domains $\Omega^+(t)$ and $\Omega^-(t)$ and unknown functions $u^\pm(x, t)$ in $Q^\pm := \cup_{0 < t \leq T} \Omega^\pm(t) \times \{t\}$ such that $\Omega = \Omega^-(t) \cup \Omega^+(t) \cup \Gamma(t)$ where $\Gamma(t) = \partial\Omega^+(t) \cap \partial\Omega^-(t) \setminus \partial\Omega$,

$$\begin{cases} u_t^\pm = \Delta u^\pm & \text{in } Q^\pm, \\ mu^+ = mu^- = -\alpha v - \kappa & \text{on } \Gamma(t), \\ N \cdot \nabla(u^+ - u^-) = -\ell v & \text{on } \Gamma(t), \end{cases} \tag{1.4}$$

where N is the unit vector normal to $\Gamma(t)$, pointing toward $\Omega^+(t)$, κ the sum of the principal curvatures of $\Gamma(t)$ (positive if $\Omega^-(t)$ is convex), v the normal velocity of $\Gamma(t)$ (positive if $\Omega^-(t)$ is expanding).

For convenience, we denote by Φ the unique solution to

$$\ddot{\Phi} - W'(\Phi) = 0 \text{ on } \mathbb{R}, \quad \Phi(\pm\infty) = 0, \quad \int_{\mathbb{R}} \rho \dot{\Phi}(\rho) d\rho = 0. \tag{1.5}$$

We shall demonstrate that the $\Phi(0)$ -level set $\Gamma_\varepsilon(t)$ of φ_ε is within an $O(\varepsilon^2)$ distance from $\Gamma(t)$ of the free boundary problem and analogously for the temperature u_ε and u^\pm , provided that

$$\alpha_1 = \frac{m\ell \int_{\mathbb{R}} (G(1) - G(\Phi(s)))(1 + \Phi(s)) ds}{2 \int_{\mathbb{R}} \dot{\Phi}^2(s) ds}, \tag{1.6}$$

$$0 = \int_{\mathbb{R}} \rho \dot{\Phi}^2(\rho) d\rho = \int_{\mathbb{R}} \rho G'(\Phi(\rho)) \dot{\Phi}(\rho) d\rho. \tag{1.7}$$

The precise statement of our main result is stated in Theorem 10.1 in §10. In numerical simulation, we can take the special choice

$$W(s) = \frac{1}{2}(1 - s^2)^2, \quad G(s) = s - \frac{1}{3}s^3, \quad \alpha_1 = \frac{5}{12}\ell m, \quad \Phi(z) = \tanh z. \tag{1.8}$$

When $m = 0$ and $\alpha_\varepsilon = 1$, the phase field equation becomes the Allen-Cahn [4] equation $\varphi_t - \Delta\varphi + W'(\varphi) = 0$. The resulting free boundary problem is the motion by mean curvature equation $v + \kappa = 0$. In this case our rapid convergence result was derived earlier by Nochetto and Verdi [28].

The rigorous proof on the convergence of solutions of (1.1) to (1.4) relies on two key assumptions: one is the existence of classical smooth solutions to solutions to (1.4) (with appropriate initial and boundary conditions) which we assume is true and the other is the existence of formal asymptotic expansions of certain order to solutions to (1.1) whose leading order expansions are that of (1.4). Hence, to show that the $\Phi(0)$ -level set of φ_ε is within an $O(\varepsilon^2)$ distance of $\Gamma(t)$, we need to construct formal asymptotic expansions of arbitrary higher order, via an inner-outer expansion technique, and show that the first order expansion of the $\Phi(0)$ -level set of φ_ε vanishes.

Arbitrary higher order inner-outer asymptotic expansions for the phase field equations were given by the authors in [9]. Although these expansions in [9] can be directly quoted here, we prefer to present a complete expansion with a new but much simpler technique.

This paper is organized as follows. In §2, we collect, for reader's convenience, a few basic notations used throughout the paper. The simpler outer expansion (e.g. solution in the phase domains $\{(x, t) \mid \varphi_\varepsilon(x, t) \approx \pm 1\}$) is summarized in §3. Since inner expansions (e.g. solution near $\{(x, t) \mid \varphi_\varepsilon \approx 0\}$) are very complicated, we divide the techniques into pieces and present them in §§4–10. As an illustration

of our result, we provide a one-dimensional traveling wave example in §11. Our concluding remarks are in §12.

2. Notation. For easy reference, we list here some main notations used in the sequel.

In the phase domain, we use the **outer expansion**

$$\begin{aligned} \varphi_\varepsilon(x, t) &\sim \pm 1 + \sum_{j \geq 1} \varepsilon^j \varphi_j^\pm(x, t), \\ u_\varepsilon(x, t) &\sim \sum_{j \geq 0} \varepsilon^j u_j^\pm(x, t) =: u_\varepsilon^\pm(x, t). \end{aligned} \tag{2.1}$$

Near the interface, we use the following notations:

- $\Gamma_0(t) = \Gamma(t)$: the limiting interface, i.e, the free boundary,
- $x = X_0(s, t)$: a local parameterization of $\Gamma(t)$, $s \in \mathbb{R}^{n-1}$,
- $s = S(x, t)$: $X_0(s, t)$ being the orthogonal projection from x onto $\Gamma(t)$,
- $r = R(x, t)$: the **signed distance** from x to $\Gamma(t)$,
- $\Gamma_\varepsilon(t)$: the $\Phi(0)$ -level set of φ_ε ,
- $r = \varepsilon h_\varepsilon(s, t)$: the graph equation for $\Gamma_\varepsilon(t)$,
- ρ : the **stretched** variable = $\frac{R(x, t) - \varepsilon h_\varepsilon(S(x, t), t)}{\varepsilon}$.

Note that $\Gamma(t)$ is the zero level set of $R(x, t)$ and Γ_ε is the zero level set of ρ .

Also we use the new independent variables (ρ, s, t) and a new function

$$\hat{u}(x, t) = u_\varepsilon(x, t) - [\theta(\rho)u_\varepsilon^+(x, t) + (1 - \theta(\rho))u_\varepsilon^-(x, t)] \tag{2.2}$$

where θ , chosen at our convenience, is any fixed smooth function satisfying $\theta(-\infty) = 0, \theta(\infty) = 1$. We use the **inner expansion**

$$\begin{aligned} \varphi_\varepsilon(x, t) &\sim \sum_{j \geq 0} \varepsilon^j \varphi_j(\rho, s, t), \\ \hat{u}^\varepsilon(x, t) &\sim \sum_{j \geq 0} \varepsilon^j \hat{u}_j(\rho, s, t), \\ \varepsilon h_\varepsilon(s, t) &\sim \sum_{j \geq 1} \varepsilon^j h_j(s, t). \end{aligned} \tag{2.3}$$

In our expansion, all $\varphi_j^\pm, u_j^\pm, \varphi_j, h_j, \hat{u}_j$ do not depend on ε . We call $(\varphi_0^\pm := \pm 1, u_0^\pm, \hat{u}_0, \varphi_0, \Gamma_0(t))$ the **leading order expansion** and $(\varphi_j^\pm, u_j^\pm, \hat{u}_j, \varphi_j, h_j)$ the **j th order expansion**, $j \geq 1$.

