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# Convergence of the phase field model to its sharp interface limits

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We consider the distinguished limits of the phase field equations and prove that the corresponding free boundary problem is attained in each case. These include the classical Stefan model, the surface tension model (with or without kinetics), the surface tension model with zero specific heat, the two phase Hele–Shaw, or quasi-static, model. The Hele–Shaw model is also a limit of the Cahn–Hilliard equation, which is itself a limit of the phase field equations. Also included in the distinguished limits is the motion by mean curvature model that is a limit of the Allen–Cahn equation, which can in turn be attained from the phase field equations.

#### 1 Introduction

The study of moving boundary problems in recent years can be grouped broadly into two categories: (i) free boundary problems in which the free boundary is to be determined and solutions must satisfy certain jump relations across the free boundary, and certain partial differential equations away from the free boundary; and (ii) systems of evolution equations, in which the solutions are smooth but experience large gradients and the interface is specified by a level set of one of the unknowns. Since typically the motion of the free boundary in the first approach is more visual, more qualitative and appears simpler than the second approach, it is desirable to connect or characterize the solutions obtained from the second approach with those obtained from the first approach, so that the underlying interfacial phenomena can be seen more clearly. On the other hand, often in the first approach, the free boundaries will develop singularities at a finite time and, therefore, pose both theoretical and numerical difficulties, whereas in the second approach, the singularities of the interfaces do not pose either analytical or numerical difficulty (since the solutions of the relevant evolution equations exist for all time). Therefore, this approach could provide sufficient information for the possible extensions of the solutions of the free boundary problems beyond any singularities.

In recent years, there has been a great deal of interest in studying interfacial phenomena by using and bridging these two approaches. In this paper, we shall rigorously bridge the dynamics of a phase field model and its sharp interface limits in a general geometric setting. The connection was shown by Caginalp [1, 2, 3] using formal asymptotic analysis. The process of rendering formal matched asymptotics intorigorous theorems is mathematically challenging. For the phase field equations this was first done for the steady state case [4, and references therein], then for travelling-wave solutions [5], and the dynamical problem in the case of one dimension and radial symmetry [6, 7].

The dynamical problem in the absence of symmetry involves complex geometrical issues. In this direction, de Mottoni & Schatzman [8] carried out an error analysis for the difference of the formal inner-outer expansion solution and the true solution of the Allen–Cahn equation [9]

$$\varphi_t^{\varepsilon} - \varDelta \varphi^{\varepsilon} + \varepsilon^{-2} f(\varphi^{\varepsilon}) = 0,$$

where f is the derivative of a symmetric double equal well potential. More recently, Alikakos *et al.* [10] carried out the same estimates for the Cahn–Hilliard equation [11]

$$\varphi_t^{\varepsilon} + \varDelta(\varepsilon \varDelta \varphi^{\varepsilon} - \varepsilon^{-1} f(\varphi^{\varepsilon})) = 0.$$

In this paper, we shall further develop this theory rigorously to verify the connections between the phase field model and several sharp interface models.

Using the scaling introduced earlier [2], the phase field equations for solidification phenomena have the form

$$C_p T_t + \frac{l}{2} \varphi_t = K \Delta T, \qquad \alpha \varepsilon \varphi_t - \varepsilon \Delta \varphi + \varepsilon^{-1} f(\varphi) = \frac{m \ [s]_E}{2\sigma} (T - T_E),$$

where the unknowns T and  $\varphi$  are, respectively, the temperature and the phase parameter, which is scaled so that  $\varphi \cong 1$  represents the liquid phase and  $\varphi \cong -1$  the solid phase. Here  $C_p, l, K, \alpha, \varepsilon, [s]_E, \sigma, T_E$ , are physical parameters representing the specific heat, the latent heat, the thermal conductivity, the relaxation time, the measure of the interface thickness, the entropy difference between phases per volume, the interfacial tension and the equilibrium melting temperature, respectively. Also,  $f(\varphi)$  is the derivative of a doubleequal-well potential  $F(\varphi)$  with global minimum zero at  $\varphi = \pm 1$ , and

$$m = \int_{-1}^{1} (2F(s))^{1/2} ds \tag{1.1}$$

is a constant depending only on the choice of the potential *F*. By introducing a dimensionless variable  $u = \frac{T-T_E}{T_E}$ , dimensionless quantities  $c(\varepsilon) = \frac{C_P T_E}{l}$ ,  $s(\varepsilon) = \frac{m[s]_E}{2\sigma} T_E$ , and dimensionless time and spatial length, the phase field equation can be written in the following dimensionless form:

$$\begin{cases} \varepsilon \alpha(\varepsilon)\varphi_t^{\varepsilon} - \varepsilon \varDelta \varphi^{\varepsilon} + \varepsilon^{-1} f(\varphi^{\varepsilon}) = s(\varepsilon)u^{\varepsilon} & \text{in } \Omega \times (0, T) =: \Omega_T, \\ c(\varepsilon)u_t^{\varepsilon} - \varDelta u^{\varepsilon} = -\varphi_t^{\varepsilon} & \text{in } \Omega \times (0, T) \end{cases}$$
(1.2)

where we have taken the appropriate time-space scale so that the thermal conductivity is scaled to unity.

The phase field model (1.2) has its origins in Landau theory [12], Cahn-Hilliard type equations [11] and the application of mean field theory to critical phenomena [13, 14]. Generally speaking, phase field and mean field theories are based on the idea that each molecule (or 'spin' in magnetic systems) behaves under the influence of all the others which effectively constitute an averaged 'field' of interactions. This is, of course, a tremendous simplification over the evaluation of the sum of all possible states in the partition function needed to obtain the free energy. Due to this great reduction, the validity of mean field theories has been of interest since their first use. The original application and justification

involved the critical temperature (i.e. the point at which gas and liquid become a single phase), and the fact that the associated correlation length (i.e. the mean distance at which molecules become 'aware' of each others' presence) is very large. Thus the use of the phase field concept for ordinary phase transitions, where correlation lengths are small, is not immediately justified by its application for critical phenomena. Furthermore, critical phenomena can rely on universality [13], which states that the critical exponents should be independent of the details of the system.

The situation is quite different for the dynamics of phase boundaries, where quantitative discrepancies generally result in qualitative and quantitative differences, since the global bifurcation diagram depends upon the parameters in the equations. Consequently, the precise identification of the physical parameters is a prerequisite for a meaningful theory. Hence, the convergence of the solutions of the phase field equations to those of the appropriate sharp interface problem (when the latter exists) with precisely the same parameter is of paramount importance for the physical theory and applications. Although the formal analyses have indicated that this is the case, these calculations do not account for the possible interaction of interfacial layers in close proximity. A similar situation prevails for the rigorous proofs in special symmetry (e.g. one dimensional space or radial symmetry). The analysis we present confirms the validity of the limits without any *a priori* assumption on the nature of the interface and the length scales involved in the initial and boundary conditions.