Note that $\Gamma_\varepsilon(t)$ is within an $O(\varepsilon^2)$ distance from $\Gamma(t)$ means that $h_1 \equiv 0$. Also that u_ε approximates $u^\pm := u_0^\pm$ by $O(\varepsilon^2)$ means that $u_1^\pm \equiv 0$. It is not necessary that $\hat{u}_1 \equiv 0$ since \hat{u}_1 depends on the choice of θ .

3. The Outer Expansion. In the “phase domain” where $\varphi_\varepsilon \sim \pm 1$, we expand the solution to (1.1) by (2.1). Upon substituting the outer expansion (2.1) into (1.1) and equating coefficients of ε^j for all j , we immediately obtain the following.

Lemma 3.1. *Assume (1.2). Then $\varphi_j^\pm(x, t) \equiv 0$ for all $j \geq 1$. Consequently,*

$$(u_j^\pm)_t = \Delta u_j^\pm \quad \text{in } Q_0^\pm \quad \forall j \geq 0 \tag{3.1}$$

where Q_0^\pm is the limiting phase domain to be determined later.

Remark 3.1. 1. If there is no phase transition, then (1.1) is equivalent to $u_{\varepsilon t} = \Delta u_\varepsilon$, whereas $\varphi_\varepsilon \equiv 1$ for the liquid and $\varphi_\varepsilon \equiv -1$ for that of solid.

2. The assertion of the lemma relies on the assumption that $G'(\pm 1) = 0$ and $W''(\pm 1) \neq 0$. For the case $G'(\pm) \neq 0$, see [9].

4. Basic Geometric Identities. We denote by $\Gamma_0(t) =: \Gamma(t)$ the **limiting interface**, and $\Omega_0^\pm(t) =: \Omega^\pm(t)$ the **limiting phase domains**, and assume, for the moment, that they exist and are smooth.

Locally, we can parameterize $\Gamma_0(t)$ by $X_0(s, t)$ where $s \in \mathbb{R}^{n-1}$. We use $N(s, t)$ to denote the unit normal to $\Gamma_0(t)$ (pointing to $\Omega_0^+(t)$ at $X_0(s, t)$). Hence, for each t , the map

$$x = X_0(s, t) + rN(s, t) \tag{4.1}$$

is locally a diffeomorphism. We denote the inverse by

$$r = R(x, t), \quad s = S(x, t) = (S^1, \dots, S^{n-1}).$$

It is easy to see that

$$R(x, t) = \begin{cases} \text{dist}(x, \Gamma_0(t)) & \text{in } \Omega^+(t), \\ -\text{dist}(x, \Gamma_0(t)) & \text{in } \Omega^-(t). \end{cases}$$

It then follows that

$$N = \nabla R, \quad |\nabla R| = 1, \quad \sum_{j=1}^n R_{x^i x^j} R_{x^j} = 0.$$

Thus, $(0, \nabla R)$ is an eigenpair of the symmetric matrix $(R_{x^i x^j})_{n \times n}$. We denote its other eigenpairs by $\{(\kappa_i, \tau_i)\}_{i=1}^{n-1}$. Since $(R_{x^i x^j})_{n \times n}$ is symmetric, we can arrange these eigenpairs such that $\{\tau_1, \dots, \tau_{n-1}, \nabla R\}$ form an orthonormal basis of \mathbb{R}^n .

In geometry, restricting x to Γ_0 , $\tau_1, \dots, \tau_{n-1}$ are called the **principal directions** of $\Gamma_0(t)$, and $\kappa_1, \dots, \kappa_{n-1}$ the **principal curvatures**. We use κ to denote the sum of all principal curvatures for $\Gamma_0(t)$, also refer to it as the $(n - 1)$ multiple) of the **mean curvature**. Then

$$\kappa(s, t) := \sum_{i=1}^{n-1} \kappa_i(X_0(s, t), t) = \Delta R(X_0(s, t), t). \tag{4.2}$$

Also, we denote

$$b(s, t) := \sum_{i=1}^{n-1} (\kappa_i(X_0(s, t), t))^2 = \sum_{i,j=1}^n R_{x^i x^j}^2(X_0(s, t), t) = -\nabla R \cdot \nabla(\Delta R). \tag{4.3}$$

Implicitly differentiating $x = X_0(s, t) + rN(s, t)|_{s=S(x,t), r=R(x,t)}$ with respect to t and taking the inner product of the resulting equation with N gives

$$-R_t(x, t) = X_{0t}(s, t) \cdot N(s, t) =: v(s, t). \tag{4.4}$$

Geometrically $v(s, t)$ represents the **velocity in the normal direction** of the motion of $\Gamma_0(t)$ at point $X_0(s, t)$. The above equation implies that $R_t(x, t) = R_t(X_0 + rN, t)$ is independent of r .

Finally, we recall the Taylor expansion, for a smooth function w ,

$$W(x + y) \sim \sum_{|\beta| \geq 0} \frac{1}{\beta!} y^\beta \frac{\partial^{|\beta|} w(x)}{\partial x^\beta} =: \sum_{k \geq 0} \frac{1}{k!} y \otimes \dots \otimes y : D^k w(x),$$

where β is a generic integer index, $y \otimes \dots \otimes y$ an order k tensor, and $:$ the shrinking operator of two order k tensors. In particular,

$$\begin{aligned} w(X_0 + rN, t) &\sim w(X_0, t) + rN \cdot \nabla w(X_0, t) + \frac{1}{2} r^2 N \otimes N : D_x^2 w(X_0, t) + \dots, \\ N \cdot \nabla w(X_0 + rN, t) &\sim N \cdot \nabla w(X_0, t) + rN \otimes N : D_x^2 w(X_0, t) + \dots \end{aligned}$$

Under the change of coordinates from (x, t) to (r, s, t) , we have

$$\begin{aligned} \partial_t &= -v \partial_r + \partial_t^\Gamma, & \partial_t^\Gamma &:= \partial_t + \sum_{i=1}^{n-1} S_t^i \partial_{s^i}, \\ \nabla &= N \partial_r + \nabla^\Gamma, & \nabla^\Gamma &:= \sum_{i=1}^{n-1} \nabla S^i \partial_{s^i}, \\ \Delta &= \partial_{rr} + \Delta R \partial_r + \Delta^\Gamma, & \Delta^\Gamma &:= \sum_{i=1}^{n-1} \Delta S^i \partial_{s^i} + \sum_{i,j=1}^{n-1} \nabla S^i \cdot \nabla S^j \partial_{s^i s^j}, \end{aligned}$$

where $\nabla S^i(x, t), S_t^i(x, t), \Delta R(x, t), R_t(x, t)$ are evaluated at $x = X_0(s, t) + rN(s, t)$, and are regarded as functions of (r, s, t) .

5. The Stretched Variable. We denote the $\Phi(0)$ -level set of φ_ε by

$$\Gamma_\varepsilon(t) := \{x \in \Omega \mid \varphi_\varepsilon(x, t) = \Phi(0)\}.$$

We expect that $\Gamma_\varepsilon(t)$ can be expressed as a graph over $\Gamma_0(t)$:

$$\Gamma_\varepsilon(t) = \{X(r, s, t) \mid r = \varepsilon h_\varepsilon(s, t)\}. \tag{5.1}$$

Hence, to find Γ_ε , it suffices to find h_ε .

We define the **stretched variable** ρ by

$$\rho := \frac{R(x, t)}{\varepsilon} - h_\varepsilon(S(x, t), t). \tag{5.2}$$

Thus, ρ represents the distance from x to Γ_ε , in the direction of N (the unit normal of Γ_0), and magnified by a factor of $1/\varepsilon$. In the sequel, we use (ρ, s, t) as independent variables for inner expansions. The change of variables can be written as

$$t = t, \quad x = X_0(s, t) + \varepsilon(\rho + h_\varepsilon(s, t))N(s, t). \tag{5.3}$$

Under this change of variables, we can calculate

$$\begin{aligned} w_t &= \left\{ -v_0 \varepsilon^{-1} - \partial_t^\Gamma h_\varepsilon \right\} w_\rho + \partial_t^\Gamma w \\ \nabla w &= \left\{ N \varepsilon^{-1} - \nabla^\Gamma h_\varepsilon \right\} w_\rho + \nabla^\Gamma w, \\ \Delta w &= \left\{ \varepsilon^{-2} + |\nabla^\Gamma h_\varepsilon|^2 \right\} w_{\rho\rho} + \left\{ \Delta R \varepsilon^{-1} - \Delta^\Gamma h_\varepsilon \right\} w_\rho - 2 \nabla^\Gamma h_\varepsilon \cdot \nabla^\Gamma w_\rho + \Delta^\Gamma w \end{aligned}$$

where $\nabla^\Gamma, \partial_t^\Gamma, \Delta^\Gamma$ are again differentiations with ρ fixed. Also,

$$\Delta R = \Delta R \Big|_{x=X_0+\varepsilon(\rho+h_\varepsilon)N} = \kappa(s, t) - \varepsilon(\rho + h_\varepsilon)b(s, t) + \dots$$

6. The Inner Expansion. Let θ be a fixed smooth function having the following properties:

$$\theta(-\infty) = 0, \quad \theta(\infty) = 1, \quad \lim_{|s| \rightarrow \infty} |s|^j \theta'(s) = 0 \quad \forall j \geq 1.$$

Near the interface $\Gamma_\varepsilon(t)$, we use the independent variables (ρ, s, t) , the new function \hat{u}_ε defined in (2.2), and the inner expansion (2.3). We point out that all ε independent functions of (x, t) are expanded via the Taylor expansion at $X_0(s, t)$ after setting $x = X_0(s, t) + \varepsilon(\rho + h_\varepsilon(s, t))N(s, t)$. Also, that $\varphi_\varepsilon = \Phi(0)$ on Γ_ε and the matching conditions of inner-outer expansions are equivalent to

$$\begin{aligned} \varphi_j(0, s, t) &= 0, & \hat{u}_j(\pm\infty, s, t) &= 0 & \forall j \geq 0, \\ \varphi_0(\pm\infty, s, t) &= \pm 1, & \varphi_j(\pm\infty, s, t) &= 0 & \forall j \geq 1. \end{aligned} \tag{6.1}$$

We call $\Gamma_0(t)$ the zeroth order expansion of Γ_ε and h_j the j th order ($j \geq 1$) expansion.

Since $(u_j^\pm)_t - \Delta u_j^\pm = 0$ in Q_0^\pm for each j , from the Taylor expansion, we see that $(u_\varepsilon^+)_t - \Delta u_\varepsilon^+ \sim 0$ and $(u_\varepsilon^-)_t - \Delta u_\varepsilon^- \sim 0$ in a neighborhood Γ_0 . Hence, the equation for \hat{u}_ε in the (x, t) variables can be written as

$$\Delta \hat{u}_\varepsilon = \hat{u}_{\varepsilon t} + \frac{1}{2} \ell \varphi_{\varepsilon t} + (u_\varepsilon^+ - u_\varepsilon^-)(\theta_t - \Delta \theta) - 2 \nabla (u_\varepsilon^+ - u_\varepsilon^-) \cdot \nabla \theta. \tag{6.2}$$

Using (ρ, s, t) as the independent variables, the phase field equations can be expressed as, after omitting the subscript ε ,

$$W'(\varphi) = \varphi_{\rho\rho} + \varepsilon \left\{ (\Delta R + \alpha_\varepsilon v_0) \varphi_\rho + G'(\varphi) (\hat{u} + \theta u^+ + (1 - \theta) u^-) \right\} \tag{6.3}$$

$$\begin{aligned}
 & + \varepsilon^2 \left\{ (\alpha_\varepsilon \partial_t^\Gamma h - \Delta^\Gamma h) \varphi_\rho + |\nabla^\Gamma h|^2 \varphi_{\rho\rho} - 2 \nabla^\Gamma h \cdot \nabla^\Gamma \varphi_\rho + \Delta^\Gamma \varphi - \alpha_\varepsilon \partial_t^\Gamma \varphi \right\}, \\
 -\hat{u}_{\rho\rho} & = (u^+ - u^-) \theta_{\rho\rho} \tag{6.4} \\
 & + \varepsilon \left\{ \frac{1}{2} \ell v_0 \varphi_\rho + (v_0 + \Delta R) (\hat{u}_\rho + (u^+ - u^-) \theta_\rho) + 2 \theta_\rho N \cdot \nabla (u^+ - u^-) \right\} \\
 & + \varepsilon^2 \left\{ \frac{1}{2} \ell \partial_t^\Gamma \varphi - \frac{1}{2} \ell \varphi_\rho \partial_t^\Gamma h + (\hat{u}_{\varepsilon\rho} + (u^+ - u^-) \theta_\rho) (\partial_t^\Gamma h - \Delta^\Gamma h) + \right. \\
 & \quad \left. |\nabla^\Gamma h|^2 \hat{u}_{\rho\rho} - 2 \nabla^\Gamma h \cdot \nabla^\Gamma \hat{u}_\rho - 2 \nabla (u^+ - u^-) \cdot \nabla^\Gamma h \theta_\rho \right. \\
 & \quad \left. + \Delta^\Gamma \hat{u} - \partial_t^\Gamma \hat{u} + (u^+ - u^-) |\nabla^\Gamma h|^2 \theta_{\rho\rho} \right\}.
 \end{aligned}$$

7. The Zeroth Order Expansion. For simplicity, we use $\llbracket w \rrbracket$ to denote the jump of w across Γ_0 ; i.e.

$$\llbracket w \rrbracket = w^+(X_0(s, t), t) - w^-(X_0(s, t), t).$$

Equating the zeroth order (ε^0) coefficients in (6.3) and (6.4) we obtain **the zeroth order inner expansion equations**:

$$\begin{aligned}
 W'(\varphi_0) & = \varphi_{0\rho\rho}, \\
 -\hat{u}_{0\rho\rho} & = \llbracket u_0 \rrbracket \theta_{\rho\rho}.
 \end{aligned}$$

The matching conditions for ϕ_0, \hat{u}_0 then yields

$$\begin{aligned}
 \varphi_0(\rho, s, t) & = \Phi(\rho), \\
 \llbracket u_0 \rrbracket & \equiv 0, \\
 \hat{u}_0 & \equiv 0,
 \end{aligned}$$

where $\Phi(\cdot)$ is the unique solution to (1.5).

To continue, we need the following lemma.