In this paper we shall consider the asymptotic limit, as  $\varepsilon \to 0$ , of the solutions of the phase field equations (1.2). Allowing  $\varepsilon \to 0$  rests on the ansatz that the atomic length scale is not crucial in determining the evolution of the interface, provided that all the other parameters are appropriately preserved.

To describe our result, let  $d^0, \alpha^0, c^0$  be non-negative constants independent of  $\varepsilon$ . With appropriate initial-boundary conditions, let  $(u, \Gamma)$  be the solution of the following free boundary problem:

$$\begin{cases} c^{0}u_{t} - \Delta u = 0 & \text{in } \Omega_{T} \setminus \Gamma, \\ v = \frac{1}{2} \left[ \frac{\partial u}{\partial n} \right]_{\Gamma} & \text{on } \Gamma, \\ u = -d^{0}(\kappa - \alpha^{0}v) & \text{on } \Gamma \end{cases}$$
(1.3)

where  $\left[\frac{\partial u}{\partial n}\right]_{\Gamma}$  is the jump of the normal derivatives of u (from solid to liquid), v is the normal velocity of  $\Gamma$  (positive of motion is directed towards the liquid), and  $\kappa$  is the sum of the principal curvatures of the interface (in space).

Let  $\hat{s}, \hat{\alpha}$ , and  $\hat{c}$  be fixed positive constants. With appropriate initial and boundary conditions for (1.2), we shall consider the following cases:

- (1)  $s(\varepsilon) = \hat{s}\varepsilon^{-1}, \alpha(\varepsilon) = O(1)$ , and  $c(\varepsilon) = \hat{c} + o(1)$ . In this case, we show that the solution  $u^{\varepsilon}$  of (1.2) tends to the solution u of (1.3) with  $c^0 = \hat{c}$  and  $d^0 = 0$ .
- (2)  $s(\varepsilon) = \hat{s}, \alpha(\varepsilon) = \hat{\alpha}$ , and  $c(\varepsilon) = \hat{c}$ . We show that  $u^{\varepsilon}$  tends to the solution of (1.3) with  $c^0 = \hat{c}, \alpha^0 = \hat{\alpha}$ , and  $d^0 = m/(2\hat{s})$  (*m* is as in (1.1)).
- (3)  $s(\varepsilon) = \hat{s}, \alpha(\varepsilon) = O(\varepsilon)$ , and  $c(\varepsilon) = \hat{c}$ . We show that  $u^{\varepsilon}$  tends to the solution of (1.3) with  $\alpha^0 = 0, c^0 = \hat{c}$ , and  $d^0 = m/(2\hat{s})$ .

- (4)  $s(\varepsilon) = \hat{s}, \alpha = \hat{\alpha}$ , and  $c(\varepsilon) = O(\varepsilon)$ . Then  $u^{\varepsilon}$  tends to solution of (1.3) with  $c^0 = 0, \alpha^0 = \hat{\alpha}$ , and  $d^0 = m/(2\hat{s})$ .
- (5)  $s(\varepsilon) = \hat{s}, \alpha(\varepsilon) = O(\varepsilon)$ , and  $c(\varepsilon) = O(\varepsilon)$ . Then  $u^{\varepsilon}$  tends to the solution of (1.3) with  $\alpha^0 = c^0 = 0$  and  $d^0 = m/(2\hat{s})$ .
- (6)  $s(\varepsilon) = O(\varepsilon), \alpha(\varepsilon) = \hat{\alpha}$ , and  $c(\varepsilon) = O(1)$ . We show that the zero level set of  $\varphi^{\varepsilon}$  tends to the solution of mean curvature equation  $\kappa = \hat{\alpha}v$ .

The corresponding dimensional limits are shown in Figure 1.

The difference between limit (1), the classical Stefan problem, and limits (2)–(5) is quite profound, since setting the interface temperature to zero in (1.3) eliminates the only length scale in the problem. Although the capillarity length  $d^0$  is often very small compared to the other length scales in the problem, it is nevertheless very significant as a stabilizing force [15]. The classical Stefan model's neglect of surface tension and surface kinetics can be partially remedied by the imposition of (1.3) with positive  $d^0$  and  $\alpha^0$ . When  $d^0 > 0$ and  $\alpha^0 = 0$ , the equilibrium free boundary condition in (1.3) becomes  $u = -d^0\kappa$ , which is known as the Gibbs–Thomson condition. Although the surface tension and kinetics model (1.3) with  $d^0 > 0$  is superficially similar to the classical Stefan model ((1.3) with  $d^0 = 0$ ) in this respect, the differences are significant, in the sense that there is no length scale in the latter and the temperature must play a dual role by determining phases.

In case (5), the limiting free boundary problem is generally known as the Hele–Shaw model, and involves a fluid between two plates (cf. [16, 17]) separated by a small distance, where the unknown u is a scaled pressure. Note that, when  $\alpha(\varepsilon) = 0, c(\varepsilon) = 0, s(\varepsilon) = 1$ , the phase field equations are simplified to  $\varphi_t^{\varepsilon} + \Delta(\varepsilon \Delta \varphi^{\varepsilon} - \frac{1}{\varepsilon} f(\varphi^{\varepsilon}) = 0$ , which is the Cahn–Hilliard equation [11]. Hence, case (5) is a generalization of the result of [10, 18] for the convergence of the solution of the Cahn–Hilliard equation to the solution of the Hele–Shaw model.

Finally, when  $s(\varepsilon) = 0$ , the two equations in (1.2) decouple, and the first equation becomes the Allen–Cahn equation. Besides the rigorous convergence result of de Mottoni & Schatzman [8], there are other proofs based either on energy estimates (Bronsard & Kohn [19] in the case of radial symmetry), on comparison principles and the construction of super and subsolutions (Chen [20] local in time, Evans *et al.* [21] and Ilmanen [22] global in time). Among them, Evans *et al.* and Ilmanen's global convergence proof considers the possibility of singularities of the mean curvature flow, as a result of the well-developed theory of mean curvature flow [23, 24, 25].

In all the six cases, we have to assume that the corresponding limit free boundary problem has a classical smooth solution. The limit of (1) is the classical Stefan problem and has been very well-studied, both for classical solutions and weak solutions; see, for example, [26, 27, and the references therein]. The limit of (2) is often referred to as the Stefan problem with surface tension and kinetic undercooling, the existence (local in time) of a unique classical solution of which was established by Chen & Reitich [28] and by Radkevitch [29]. For the limit of (3), known as the Stefan problem with Gibbs–Thomson law for equilibrium temperature, the existence (local in time) of a unique classical solution was established by Radkevitch [29], whereas that of global (in time) weak solutions were established by Luckhaus [30] and Almgren & Wang [31]. For the limit of (5), usually known as the Hele–Shaw problem, the existence, local in time, of weak solutions in the





two dimensional case was established by Duchon & Robert [32] (one phase problem) and by Chen [33] (two phase problem); more recently, Chen *et al.* [34] established the existence of a unique classical solution, local in time, for arbitrary space dimensions. For the limit of (6), known as the mean curvature flow, there are well-developed theories; see, for example, Brakke [35], Chen *et al.* [23], Evans & Spruck [24] and Soner [25], and the references therein. In summary, the existence of classical smooth solutions for the limiting free boundary problems in all the cases – except possibly case (4) – has been established.

This paper is organized as follows. We state our main theorems in the next section. In § 3, we give an estimate for the difference between approximate solutions and true solutions, and a review for the eigenvalue estimates established in [36]. In § 4, we construct an approximation solution by using asymptotic expansions similar to, but different in character from, the traditional ones [3]. Finally, we prove the main theorems in § 5.

**Remark 1.1** After this paper was submitted, we learned that Soner [37] had proved weak convergence of solutions of a system of phase field equations to the sharp interface limit in a completely general setting that is applicable even when the classical solution does not exist. The result we present involves strong convergence to unique classical solutions. Neither result implies the other, as the weak limit is more general but may not be unique. Also, we learned that Omel'yanov *et al.* [38] studied the convergence of solutions of a conserved phase field system.

#### 2 Statement of main results

Throughout this paper, we always assume that f is the derivative of a smooth potential F having global minimum 0 only at  $\pm 1$ ; more precisely, we assume that  $f \in C^{\infty}(\mathbb{R}^{1})$  satisfies

$$f(\pm 1) = 0, \quad f'(\pm 1) > 0, \quad \int_{-1}^{u} f(s)ds = \int_{1}^{u} f(s)ds > 0 \quad \forall \ u \in (-1, 1).$$

We denote by *m* the constant in (1.1), where  $F(u) := \int_{-1}^{u} f(s) ds$ .

Also, we always assume that  $\Omega$  is a bounded domain in  $\mathbb{R}^N$   $(N \ge 1)$  with smooth boundary  $\partial \Omega$  and  $\Gamma_0^0$  is an N-1 dimensional manifold which is the boundary of an open set  $\Omega_0^- \subset \subset \Omega$ . We define  $\Omega_0^+ = \Omega \setminus (\Gamma_0^0 \cup \Omega_0^-)$ . In this paper, we shall prove the following two theorems.

**Theorem 2.1** Let  $c^0$ ,  $d^0$ ,  $\alpha^0$  be fixed positive constants. Let  $g \in C^{\infty}(\overline{\Omega_0^{\pm}} \times [0, T])$  be any given function satisfying certain compatibility conditions, with  $\Gamma_0^0$  such that there is a smooth solution  $(u, \Gamma^0)$  ( $\Gamma^0 = \bigcup_{0 \le t \le T} (\Gamma_t^0 \times \{t\})$ ) to the free boundary problem (1.2) with initial-boundary condition

$$u(x,t) = g \quad on \quad \partial_p \Omega_T \equiv (\Omega \times \{0\}) \cup (\partial \Omega \times [0,T]). \tag{2.1}$$

(Note that the expression of  $\Gamma$  implies the initial condition  $\Gamma \cap \{t = 0\} = \Gamma_0^0 \times \{0\}$ .) Assume that  $\Gamma \subset \Omega \times [0, T]$ . Then there exists a family of functions  $\{g_0^{\varepsilon}, \varphi_0^{\varepsilon}\}_{0 \le \varepsilon \le 1}$  defined on  $\partial_p \Omega_T$ 

such that the solution of the phase field equations

$$\begin{aligned} \varepsilon \alpha(\varepsilon)\varphi_t^{\varepsilon} - \varepsilon \Delta \varphi^{\varepsilon} + \varepsilon^{-1} f(\varphi^{\varepsilon}) &= s(\varepsilon)u^{\varepsilon} & \text{ in } \Omega_T, \\ c(\varepsilon)u_t^{\varepsilon} - \Delta u^{\varepsilon} &= -(\varphi^{\varepsilon})_t & \text{ in } \Omega_T, \\ \varphi^{\varepsilon} &= \varphi_0^{\varepsilon}, \quad u^{\varepsilon} &= g_0^{\varepsilon} & \text{ on } \partial_p \Omega_T, \end{aligned}$$
(2.2)

with

$$\alpha(\varepsilon) = \alpha^0, \quad s(\varepsilon) = \frac{m}{2d_0}, \quad c(\varepsilon) = c^0$$

has the property that, as  $\varepsilon \to 0$ ,

$$\|u^{\varepsilon} - u\|_{C^{0}(\bar{\Omega}_{T})} \longrightarrow 0,$$
  
 $\varphi^{\varepsilon} \longrightarrow \pm 1$  uniformly in any compact subset of  $\bar{\Omega}_{T} \setminus \Gamma^{0}.$ 

**Theorem 2.2** Theorem 2.1 remains valid if one of the following revisions is made:

(1) The Dirichlet boundary conditions for u and  $u^{\varepsilon}$  are replaced by the mixed boundary conditions

$$\begin{cases} u = u^{\varepsilon} = g_{0}^{+} & \text{on } S \times (0, T), \\ \frac{\partial u}{\partial n} + \beta u = \frac{\partial u^{\varepsilon}}{\partial n} + \beta u^{\varepsilon} = \bar{g}_{0} & \text{on } (\partial \Omega \setminus S) \times (0, T) \end{cases}$$
(2.3)

where S is a smooth open part of  $\partial \Omega$ , and  $\beta$  and  $\bar{g}_0$  are smooth functions on  $\partial \Omega \times [0, T]$ ;

- (2)  $d^0 = 0$  and  $s(\varepsilon) = \varepsilon^{-1/2}$ ;
- (3)  $\alpha^0 = 0$  and  $\alpha(\varepsilon) = \varepsilon^k$  for any integer  $k \ge 1$ ;
- (4)  $c^0 = 0$  and  $c(\varepsilon) = \varepsilon^k$  for any integer  $k \ge 1$ ;
- (5)  $c^0 = \alpha^0 = 0$ ,  $c(\varepsilon) = \varepsilon^k$ ,  $\alpha(\varepsilon) = \varepsilon^m$  for any integers  $k, m \ge 1$ ;
- (6)  $s(\varepsilon) = \varepsilon^k$  for some integer  $k \ge 1$  and replace the equilibrium condition  $u = -d^0(\kappa_{\Gamma} \alpha^0 v)$ by  $\kappa_{\Gamma} = \alpha^0 v$ .