Lemma 7.1. *Assume W satisfies (1.2). Then (1.5) admits a unique solution, and the solution satisfies $\dot{\Phi} = \sqrt{2W(\Phi)}$.*

In addition, define the linear operator

$$\mathbf{L}\phi = -\phi_{\rho\rho} + W''(\Phi(\rho))\phi.$$

Then for any bounded continuous function g on \mathbb{R} satisfying $g(\pm\infty) = 0$, the following problem, for ϕ ,

$$\mathbf{L}\phi = g \quad \text{on } \mathbb{R}, \quad \phi(\pm\infty) = 0 = \phi(0)$$

is solvable if and only if

$$\int_{\mathbb{R}} g(\rho) \dot{\Phi}(\rho) d\rho = 0.$$

Moreover, if solvable, the solution is unique.

This Lemma can be proven by using the variation of constant technique for second linear order ODE's. We omit the details.

In the sequel, we denote by Φ_1 the unique solution to

$$\mathbf{L}\Phi_1 = G'(\Phi) - \dot{\Phi}, \quad \Phi_1(\pm\infty) = 0 = \Phi_1(0). \tag{7.1}$$

Note that by the assumption (1.2), this problem has a unique solution.

In particular, the choice

$$G(s) = \int_0^s \sqrt{2W(z)} dz \quad \forall s \in \mathbb{R} \tag{7.2}$$

implies $G'(\Phi) = m\sqrt{2W(\Phi)} = \dot{\Phi}$ so that $\Phi_1 \equiv 0$.

For the higher order expansions, we notice that, by the Taylor expansion,

$$\begin{aligned} u_\varepsilon^+ - u_\varepsilon^- &\sim \llbracket u_0 \rrbracket + \varepsilon\{\llbracket u_1 \rrbracket + (\rho + h_1)\llbracket N \cdot \nabla u_0 \rrbracket\} \\ &\quad + \varepsilon^2\{\llbracket u_2 \rrbracket + h_2\llbracket N \cdot \nabla u_0 \rrbracket + \frac{1}{2}(\rho + h_1)^2\llbracket N \otimes N : D_x^2 u_0 \rrbracket\} + \\ &\quad \dots + \varepsilon^j\{\llbracket u_j \rrbracket + h_j\llbracket N \cdot \nabla u_0 \rrbracket + \dots\} + \dots, \\ N \cdot \nabla(u_\varepsilon^+ - u_\varepsilon^-) &\sim \llbracket N \cdot \nabla u_0 \rrbracket + \varepsilon\{\llbracket N \cdot \nabla u_1 \rrbracket + (\rho + h_1)\llbracket N \otimes N : D_x^2 u_0 \rrbracket\} + \\ &\quad \dots + \varepsilon^j\{\llbracket N \cdot \nabla u_j \rrbracket + \dots\} + \dots \end{aligned}$$

To calculate $\llbracket N \otimes N : D_x^2 u_0 \rrbracket$, we differentiate $\llbracket u_0 \rrbracket = 0$ to obtain

$$\begin{aligned} 0 &= \llbracket \nabla^{\Gamma_0} u_0 \rrbracket, \\ 0 &= \llbracket \partial_t^{\Gamma_0} u_0 \rrbracket = \llbracket X_{0t} \cdot \nabla u_0 + u_{0t} \rrbracket = v_0\llbracket N \cdot \nabla u_0 \rrbracket + \llbracket u_{0t} \rrbracket, \\ 0 &= \llbracket \Delta^{\Gamma_0} u_0 \rrbracket = \llbracket \Delta u_0 - N \otimes N : D_x^2 u_0 - \kappa_0 N \cdot \nabla u_0 \rrbracket. \end{aligned}$$

Using the equation $u_{0t}^\pm = \Delta u_0^\pm$, we then obtain

$$\llbracket N \otimes N : D_x^2 u_0 \rrbracket = \llbracket u_{0t} \rrbracket - \kappa\llbracket N \cdot \nabla u_0 \rrbracket = -(v + \kappa)\llbracket N \cdot \nabla u_0 \rrbracket. \tag{7.3}$$

8. The First Order Expansion. Denote $u_0^{\Gamma_0} = u_0^\pm(X_0(s, t), t)$. The equations for the coefficient of ε^1 in (6.3) and (6.4) read

$$\begin{aligned} \mathbf{L}\varphi_1 &= (\alpha_0 v + \kappa)\dot{\Phi} + mG'(\Phi)u_0^{\Gamma_0}, \\ -\hat{u}_{1\rho\rho} &= \frac{1}{2}\ell v\dot{\Phi} + \{\llbracket u_1 \rrbracket + (\rho + h_1)\llbracket N \cdot \nabla u_0 \rrbracket\}\theta_{\rho\rho} + 2\llbracket N \cdot \nabla u_0 \rrbracket\theta_\rho. \end{aligned}$$

The solvability of φ_1 requires

$$\alpha v + \kappa = -m u_0^{\Gamma_0} \quad \text{on } \Gamma_0(t). \tag{8.1}$$

Under such conditions, the solution φ_1 is given uniquely by

$$\varphi_1(\rho, s, t) = m u_0^{\Gamma_0} \Phi_1(\rho).$$

In the special case when G is given by (1.2) or more general (7.2), one has $\varphi_1 \equiv 0$.

Integrating the equation for $\hat{u}_{1\rho\rho}$ and using $u_{1\rho}|_{\rho=-\infty} = 0$ gives

$$-\hat{u}_{1\rho} = \frac{1}{2}\ell v_0(1 + \Phi) + \llbracket u_1 \rrbracket\theta_\rho + \llbracket N \cdot \nabla u_0 \rrbracket\{\theta + (\rho + h_1)\theta_\rho\}.$$

The condition $\hat{u}_{1\rho}|_{\rho=\infty} = 0$ then requires

$$\llbracket N \cdot \nabla u_0 \rrbracket = -\ell v \quad \text{on } \Gamma_0(t). \tag{8.2}$$

Consequently, one has the equations

$$-\hat{u}_{1\rho} = \llbracket u_1 \rrbracket \theta_\rho + \llbracket N \cdot \nabla u_0 \rrbracket \left\{ \theta - \frac{1}{2}(1 + \Phi) + (\rho + h_1)\theta_\rho \right\}, \tag{8.3}$$

$$-\hat{u}_1 = \llbracket u_1 \rrbracket \theta + \llbracket N \cdot \nabla u_0 \rrbracket \left\{ h_1 \theta + \rho \left(\theta - \frac{1}{2}(1 + \Phi) \right) + \frac{1}{2} \int_{-\infty}^\rho s \dot{\Phi}(s) ds \right\}. \tag{8.4}$$

The condition $\hat{u}_1|_{\rho=\infty} = 0$ requires, using $\llbracket N \cdot \nabla u_0 \rrbracket = -\ell v$,

$$\llbracket u_1 \rrbracket + \llbracket N \cdot \nabla u_0 \rrbracket h_1 = 0 \quad \text{on } \Gamma_0. \tag{8.5}$$

In summary, $(u^+, u^-, \Gamma) := (u_0^+, u_0^-, \Gamma_0)$ solves the free boundary problem (1.4). In the sequel, we shall assume that appropriate initial and boundary conditions are supplied to (1.4), so that it admits a unique smooth solution in $\bar{\Omega} \times [0, T]$ for some $T > 0$.

9. The Second Order Expansion. At this stage, we shall assume (1.7). These conditions are satisfied if both W and G' are even. The second equality in (1.7) implies

$$0 = \int_{\mathbb{R}} \rho \dot{\Phi} [G'(\Phi) - \dot{\Phi}] = \int_{\mathbb{R}} \rho \dot{\Phi} \mathbf{L} \Phi_1 = \int_{\mathbb{R}} (2\dot{\Phi}_1 \dot{\Phi} + \rho \Phi_1 \mathbf{L} \dot{\Phi}) = 2 \int_{\mathbb{R}} \dot{\Phi}_1 \dot{\Phi}.$$

The equation for φ_2 reads

$$\begin{aligned} \mathbf{L} \varphi_2 &= -\frac{1}{2} W'''(\Phi) \varphi_1^2 + (\alpha_0 v + \kappa) \varphi_{1\rho} + m G''(\Phi) u_0^{\Gamma_0} \varphi_1 + \\ &\quad m G'(\Phi) u_1 + \dot{\Phi} \{ \alpha_1 v_0 - (\rho + h_1) b + \alpha_0 \partial_t^{\Gamma_0} h_1 - \Delta^{\Gamma_0} h_1 \} + |\nabla^{\Gamma_0} h_1|^2 \ddot{\Phi} \end{aligned}$$

where

$$\begin{aligned} u_1 &= \theta \{ u_1^{+\Gamma_0} + (\rho + h_1) N \cdot \nabla u_0^{+\Gamma_0} \} + (1 - \theta) \{ u_1^{-\Gamma_0} + (\rho + h_1) N \cdot \nabla u_0^{-\Gamma_0} \} + \hat{u}_1 \\ &= u_1^{-\Gamma_0} + (\rho + h_1) N \cdot \nabla u_0^{-\Gamma_0} + \llbracket N \cdot \nabla u_0 \rrbracket \left\{ \frac{1}{2} \rho (1 + \Phi) - \frac{1}{2} \int_{-\infty}^\rho s \dot{\Phi}(s) ds \right\} \\ &= u_1^{-\Gamma_0} + (\rho + h_1) N \cdot \nabla u_0^{-\Gamma_0} - \frac{1}{2} \ell v_0 \int_{-\infty}^\rho (1 + \Phi(s)) ds \end{aligned}$$

by the expression for \hat{u}_1 and $\llbracket N \cdot \nabla u_0 \rrbracket = -\ell v_0$. Hence,

$$\int_{\mathbb{R}} \dot{\Phi} G'(\Phi) u_1 = [G(1) - G(-1)] \{ u_1^{-\Gamma_0} + h_1 N \cdot \nabla u_0^{-\Gamma_0} \} + \frac{1}{2} \ell v_0 \int_{\mathbb{R}} (G(\Phi) - G(1)) (1 + \Phi) d\rho$$

We can also compute

$$\begin{aligned} &\int_{\mathbb{R}} \dot{\Phi} \left\{ -\frac{1}{2} W'''(\Phi) \varphi_1^2 + (\alpha_0 v + \kappa) \varphi_{1\rho} + G''(\Phi) u_0^{\Gamma_0} \varphi_1 \right\} \\ &= \int_{\mathbb{R}} \left\{ \varphi_1 \varphi_{1\rho} W'''(\Phi) + (\alpha_0 v + \kappa) \dot{\Phi} \varphi_{1\rho} - u_0^{\Gamma_0} G'(\Phi) \varphi_{1\rho} \right\} \\ &= \int_{\mathbb{R}} \left\{ \varphi_{1\rho} \varphi_{1\rho\rho} + 2(\alpha_0 v + \kappa) \dot{\Phi} \varphi_{1\rho} \right\} \\ &= -2m(u_0^{\Gamma_0})^2 \int_{\mathbb{R}} \dot{\Phi} \dot{\Phi}_1 = 0. \end{aligned}$$

Thus, the solvability condition for φ_2 can be written as, using

$$\llbracket u_1 \rrbracket + h_1 \llbracket N \cdot \nabla u_0 \rrbracket = 0,$$

$$\mathcal{L}^{\Gamma_0} h_1 + \frac{1}{2} m (u_1^- + u_1^+) = (\hat{\alpha}_1 - \alpha_1) v \tag{9.1}$$

$$\mathcal{L}^{\Gamma_0} := \alpha_0 \partial_t^{\Gamma_0} - \Delta^{\Gamma_0} - b + \frac{1}{2} m N \cdot \nabla (u_0^{-\Gamma_0} + u_0^{+\Gamma_0}), \tag{9.2}$$

$$\hat{\alpha}_1 = \frac{m \ell \int_{\mathbb{R}} (G(1) - G(\Phi))(1 + \Phi) d\rho}{2 \int_{\mathbb{R}} \dot{\Phi}^2 d\rho} \tag{9.3}$$

Finally, we consider the equation for \hat{u}_2 . The equation reads, since $\hat{u}_0 \equiv 0$ and $\llbracket u_0 \rrbracket = 0$,

$$\begin{aligned} -\hat{u}_{2\rho\rho} &= \frac{1}{2} \ell v_0 \varphi_{1\rho} + \theta_{\rho\rho} \{ \llbracket u_2 \rrbracket + h_2 \llbracket N \cdot \nabla u_0 \rrbracket + (\rho + h_1) \llbracket N \cdot \nabla u_1 \rrbracket \\ &\quad + \frac{1}{2} (\rho + h_1)^2 \llbracket N \otimes N : D_x^2 u_0 \rrbracket \} \\ &\quad + 2\theta_{\rho} \{ \llbracket N \cdot \nabla u_1 \rrbracket + (\rho + h_1) \llbracket N \otimes N : D_x^2 u_0 \rrbracket \} \\ &\quad + (v_0 + \kappa_0) (\hat{u}_{1\rho} + (\llbracket u_1 \rrbracket + (\rho + h_1) \llbracket N \cdot \nabla u_0 \rrbracket) \theta_{\rho}). \end{aligned}$$

Substituting the expression for $\hat{u}_{1\rho}$ and integrating we obtain

$$\begin{aligned} -\hat{u}_{2\rho} &= \frac{1}{2} \ell v_0 \varphi_1 + \{ \llbracket u_2 \rrbracket + h_2 \llbracket N \cdot \nabla u_0 \rrbracket \} \theta_{\rho} \\ &\quad + \llbracket N \cdot \nabla u_1 \rrbracket \{ (\rho + h_1) \theta_{\rho} + \theta \} + \llbracket N \otimes N : D_x^2 u_0 \rrbracket \{ \frac{1}{2} (\rho + h_1)^2 \theta_{\rho} \\ &\quad + h_1 \theta + \int_{-\infty}^{\rho} s \theta_s(s) ds \} \\ &\quad + (v_0 + \kappa_0) \llbracket N \cdot \nabla u_0 \rrbracket \int_{-\infty}^{\rho} (\frac{1}{2} (1 + \Phi) - \theta). \end{aligned}$$

Using (7.3), the condition $\hat{u}_{2\rho}|_{\rho=\infty} = 0$ is equivalent to

$$\begin{aligned} \llbracket N \cdot \nabla u_1 \rrbracket &= (v_0 + \kappa_0) \llbracket N \cdot \nabla u_0 \rrbracket \left\{ h_1 + \int_{\mathbb{R}} s \theta_s - \int_{\mathbb{R}} (\frac{1}{2} (1 + \Phi) - \theta) \right\} \\ &= (v_0 + \kappa_0) \llbracket N \cdot \nabla u_0 \rrbracket h_1 = -(v_0 + \kappa_0) \llbracket u_1 \rrbracket. \end{aligned}$$