In addition, in cases (2)–(6), the Dirichlet boundary conditions for u and  $u^{\varepsilon}$  can be replaced by boundary conditions (2.3).

# Remark 2.3

(1) If we let d(x) be the signed distance to the manifold  $\Gamma_0^0$ , then  $g_{\varepsilon}(x,0)$  in Theorem 2.1 can be taken as

$$g_{\varepsilon}(x,0) = \zeta \left( \delta^{-1} d(x) \right) \left[ \frac{1}{2} (g_0^+ + g_0^-) + \frac{1}{2} (g_0^+ - g_0^-) \theta_0 \left( \varepsilon^{-1} d(x) \right) \right] \\ + \left[ 1 - \zeta \left( \delta^{-1} d(x) \right) \right] \left[ g_0^+ \chi_{\{d>0\}} + g_0^- \chi_{\{d<0\}} \right]$$

where  $\delta$  is any fixed small constant independent of  $\varepsilon$ ,  $\chi_A$  is the characteristic function of *A*,  $\zeta(s)$  is a cut-off function satisfying

$$\zeta(s) = 0 \quad \text{if } |s| \ge 1, \quad \zeta(s) = 1 \quad \text{if } |s| \le 1/2, \quad s\zeta'(s) \ge 0 \quad \text{in } \mathbb{R}^1, \tag{2.4}$$

and  $\theta_0(z)$  is the unique solution to

$$-\theta_0'' + f(\theta_0) = 0 \text{ in } \mathbf{R}^1, \quad \theta_0(\pm \infty) = \pm 1, \quad \theta_0(0) = 0.$$
(2.5)

In particular, away from a  $\delta$ -distance of the initial interface  $\Gamma_0^0$ , one has  $g^{\varepsilon}(x,0) = g(x,0)$ . Since  $\nabla_x g(x,0)$  experiences a jump across  $\Gamma_0^0$ , it is necessary (for the simplicity of analysis) to take a specific profile  $g^{\varepsilon}(x,0)$  near the initial interface  $\Gamma_0^0$ , as shown.

- (2) Since we assume that  $\Gamma \subset \Omega \times [0, T]$ , as we shall see in our proof, we can take  $g^{\varepsilon} = g$  on  $\partial \Omega \times [0, T]$ .
- (3) The function  $\varphi_0^{\varepsilon}(x,0)$  in Theorem 2.1 is complicated, but has the structure

$$\varphi_0^{\varepsilon}(x,0) = \zeta \left( \delta^{-1} d(x) \right) \theta_0 \left( \varepsilon^{-1} d(x) \right) + \left[ 1 - \zeta \left( \delta^{-1} d(x) \right) \right] \left[ \chi_{\{d>0\}} - \chi_{\{d<0\}} \right] + O(\varepsilon).$$

In particular, away from the initial interface  $\Gamma_0^0$ ,  $\varphi^{\varepsilon}(x,0)$  is close to  $\pm 1$  in  $\Omega_0^{\pm}$ .

If one insists on assigning an 'arbitrary' initial data for  $\varphi^{\varepsilon}$ , then generation of the interface will take place in a very short time, and we expect that our analysis will apply thereafter.

- (4) In the statement of our theorems, the boundary value of φ<sup>ε</sup> on ∂Ω × [0, T] is not arbitrarily given, but depends upon g, the boundary value of u. However, if one imposes 'general' (but compatible with phase) boundary data such as φ<sup>ε</sup> = 1 or <sup>∂</sup>/<sub>∂n</sub>φ<sup>ε</sup> = 0 on∂Ω × [0, T], then our assertions of the theorems remain true, but in our proof we need a boundary layer expansion similar to that in [10]. As a compromise between simplicity and completeness, we shall briefly describe the boundary layer expansions.
- (5) For the second case (i.e. the case where the limit is the classical Stefan problem (u = 0 on the interface), the expansion is obtained in terms of  $\hat{\varepsilon} := \varepsilon^{1/2}$ , but we do not present these expansions in our current paper. When the potential f is of double obstacle type, i.e.

$$\begin{split} f(\varphi) &= \varphi \quad \text{if} \quad \varphi \in (-1,1), \qquad f(\varphi) = \pm \infty \quad \text{if} \quad \pm \varphi > 1, \\ f(1) &= [-1,\infty), \quad f(-1) = (-\infty,1], \end{split}$$

Blowey & Elliott [39] proved that the limit of the phase field model is the weak solution of the classical Stefan problem, global in time  $t \in (0, \infty)$ . The method is based on an energy estimate, and is totally different from what we present in this paper.

Theorems 2.1 and 2.2 will be proved in § 5. The basic idea is to construct approximation solutions by matched asymptotics (which will be done in § 4), to estimate the upper bound of the eigenvalues of the linearized operator of the phase field equations at the approximated solutions (which is done in [36]), and then to estimate the difference between the true solutions and the approximate ones (which will be done in the next section). Though the approximation obtained by conventional asymptotic expansion techniques [8, 3] may be used in our situation, we prefer to use a new asymptotic expansion technique developed in [10]. For more detailed discussion on these two asymptotic expansions, see [10] and § 4 below.

## **3** Error estimates

It is convenient to use the variable  $\varphi$  and  $v = \int_0^t u$ , so that the phase field equations in (1.1) can be written as

$$\begin{cases} \epsilon \alpha(\epsilon) \varphi_t^{\epsilon} - \epsilon \Delta \varphi^{\epsilon} + \epsilon^{-1} f(\varphi^{\epsilon}) = s(\epsilon) v_t^{\epsilon} & \text{in } \Omega_T, \\ c(\epsilon) v_t^{\epsilon} = \Delta v^{\epsilon} - \varphi^{\epsilon} + e_0^{\epsilon} & \text{in } \Omega_T \end{cases}$$
(3.1)

where  $e_0^{\varepsilon} = \varphi^{\varepsilon}(\cdot, 0) + c(\varepsilon)u^{\varepsilon}(\cdot, 0)$  is the initial enthalpy.

In this section,  $\|\cdot\|_{p,Q}$  represents the  $L^p(Q)$  norm.

**Theorem 3.1** Assume that  $f \in C^{\infty}(\mathbb{R}^1)$  satisfies, for some positive  $C_0$ ,  $sf''(s) \ge 0$  for all  $s \in (-\infty, -C_0] \cup [C_0, \infty)$ , and that  $s(\varepsilon) \ge 0, c(\varepsilon) \ge 0, \alpha(\varepsilon) \in (0, \alpha^0]$  for all  $\varepsilon \in (0, 1]$ . Define  $K_1 = \frac{19}{5}, K_2 = 5, K_3 = 7, K_4 = 11$ , and  $K_n = \frac{n^2+6n+4}{4}$  for all  $n \ge 5$ . Let  $(\varphi^{\varepsilon}, v^{\varepsilon})$  be a  $C^2(\bar{\Omega}_T)$  solution of (3.1) and  $(\varphi^{\varepsilon}_A, v^{\varepsilon}_A)$  be a  $k^{th}$  order  $(k > K_N)$  approximation of (3.1) in the following sense:

(i)  $|\varphi_A^{\varepsilon}|$  is bounded by  $C_0$ ;

(ii)  $(\varphi_A^{\varepsilon}, v_A^{\varepsilon})$  satisfies exactly the same initial and boundary condition as  $(\varphi^{\varepsilon}, v^{\varepsilon})$ , i.e.

$$\begin{aligned} (\varphi_A^{\varepsilon} - \varphi^{\varepsilon}) \frac{\partial}{\partial n} (\varphi_A^{\varepsilon} - \varphi^{\varepsilon}) &= (v_A^{\varepsilon} - v^{\varepsilon}) \frac{\partial}{\partial n} (v_A^{\varepsilon} - v^{\varepsilon}) = 0 \qquad on \quad \partial \Omega_T, \\ \varphi_A^{\varepsilon} - \varphi^{\varepsilon} &= v_A^{\varepsilon} - v^{\varepsilon} = 0 \qquad on \quad \bar{\Omega} \times \{0\}; \end{aligned}$$

(iii)  $(\varphi_A^{\varepsilon}, v_A^{\varepsilon})$  satisfies the approximation equations

$$\begin{cases} \varepsilon \alpha(\varepsilon) \varphi_{At}^{\varepsilon} - \varepsilon \Delta \varphi_{A}^{\varepsilon} + \varepsilon^{-1} f(\varphi_{A}^{\varepsilon}) = s(\varepsilon) v_{At}^{\varepsilon} + \delta_{A}^{\varepsilon} & \text{in } \Omega_{T}, \\ c(\varepsilon) v_{A}^{\varepsilon} = \Delta v_{A}^{\varepsilon} - \varphi_{A}^{\varepsilon} + e_{0}^{\varepsilon} & \text{in } \Omega_{T}, \end{cases}$$
(3.2)

where  $\delta_A^{\varepsilon}$  is a function which satisfies, for  $p = \min\{3, 2 + \frac{4}{N}\}$  and some  $k > K_N$ ,

$$\|\delta_A^{\varepsilon}\|_{\frac{p}{p-1},\Omega_T} \leq (\alpha(\varepsilon))^{\frac{p-1}{p-2}} \varepsilon^k;$$

(iv) For each  $t \in [0, T]$ ,  $\varphi^{\varepsilon}_{A}(\cdot, t)$  satisfies the spectral condition

$$\inf_{\boldsymbol{\psi}\in H^{1}(\Omega), \ \boldsymbol{w}\in H^{2}(\Omega)} \frac{\int_{\Omega} \{\varepsilon |\nabla \boldsymbol{\psi}|^{2} + \varepsilon^{-1} f'(\boldsymbol{\varphi}_{A}^{\varepsilon}(\cdot,t)) \boldsymbol{\psi}^{2} + \frac{s(\varepsilon)}{c(\varepsilon)} |\Delta \boldsymbol{w} - \boldsymbol{\psi}|^{2} \}}{\int_{\Omega} \{\varepsilon \alpha(\varepsilon) \boldsymbol{\psi}^{2} + s(\varepsilon) |\nabla \boldsymbol{w}|^{2} \}} \ge -C_{0}$$

Here in the case  $c(\varepsilon) = 0$ , one assumes that  $\psi = \Delta w$  and removes the term  $\frac{s(\varepsilon)}{c(\varepsilon)} |\Delta w - \psi|^2$ . Then there exists a positive constant  $\varepsilon_0$  which depends only upon  $\Omega$ , T,  $C_0$ , k, and  $||f||_{C^2([-2C_0, 2C_0])}$ such that, if  $\varepsilon \in (0, \varepsilon_0]$ , then

$$\|\varphi^{\varepsilon} - \varphi^{\varepsilon}_{A}\|_{p,\Omega_{T}} \leq (\alpha(\varepsilon))^{\frac{1}{p-2}} \varepsilon^{\frac{k+1}{p-1}}.$$
(3.3)

**Proof** Set  $\psi = \varphi^{\varepsilon} - \varphi^{\varepsilon}_A$  and  $w = v^{\varepsilon} - v^{\varepsilon}_A$ . Then  $(\psi, w)$  satisfies

$$\begin{cases} \varepsilon \alpha(\varepsilon) \psi_t - \varepsilon \varDelta \psi + \varepsilon^{-1} f'(\varphi_A^{\varepsilon}) \psi + \varepsilon^{-1} N(\varphi_A^{\varepsilon}, \psi) = s(\varepsilon) w_t + \delta_A^{\varepsilon} & \text{in } \Omega_T, \\ c(\varepsilon) w_t = \varDelta w - \psi & \text{in } \Omega_T \end{cases}$$
(3.4)

where  $N(\varphi_A^{\varepsilon}, \psi) = f(\varphi_A^{\varepsilon} + \psi) - f(\varphi_A^{\varepsilon}) - f'(\varphi_A^{\varepsilon})\psi$ . Since  $sf''(s) \ge 0$  in  $(-\infty, -C_0] \cup [C_0, \infty)$  and

 $\varphi_A^{\varepsilon}$  is bounded by  $C_0$ ,  $N(\varphi_A^{\varepsilon}, \psi)\psi \ge -C|\psi|^p$  for every  $p \in [2, 3]$  and every  $\psi \in (-\infty, \infty)$ , where C is a positive constant depending only on  $C_0$  and  $||f||_{C^2([-2C_0, 2C_0])}$  (cf. [10, Lemma 2.3]).

Replacing  $w_t$  in (3.4a) by the right-hand side of (3.4b) and multiplying the resulting equation by  $\psi$ , adding (3.4b) multiplied by  $-s(\varepsilon)\Delta w/c(\varepsilon)$ , integrating by parts over  $\Omega$ , and using the boundary conditions  $\psi \frac{\partial \psi}{\partial n} = w \frac{\partial w}{\partial n} = 0$  on  $\partial \Omega \times [0, T]$ , we obtain after a routine calculation

$$\frac{1}{2}\frac{d}{dt}\int_{\Omega} \left[\varepsilon\alpha(\varepsilon)\psi^{2} + s(\varepsilon)|\nabla w|^{2}\right] + \int_{\Omega} \left[\varepsilon|\nabla\psi|^{2} + \varepsilon^{-1}f'(\varphi_{A}^{\varepsilon})\psi^{2} + \frac{s(\varepsilon)}{c(\varepsilon)}|\Delta w - \psi|^{2}\right] \\
= \int_{\Omega} \left[\delta_{A}^{\varepsilon}\psi - \varepsilon^{-1}N(\varphi_{A}^{\varepsilon},\psi)\psi\right] \leqslant C\int_{\Omega} \left[|\delta_{A}^{\varepsilon}\psi| + \varepsilon^{-1}|\psi|^{p}\right], \ \forall t \in (0,T].$$
(3.5)

We note that if  $c(\varepsilon) = 0$ , then one has  $\Delta w = \psi$  so that the above identity remains true if one removes the term involving  $|\Delta w - \psi|$ .