At this stage, we conclude that (u_1^-, u_1^+, h_1) solves the linear system

$$\begin{cases} (u_1^{\pm})_t = \Delta u_1^{\pm} & \text{in } Q_0^{\pm} := \cup_{0 < t < T} \Omega_0^{\pm}(t) \times \{t\}, \\ \llbracket u_1 \rrbracket + \llbracket N \cdot \nabla u_0 \rrbracket h_1 = 0 & \text{on } \Gamma_0, \\ \llbracket N \cdot \nabla u_1 \rrbracket + (v + \kappa) \llbracket u_1 \rrbracket = 0 & \text{on } \Gamma_0, \\ \mathcal{L}^{\Gamma_0} h_1 + \frac{1}{2} m (u_1^- + u_1^+) = (\hat{\alpha}_1 - \alpha_1) v_0 & \text{on } \Gamma_0. \end{cases} \tag{9.4}$$

Now if we take $\alpha_1 = \hat{\alpha}_1$ and homogeneous boundary and initial data for u_1^{\pm} , then we obtain

$$u_1^{\pm} \equiv 0, \quad h_1 \equiv 0.$$

Consequently, the distance from Γ_0 to Γ_{ε} is

$$R = \varepsilon h_{\varepsilon} = \varepsilon^2 h_2 + \dots = O(\varepsilon^2).$$

If in particular we take $\theta = \frac{1}{2} (1 + \Phi)$, then

$$\hat{u}_1(\rho, s, t) = \frac{1}{2} \llbracket N \cdot \nabla u_0 \rrbracket \int_{-\infty}^{\rho} s \dot{\Phi}(s) ds. \tag{9.5}$$

10. **Higher Order Expansions.** For each $j \geq 2$, the solvability conditions

$$\int_{\mathbb{R}} \hat{u}_{j+1,\rho\rho} d\rho = 0, \quad \int_{\mathbb{R}} \hat{u}_{j\rho} d\rho = 0, \quad \int_{\mathbb{R}} \dot{\Phi} \mathbf{L} \varphi_{j+1} = 0$$

provide a closed system for (u_j^+, u_j^-, h_j) in the form

$$\begin{cases} (u_j^\pm)_t = \Delta u_j^\pm & \text{in } Q_0^\pm \\ \llbracket u_j \rrbracket + \llbracket N \cdot \nabla u_0 \rrbracket h_j = \dots & \text{on } \Gamma_0, \\ \llbracket N \cdot \nabla u_j \rrbracket + (v_0 + \kappa_0) \llbracket u_j \rrbracket = \dots & \text{on } \Gamma_0, \\ \mathcal{L}^{\Gamma_0} h_j + \frac{1}{2} m(u_j^- + u_j^+) = \dots & \text{on } \Gamma_0. \end{cases} \tag{10.1}$$

where all \dots depend only on the lower order expansions. This is a well-posed linear problem and admits a unique solution for appropriately given initial and boundary conditions. By a mathematical induction, we can find arbitrarily higher order expansions, provided that the solution (u_0^+, u_0^-, Γ_0) to (1.4) is sufficiently smooth. Following a general rigorous result of [10] which states that *if one can find arbitrary higher order expansion for the phase field system, then the expansion is asymptotic, e.g. the expansion converges to the limit*, we then can show that the asymptotic expansion is valid. Hence, we can summarize our result as follows:

Theorem 10.1. *Assume (1.2), (1.7), and $\alpha_\varepsilon = \alpha + \varepsilon \alpha_1$ where α_1 is given in (1.6).*

Suppose a set of initial and boundary data is supplied to (1.4) such that (1.4) admits a smooth solution, denoted by (u_0^+, u_0^-, Γ_0) , in $\Omega \times [0, T]$, where $\Gamma_0(t) \cap \partial\Omega = \emptyset$ for all $t \in [0, T]$.

Let $R_0(x)$ be the signed distance from x to $\Gamma_0(0)$ and $S_0(x)$ the orthogonal projection from x onto $\Gamma_0(x)$. For (1.1) supply u_ε the same boundary data as that for (1.4), but with the initial data

$$\begin{aligned} u_\varepsilon(x, 0) &= \frac{1}{2}(1 + \Phi(R_0/\varepsilon))u_0^+(x, 0) + \frac{1}{2}(1 - \Phi(R_0/\varepsilon))u_0^-(x, 0) \\ &\quad + \varepsilon \llbracket N \cdot \nabla u_0 \rrbracket \Big|_{(S_0(x), 0)} \int_{-\infty}^{R_0/\varepsilon} s \dot{\Phi}(s) ds. \end{aligned}$$

Also impose on φ_ε the homogeneous Neumann boundary condition and the initial data

$$\phi_\varepsilon(x, 0) = \Phi(R_0(x)/\varepsilon) + \varepsilon u_0(S_0(x), 0) \Phi_1(R_0/\varepsilon).$$

Denote by $(u_\varepsilon, \varphi_\varepsilon)$ the solution to (1.1) with the above mentioned initial and boundary conditions, and by Γ_ε the $\Phi(0)$ -level set of φ_ε . Then

- (i) *the distance from $\Gamma_0(t)$ to $\Gamma_\varepsilon(t)$ is $O(\varepsilon^2)$ for $t \in [0, T]$;*
- (ii) *Denoting by $R(x, t)$ the signed distance from x to $\Gamma_0(t)$ and by $S(x, t)$ the orthogonal projection from x onto $\Gamma_0(t)$, there holds*

$$\begin{aligned} \varphi_\varepsilon - \Phi(R/\varepsilon) - u_0(S(x, t), t) \Phi_1(R/\varepsilon) &= O(\varepsilon^2), \\ u_\varepsilon - \frac{1}{2}(1 + \Phi(R/\varepsilon)) u_0^+(x, t) - \frac{1}{2}(1 - \Phi(R/\varepsilon)) u_0^-(x, t) \\ &\quad + \varepsilon \llbracket N \cdot \nabla u(S(x, t), t) \rrbracket \int_{-\infty}^{R/\varepsilon} s \dot{\Phi}(s) ds = O(\varepsilon^2). \end{aligned}$$

In particular,

$$u_\varepsilon - u_0^\pm = O(\varepsilon^2) \quad \text{if } \pm R(x, t) > C\varepsilon |\ln \varepsilon|.$$

Furthermore, if $G'(s) = \sqrt{2W(s)}$ so that $\Phi_1 \equiv 0$, then a similar relation holds for φ_ε :

$$\varphi_\varepsilon(x, t) - \Phi(R(x, t)/\varepsilon) = O(\varepsilon^2).$$

Remark 10.1. 1. If $\Gamma_0(t)$ touches the boundary $\partial\Omega$, then not only the boundary layer expansion is needed, but also the boundary condition for φ_ε has to be compatible with that of u_0^\pm . For the simplicity of our presentation, we choose to omit the boundary layer expansions. For the corresponding techniques, see Caginalp and Chen [10]

2. Due to the introduction of new functions \hat{u}_ε and h_ε , the asymptotic expansion technique used here is different from and much simpler than that used in Caginalp-Chen [9] for the phase field equation, Alikakos-Bates-Chen [1] for the Cahn-Hilliard equation, and deMottoni-Schatzman [17] for the Allen-Cahn equation where the new independent variables (ρ, s, t) are defined as $\rho = R_\varepsilon/\varepsilon$, $R_\varepsilon \sim \sum_{j \geq 0} \varepsilon^j R_j(x, t)$ the signed distance from x to Γ_ε and $x = X_\varepsilon(s, t) \sim \sum_{j \geq 0} \varepsilon^j X_j(s, t)$, $s \in \mathbb{R}^{n-1}$, a local representation of Γ_ε .