Using the spectral condition and Gronwall's inequality, we then obtain, for all  $t \in (0, T]$ ,

$$\sup_{0 \le \tau \le T} \int_{\Omega} \left[ \varepsilon \alpha(\varepsilon) \psi^2(\cdot, \tau) + s(\varepsilon) |\nabla w(\cdot, \tau)|^2 \right] \le C(T) \iint_{\Omega_T} \left[ \varepsilon^{-1} |\psi|^p + |\delta_A^{\varepsilon} \psi| \right] \equiv C(T) I(T),$$

where  $I(t) \equiv \iint_{\Omega_t} [\varepsilon^{-1} |\psi|^p + |\delta_A^{\varepsilon} \psi|].$ 

Integrating (3.5) from 0 to t, we also obtain

$$\iint_{\Omega_t} \varepsilon |\nabla \psi|^2 \leqslant -\varepsilon^{-1} \iint_{\Omega_t} f'(\psi_A^{\varepsilon}) \psi^2 + CI(t) \leqslant C \left[ \varepsilon^{-1} \|\psi\|_{2,\Omega_t}^2 + I(t) \right]$$

since  $\varphi_A^{\varepsilon}$  is bounded by  $C_0$  and f is smooth. Recall the Sobolev Imbedding Theorem [40, p. 74]: for every  $p \in [2, 2 + \frac{4}{N}]$  and  $t \in (0, T]$ ,

$$\|\psi\|_{p,\Omega_t}^2 = C(\Omega,T) \Big( \sup_{0 \leqslant \tau \leqslant T} \|\psi(\cdot,\tau\|_{2,\Omega}^2)^{1-\theta} \Big( \|\nabla\psi\|_{2,\Omega_t}^2 + \|\psi\|_{2,\Omega_t}^2 \Big)^{\theta}$$

where  $\theta = \frac{N}{2} - \frac{N}{p}$  and  $C(\Omega, T)$  depends only upon  $\Omega$  and T. The last two estimates then yield

$$\|\psi\|_{p,\Omega_t}^2 \leqslant C \left[\varepsilon^{-1} \alpha(\varepsilon)^{-1} I(t)\right]^{1-\theta} \left[\varepsilon^{-2} \|\psi\|_{p,\Omega_t}^2 + \varepsilon^{-1} I(t) + \|\psi\|_{p,\Omega_t}^2\right]^{\theta}.$$
(3.6)

Define  $T_{\varepsilon} = \sup\{t \leq T ; \|\psi\|_{p,\Omega_t} \leq (\alpha(\varepsilon))^{\frac{1}{p-2}} \varepsilon^{\frac{k+1}{p-1}}\}$ . Using the assumption on  $\delta_A^{\varepsilon}$ , we have that  $I(T_{\varepsilon}) \leq \varepsilon^{-1} \|\psi\|_{p,\Omega_{T_{\varepsilon}}}^{p} + \|\delta_A^{\varepsilon}\|_{\frac{p}{p-1},\Omega_{T_{\varepsilon}}}^{p} \|\psi\|_{p,\Omega_{T_{\varepsilon}}} \leq 2(\alpha(\varepsilon))^{\frac{p}{p-2}} \varepsilon^{\frac{kp+1}{p-1}}$ . Consequently,  $\varepsilon^{-2} \|\psi\|_{p,\Omega_{T_{\varepsilon}}}^{2} + \varepsilon^{-1}I(t) + \|\psi\|_{p,\Omega_{T_{\varepsilon}}}^{2} \leq C\alpha(\varepsilon)^{\frac{2}{p-2}} \varepsilon^{\frac{2(k+1)}{p-1}-2}$ , since  $2 , and <math>0 < \varepsilon \leq 1$ . Substituting these estimates into (3.6) then yields

$$\begin{aligned} \|\psi\|_{p,\Omega_t}^2 &\leqslant C \left[ \varepsilon^{-1} \alpha(\varepsilon)^{-1} \alpha(\varepsilon)^{\frac{p}{p-2}} \varepsilon^{\frac{kp+1}{p-1}} \right]^{1-\theta} \left[ \alpha(\varepsilon)^{\frac{2}{p-2}} \varepsilon^{\frac{2(k+1)}{p-1}-2} \right]^{\theta} \\ &= C \left[ \alpha(\varepsilon)^{\frac{1}{p-2}} \varepsilon^{\frac{k+1}{p-1}} \right]^2 \varepsilon^{\frac{p-2}{p-1}(1-\theta)[k-\frac{p+(p-2)\theta}{(p-2)(1-\theta)}]}. \end{aligned}$$

Since  $\theta = \frac{N}{2} - \frac{N}{p}$  and  $p = \min\{3, 2 + \frac{4}{N}\}$ , by the definition of  $K_N$ ,  $\frac{p+(p-2)\theta}{(p-2)(1-\theta)} = K_N$ . It then follows that  $\|\psi\|_{p,\Omega_t}^2 \leq C[\alpha(\varepsilon)^{\frac{1}{p-2}}\varepsilon^{\frac{k+1}{p-1}}]^2\varepsilon^{\frac{p-2}{p-1}(1-\theta)(k-K_N)} \leq \frac{1}{2}(\alpha(\varepsilon)^{\frac{1}{p-2}}\varepsilon^{\frac{k+1}{p-1}})^2$  if  $\varepsilon$  is sufficiently small. Hence by the definition of  $T_{\varepsilon}$ , we must have  $T = T_{\varepsilon}$ . This completes the proof of the theorem.

## Remark 3.2

- (1) With the fundamental estimate (3.3), one can use interpolation and a bootstrap argument for the regularity (depending on  $\varepsilon$ ) of the solution of (3.2) to establish estimates for  $\|\varphi^{\varepsilon} \varphi^{\varepsilon}_{A}\|_{C^{m}(\bar{\Omega}_{T})}$  and  $\|v^{\varepsilon} v^{\varepsilon}_{A}\|_{C^{m}(\bar{\Omega}_{T})}$ , provided that  $\|\delta^{\varepsilon}_{A}\|_{C^{m}(\bar{\Omega}_{T})}$  is sufficiently small. For more details, see [10, Remark 2.1].
- (2) From the proof of the theorem, one sees that adding small perturbations to the initial and boundary data for  $\varphi^{\varepsilon} \varphi^{\varepsilon}_{A}$  and  $v^{\varepsilon} v^{\varepsilon}_{A}$  will not alter the conclusion of the theorem.
- (3) Theorem 2.2 allows for both Dirichlet and Neumann boundary conditions. From the proof (in particular the derivation of (3.5)), one can verify that it also holds for mixed boundary conditions.
- (4) In Theorem 3.1, we have to assume that α(ε) > 0. Part of the reason that we cannot let α(ε) = 0 is that if α(ε) = 0, then the equation for φ<sup>ε</sup> is elliptic and may not have a unique solution. For the special case α(ε) = c(ε) = 0, namely, the Cahn-Hilliard equation, see [10].

There are two essential requirements in applying Theorem 3.1. The first is the construction of asymptotic expansion for the solution up to very high order, and the second is the verification of the spectral condition. The former will be discussed in detail in subsequent sections, whereas the latter has already been established by Chen [36]. Here we just cite the result in Chen [36] for our application.

Let  $\gamma$  be an N-1 dimensional compact manifold embedded in  $\Omega \subset \mathbb{R}^N$ , and let d(x) be the signed distance from x to  $\gamma$ . Let  $\delta$  be a small positive constant such that  $\gamma(\delta) = \{x \in \mathbb{R}^N ; |d(x)| < \delta\}$  is contained in  $\Omega$ , and that S(x), the projection from x to  $\gamma$  along the normal of  $\Gamma$ , is well-defined in  $\gamma(\delta)$ . Set  $\|\gamma\|_3 \equiv \delta^{-1} + \|d\|_{C^3(\gamma(\delta))}$ .

Let  $\theta_0(z)$  be the unique solution to (2.5). Since f is the derivative of a double-equal-well potential with its global minimum 0 at  $\pm 1$ ,  $\theta_0$  is well-defined, smooth, and monotonic in z. (In case  $f = 2\theta(\theta^2 - 1), \theta_0(z) = \tanh z$ .)

Let  $\theta_1(z)$  be a bounded function in  $\mathbb{R}^1$  such that

$$\int_{-\infty}^{\infty} f''(\theta_0)(\theta'_0)^2 \theta_1 dz = 0.$$
(3.7)

In our applications, one can verify that the above 'orthogonality' condition is satisfied (see  $[10, \S6]$  for a proof).

Let  $p^{\varepsilon}(x), q^{\varepsilon}(x), \varphi^{\varepsilon}_{+}(x)$  be  $C^{1}$  functions such that

$$\begin{cases} |p^{\varepsilon}(x)| + \frac{|q^{\varepsilon}(x)|}{1 + \varepsilon^{-1}|d(x)|} + \varepsilon |\nabla^{\gamma} p^{\varepsilon}(x)| + \varepsilon^{2} |\nabla^{\gamma} q^{\varepsilon}(x)| \leq C_{0} & \text{in } \gamma(\delta), \\ f'(\varphi^{\varepsilon}_{\pm}) \geq 1/C_{0} & \text{in } \Omega \end{cases}$$
(3.8)

where  $\nabla^{\gamma} \equiv \nabla - \nabla d(\nabla d \cdot \nabla)$  is the tangential derivative along  $\gamma$ .

Let  $\zeta(\cdot) \in C_0^{\infty}(\mathbb{R}^1)$  be a cut-off function satisfying (2.4). We construct  $\varphi^{\varepsilon}(x)$  as follows:

$$\varphi^{\varepsilon}(x) = \zeta \left( \delta^{-1} d(x) \right) \left[ \theta_0 \left( \varepsilon^{-1} d(x) \right) + \varepsilon p^{\varepsilon}(S(x)) \theta_1 \left( \varepsilon^{-1} d(x) \right) + \varepsilon^2 q^{\varepsilon}(x) \right] + \left[ 1 - \zeta (\delta^{-1} d(x)) \right] \left[ \varphi^{\varepsilon}_+(x) \chi_{\{d(x) > 0\}} + \varphi^{\varepsilon}_-(x) \chi_{\{d(x) < 0\}} \right].$$
(3.9)

**Proposition 3.1** Let  $\varphi^{\varepsilon}(x)$  be constructed as in (3.9) and (3.7), (3.8) hold. Then there exists a positive constant  $\hat{C}$  which depends only upon  $\|\gamma\|_3, \theta_0, \theta_1, f, C_0, N$  and  $\Omega$  such that, for every  $\varepsilon \in (0, 1], \psi \in H^1(\Omega), w \in H^2(\Omega)$ ,

$$\int_{\Omega} \left[ \varepsilon |\nabla \psi|^2 + \varepsilon^{-1} f'(\varphi^{\varepsilon}) \psi^2 + \frac{s(\varepsilon)}{c(\varepsilon)} |\Delta w - \psi|^2 \right] > -\hat{C} \int_{\Omega} \left[ \varepsilon \alpha(\varepsilon) \psi^2 + s(\varepsilon) |\nabla w|^2 \right]$$

provided that one of the following conditions holds:

- (1)  $\alpha(\varepsilon) \ge \frac{1}{C_0}$ ,  $s(\varepsilon) \ge 0$ ,  $c(\varepsilon) \ge 0$ ,
- (2)  $\alpha(\varepsilon) \ge 0$ ,  $s(\varepsilon) \ge 1/C_0$ ,  $\frac{s(\varepsilon)}{c(\varepsilon)} \ge 1/C_0$ .

**Proof** In case (1), i.e.  $\alpha(\varepsilon) \ge \frac{1}{C_0}$ , the assertion follows from the following stronger inequality, which was originally established by de Mottoni & Schatzman [8] for the special case when f is anti-symmetric, e.g.  $f(\phi) = \phi^3 - \phi$ , and later by Chen [36] with a slightly simpler proof and for more general f: For every  $\psi \in H^1(\Omega)$ ,

$$\int_{\Omega} \left[ \varepsilon |\nabla \psi|^2 + \varepsilon^{-1} f'(\varphi^{\varepsilon}) \psi^2 \right] \ge -C_1 \varepsilon \int_{\Omega} \psi^2.$$

In case (2), i.e.  $s(\varepsilon) \ge \frac{1}{C_0}, \frac{s(\varepsilon)}{c(\varepsilon)} \ge \frac{1}{C_0}$ , the assertion follows immediately from the following inequality established by Chen [36]: for every  $\mu \in (0, \infty]$ ,  $\varepsilon \in (0, 1]$ ,  $\psi \in H^1(\Omega)$ , and  $w \in H^2(\Omega)$ ,

$$\int_{\Omega} [\varepsilon |\nabla \psi|^2 + \varepsilon^{-1} f'(\varphi^{\varepsilon}) \psi^2 + \mu |\Delta w - \psi|^2] \ge -\bar{C}(\mu) \min\left\{\varepsilon \int_{\Omega} \psi^2, \int_{\Omega} |\nabla w|^2\right\}$$
(3.10)

where  $C_1$  is a constant and  $C(\mu)$  is a monotone decreasing function of  $\mu$  defined on  $(0, \infty]$ .