11. A 1-D Example. We consider the one-dimensional case, taking

$$m = 1, \quad G'(s) = \sqrt{2W(s)}.$$

For fixed positive constants α and v , the free boundary problem (1.4) admits a traveling wave of speed $v > 0$, modeling solidification of supercooled liquid:

$$u(x, t) = \begin{cases} -\alpha v & \text{if } x \leq vt, \\ -\alpha v + \ell(e^{v(vt-x)} - 1) & \text{if } x > vt, \end{cases} \quad \varphi = \begin{cases} -1 & \text{if } x < vt, \\ 1 & \text{if } x > vt. \end{cases}$$

Here the value φ is needed to indicate that the region $\{x < vt\}$ is occupied by solid whose temperature is the constant $-\alpha v$, and the region $\{x > vt\}$ is occupied by liquid which is supercooled near $x = \infty$ since its temperature is $-\ell - \alpha v$ which is below $-\ell$. Thus the traveling wave solution describes the phenomenon that the supercooled liquid is solidifying, releasing latent heat to increase the temperature in solid, and the free boundary, located at vt , is moving to the right with a constant velocity $v > 0$.

Correspondingly, (1.1) also admits a traveling wave, with the prescribed temperature at $x = \pm\infty$. The existence of traveling waves to (1.1) has been studied by Caginalp and Nishiura [12]. Here for the readers convenience and also to find the corresponding traveling wave speed $c_\varepsilon =: c$, we provide details.

We are looking for solutions to (1.1) that have the form

$$u_\varepsilon(x, t) = w(x - ct), \quad \varphi_\varepsilon(x, t) = \phi(x - ct).$$

The equation for u_ε reads $w'' + cw' + \frac{1}{2}c\ell\phi' = 0$, which after integration and using the condition at $x = -\infty$ gives

$$w' + c(w + \alpha v) + \frac{1}{2}c\ell(\phi + 1) = 0.$$

Note that this equation gives automatically the condition $w(\infty) = -\alpha v - \ell$ provided that $\phi(\infty) = 1$. This equation can be integrated to give a unique bounded solution, in an integrated form,

$$w(z) = -\alpha v - \frac{1}{2}c\ell \int_{-\infty}^z e^{c(y-z)}(\phi(y) + 1) dy.$$

The equation for φ_ε then translates to an integro-differential equation:

$$W'(\phi) = \varepsilon^2(c\alpha_\varepsilon\dot{\phi} + \ddot{\phi}) - \varepsilon G'(\phi)\left\{\alpha v + \frac{1}{2}c\ell \int_{-\infty}^z e^{c(y-z)}(\phi(y) + 1) dy\right\}.$$

To solve this equation, we use the stretched variable $\rho = z/\varepsilon$. Hence, writing $\phi(z) = \Psi(z/\varepsilon)$ we obtain the integro-differential equation

$$W'(\Psi) - \ddot{\Psi} = c\alpha_\varepsilon\varepsilon\dot{\Psi} - \varepsilon G'(\Psi)\left\{\alpha v + \frac{1}{2}\ell \int_{-\infty}^\rho c\varepsilon e^{c\varepsilon(\eta-\rho)}(\Psi(\eta) + 1) d\eta\right\}. \tag{11.1}$$

Since ε is small, this equation can be solved by a regular iteration procedure.

Set $\Psi(\rho) = \Phi(\rho) + \varepsilon\Psi_1(\rho)$. We can write the equation as

$$\mathbf{L}\Psi_1 = c\alpha_\varepsilon\dot{\Phi} - M(c, \Psi_1)$$

where

$$\begin{aligned} M(c, \Psi_1) &:= \frac{1}{\varepsilon}\left\{W'(\Phi + \varepsilon\Psi_1) - W'(\Phi) - \varepsilon W''(\Phi)\Psi_1\right\} - \varepsilon c\alpha_\varepsilon\dot{\Psi}_1 \\ &\quad + G'(\Phi + \varepsilon\Psi_1)\left\{\alpha v + \frac{1}{2}\ell \int_{-\infty}^\rho c\varepsilon e^{c\varepsilon(\eta-\rho)}(\Phi + 1 + \varepsilon\Psi_1(\eta)) d\eta\right\} \\ &= G'(\Phi)\left\{\alpha v + \frac{1}{2}\ell \int_{-\infty}^\rho c\varepsilon e^{c\varepsilon(\eta-\rho)}(\Phi(\eta) + 1) d\eta\right\} + O(|\varepsilon\Psi_1| + |\varepsilon\dot{\Psi}_1|). \end{aligned}$$

For each $c \in [v/2, v + \ell/v + 1]$ and a function Ψ_1 satisfying $|\Psi_1| + |\dot{\Psi}_1| \leq \varepsilon^{-1/3}$, we define \bar{c} by

$$\bar{c} = \frac{\int_{\mathbb{R}} M(c, \Psi_1)\dot{\Phi}}{\alpha_\varepsilon \int_{\mathbb{R}} \dot{\Phi}^2}$$

and define $\bar{\Psi}_1$ as the unique solution to

$$\mathbf{L}\bar{\Psi}_1 = \alpha_\varepsilon\bar{c}\dot{\Phi} - M(c, \Psi_1) \text{ on } \mathbb{R}, \quad \bar{\Psi}_1(0) = 0.$$

By the definition of \bar{c} and solvability, this equation has a unique solution. Notice that

$$M(c, \Psi_1) = M(0, 0) + O(\varepsilon|\Psi_1| + \varepsilon|\dot{\Psi}_1|).$$

It is easy to show that that for small ε , the mapping $(c, \Psi_1) \rightarrow (\bar{c}, \bar{\Psi}_1)$ is a contraction in terms of the L^∞ norms for each ε small enough, so that there is a unique fixed point. This established the existence of a traveling wave. We denote the solution by Ψ_1 .

Since $|M(c, \Psi_1) - M(c, 0)| = O(\varepsilon)(|\Psi_1| + |\dot{\Psi}_1|)$ we see that the solution Ψ is uniformly bounded. Consequently,

$$M(c, \Psi_1) - M(c, 0) = O(\varepsilon).$$

Note that for $z < 0$, $e^z = 1 + O(1)z$ where $O(1)$ is uniformly bounded. We can estimate

$$\begin{aligned} \int_{-\infty}^\rho c\varepsilon e^{c\varepsilon(\eta-\rho)}(\Phi(\eta) + 1) d\eta &= \Phi + 1 - \int_{-\infty}^\rho e^{c\varepsilon(\eta-\rho)}\dot{\Phi}(\eta) d\eta \\ &= \Phi + 1 - \int_{-\infty}^\rho \{1 + c\varepsilon O(1)(\rho - \eta)\}\dot{\Phi}(\eta) d\eta \\ &= O(\varepsilon)\rho(\Psi(\rho) + 1) + O(\varepsilon). \end{aligned}$$

Hence,

$$M(c, \Psi_1) = M(c, 0) + O(\varepsilon) = G'(\Phi)\alpha v + O(\varepsilon)\rho G'(\Phi) = \dot{\Phi}\alpha v + O(\varepsilon).$$

since $G'(\Phi) = \dot{\Phi}$. Therefore, we obtain

$$\mathbf{L}\Psi_1 = \dot{\Phi} \{ \alpha_\varepsilon c - \alpha v \} + O(\varepsilon).$$

From this, we conclude that

$$c = v + O(\varepsilon), \quad |\Psi_1| + |\dot{\Psi}_1| = O(\varepsilon).$$

By linearization, one can show that the solution Ψ_1 decays exponentially fast near $\rho = \pm\infty$.

Finally, multiplying (11.1) by $\dot{\Psi}/\varepsilon$ and integrating over \mathbb{R} , we obtain

$$\begin{aligned} c\alpha_\varepsilon \int_{\mathbb{R}} \dot{\Psi}^2 &= \int_{\mathbb{R}} \dot{\Psi} G'(\Psi) \left\{ \alpha v + \frac{\ell}{2} \int_{-\infty}^{\rho} c\varepsilon e^{c\varepsilon(\eta-\rho)} (\Psi(\eta) + 1) d\eta \right\} d\rho \\ &= \alpha v \{ G(1) - G(-1) \} \\ &\quad - \frac{\ell}{2} \int_{\mathbb{R}} \{ G(\Psi) - G(1) \} \left\{ c\varepsilon (\Psi + 1) - \int_{-\infty}^{\rho} (c\varepsilon)^2 e^{c\varepsilon(\eta-\rho)} (\Psi(\eta) + 1) d\eta \right\} \\ &= \alpha v \{ G(1) - G(-1) \} + \frac{\ell}{2} \{ c\varepsilon + O(\varepsilon^2) \} \int_{\mathbb{R}} (G(1) - G(\Psi)) (\Psi + 1) d\rho \end{aligned}$$

Since $\Psi = \Phi + \varepsilon\Psi_1 = \Phi + O(\varepsilon^2)$, we then obtain

$$\alpha v = c \{ \alpha_\varepsilon - \hat{\alpha}_1 \varepsilon + O(\varepsilon^2) \}$$

where

$$\hat{\alpha}_1 := \frac{\ell \int_{\mathbb{R}} (G(1) - G(\Phi)) (\Phi + 1)}{2 \int \dot{\Phi}^2}.$$

Hence, if $\alpha_\varepsilon = \alpha + \varepsilon\hat{\alpha}_1$, then $c = v + O(\varepsilon^2)$.

12. Conclusion. In this paper we have derived a set of phase field models and proven that these approximate the motion of a sharp interface to $O(\varepsilon^2)$ rather than $O(\varepsilon)$, where ε is a measure of interface thickness. Since it is difficult to implement values smaller than $\varepsilon = 10^{-3}$ due to grid size and computational time constraints, the computational advantage is highly significant. The key here is to set

$$\alpha_\varepsilon = \alpha_0 + \varepsilon\alpha_1$$

where α_1 is given by (1.6). Past computation simulations are exclusively done with $\alpha_1 = 0$. As demonstrated in this paper, setting $\alpha_1 = \hat{\alpha}_1$ improves the approximation of the phase field model to the limiting sharp interface model from $O(\varepsilon)$ to $O(\varepsilon^2)$.

To summarize, we write the sharp interface problem in fully dimensional form as

$$\begin{cases} \rho c_m T_t = K\Delta T & \text{in } Q^\pm \\ -\rho l_m v = N \cdot \nabla(u^+ - u^-) & \text{on } \Gamma_0(t) \\ T = T_E - \frac{\sigma}{[s]_E} (\kappa - \alpha v) & \text{on } \Gamma_0(t) \end{cases} \quad (12.1)$$

where $\rho, c_m, l_m, T_E, \sigma$, and $[s]_E$ are physical constants defined in [9].

This sharp interface problem will be approximated by a phase field model of the form

$$\begin{cases} \varepsilon^2(\alpha_\varepsilon \varphi_t - \Delta \varphi) + W'(\varphi) = \varepsilon G'(\varphi)(T - T_E) \\ \rho c_m T_t + \frac{\rho l_m}{2} \varphi_t = K\Delta T \end{cases} \quad \text{in } \Omega \times (0, \infty) \quad (12.2)$$

where G is an arbitrary smooth function such that $G(1) > G(-1)$ and W is a smooth double-well function satisfying (1.2).

For a given $\sigma/[s]_E$ we can scale either W or G by a constant so there holds the relation

$$m := \frac{G(1) - G(-1)}{\int_{-1}^1 \sqrt{2W(s)} ds} = \frac{[s]_E}{\sigma} \quad (12.3)$$

Subsequently, a particular undercooling term $\beta := (\alpha\sigma/[s]_E)$ specifies α . Then we write $\alpha_\varepsilon := \alpha_0 + \varepsilon\alpha_1$ in (12.2) via $\alpha_0 := \alpha$ and $\alpha_1 := \hat{\alpha}_1$ defined by (1.6). Hence, all of the parameters of (12.1) are thereby completely identified by (12.2), (12.3).

Given any set of initial and boundary data such that (12.1) admits a smooth solution (u^+, u^-, Γ_0) , we have proven (Theorem 10.1) that the solution $(u_\varepsilon, \varphi_\varepsilon)$ to (12.2) has the property that the distance between the zero level set of φ_ε , namely, $\Gamma_\varepsilon(t)$, and $\Gamma_0(t)$, is $O(\varepsilon^2)$.

Alternative distinguished limits. It has been known for some time that a broad spectrum of sharp interface models, of which (12.1) is just one, can be obtained as distinguished limits of phase field equations such as (12.2). One of the other models, sometimes preferred by physicists is (12.1) with $\alpha := 0$. In other words the dynamical condition is replaced by the traditional (equilibrium) Gibbs-Thomson relation. In this case one has simply $\alpha_0 := 0$ and $\alpha_1 := \hat{\alpha}_1$ again. Since we have not assumed a positive lower bound on α or α_0 , Theorem 10.1 remains valid. Another similar model, often called the quasi-static limit, is attained by setting $c_m = 0$ as well as $\alpha = 0$. The degeneracy (from parabolic to elliptic) in (12.2) does not affect the rigorous asymptotic expansion so that Theorems 1 holds.

The phase field equations have numerous additional distinguished limits as shown in Figure 1 of [9] and [8]. Among these is the sharp interface problem known as the Allen-Cahn equation obtained by setting $T := T_E$ for the initial and boundary conditions and assuming $l_m := 0$. Then the limit $\varepsilon \rightarrow 0$ yields the motion by mean curvature. Hence the choice $\alpha_1 := 0$ in $\alpha_\varepsilon = \alpha_0 + \varepsilon\alpha_1$ yields an $O(\varepsilon^2)$ approximation to the interface. For the Allen-Cahn equation this fact had been noted [17, 28]. Our methodology can be applied to the other limits in [9], the main consideration being the preservation of bounds as quantities such as c_m approach zero.

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E-mail address: xinfu@pitt.edu

E-mail address: caginalp@pitt.edu

E-mail address: eck@am.uni-erlangen.de