It is easy to check that in all the six cases in Theorems 2.1 and 2.2,  $s(\varepsilon)$ ,  $c(\varepsilon)$  and  $\alpha(\varepsilon)$  satisfy one of the conditions in Proposition 3.1, so that as long as  $\varphi_A^{\varepsilon}$  has the properties (3.7), (3.8) and (3.9), the spectral condition required by Theorem 3.1 is satisfied. In the sequel, we shall construct approximate solutions ( $\varphi_A^{\varepsilon}, v_A^{\varepsilon}$ ) such that for each  $t \in [0, T]$ ,  $\varphi_A^{\varepsilon}(\cdot, t)$ satisfies (3.7), (3.8) and (3.9).

## 4 Construction of approximate solutions

In this section, we shall use matched asymptotic expansions to construct approximate solutions, up to an arbitrary higher order k in the sense of Theorem 3.1 and in the case

$$\alpha(\varepsilon) = \alpha^0 = 1, \qquad s(\varepsilon) = s^0, \qquad c(\varepsilon) = c^0$$

where  $\alpha^0$ ,  $s^0$ , and  $c^0$  are positive constants. This corresponds to the distinguished limit of the surface tension and kinetic model (1.3) with  $d^0 > 0$  and  $\alpha^0 > 0$ . The other limits stated in Theorem 2.2 are constructed in a similar manner and are omitted. We consider here only Dirichlet boundary conditions. Other types of boundary conditions can be discussed similarly.

A matched asymptotic expansion has three components: outer expansion, inner expansion and matching; see, for example, Wasow [41].

The outer expansion is used in the 'bulk' regions, i.e. regions of 'pure' solid (denoted by -) and 'pure' liquid region (denoted by +). Just by inserting  $\varphi^{\varepsilon} = \pm 1 + O(\varepsilon) \sim \pm 1 + \varepsilon \sum_{i \ge 0} \varepsilon^i \varphi^i_{\pm}$ ,  $u^{\varepsilon} = O(1) = \sum_{i \ge 0} \varepsilon^i u^i_{\pm}$  into the phase field equations, one can consecutively obtain equations for  $(\varphi^i_{\pm}, u^i_{\pm})$ . These equations, which we call outer expansion equations, can be uniquely solved provided that the regions  $Q^i_{\pm}$ , where the equations are to be solved and certain supplementary conditions such as initial boundary conditions are given.

In our approach, all  $(\varphi_{\pm}^{i}.u_{\pm}^{i})$  for  $i \ge 0$  are independent of  $\varepsilon$  and are defined in an  $\varepsilon$  and i independent domain. More precisely, we solve the outer equations, for each order  $i \ge 0$ , in the domain  $Q_{\pm}^{0}$ , the leading order approximation of the liquid/solid region. Nevertheless, one has to realize that the outer expansion and the outer expansion equations could only be valid in  $Q_{\pm}^{\pm}$  minus a thin neighbourhood of the interface  $\Gamma^{\varepsilon} := \{(x, t) \mid \varphi^{\varepsilon}(x, t) = 0\}.$ 

The inner expansion is used in a thin neighbourhood of the interface  $\Gamma^{\varepsilon}$ . As  $\varphi^{\varepsilon}$  has a large gradient (of order  $\varepsilon^{-1}$ ) in the direction normal to the interface  $\Gamma_t^{\varepsilon} := \{x \mid \varphi^{\varepsilon}(x,t) = 0\},\$ one uses the method of stretched coordinates, writing  $Z := d^{\varepsilon}(x,t)/\varepsilon$  where  $d^{\varepsilon}(x,t)$  is the signed distance to the interface  $\Gamma_t^{\varepsilon}$ . Classically, for example, in the paper by Caginalp [3], a change of variable  $(x,t) \to (S,Z,t) \in \mathcal{M} \times \mathbb{R} \times \mathbb{R}^+$  is used in the inner expansion. Here  $\mathcal{M} \subset \Omega$  is a reference Riemanian N-1 manifold differomorphic to  $\Gamma_t^{\varepsilon}$ . (We are working in local time and in the classical limit, so no topological changes in  $\Gamma_t^{\varepsilon}$  are considered). The map  $x \to S$  is usually the normal projection onto  $\mathcal{M}$ . Under this change of variables and under the assumption that  $\varphi^{\varepsilon} \sim \theta_0(Z) + \varepsilon \sum_{i \ge 0} \varepsilon^i \varphi_i(S, Z, t)$  ( $\theta_0$  is defined in (2.5)),  $u^{\varepsilon} \sim \sum_{i \ge 0} \varepsilon^{i} u_{i}(S, Z, t)$ , one can obtain inner expansion equations for  $(\varphi_{i}, u_{i})$ . Notice that, since the change of variable  $x \to Z$  depends upon  $\varepsilon$ , an  $\varepsilon$ -power expansion for the function  $d^{\varepsilon}(x,t)$  is needed.<sup>1</sup> Also, a solvability condition for each order of inner expansion equation provides an equation for the corresponding order of expansion for  $d^{\varepsilon}$ . The inner equations, usually ordinary differential equations in the Z variable (whereas S is only treated as a parameter), can be solved uniquely, provided that compatible conditions at  $Z = \pm \infty$  are given. (Our inner expansion, as explained later, is different from this approach.)

The matching is used to obtain the supplementary conditions needed by the outer and inner expansion equations, in such a way that both inner and outer expansions are consistent. For this, it is sufficient to ensure that the outer expansion and inner expansion matches in their overlap domain. A classical way to proceed with this would be as follows. Let  $x = X^{\varepsilon}(S, Z, t)$  be the inverse map of  $x \to (S, Z)$  used in inner expansion. Suppose, for simplicity, we take  $\mathscr{M}$  to be  $\Gamma_t^0$ , the leading order approximation of the interface  $\Gamma_t^{\varepsilon}$ , which is also the (t cross-section) of the intersection of the boundary of  $Q_-^0$  and  $Q_+^0$ . Then, the definition of Z gives the expansion  $X^{\varepsilon} = X_0(S,t) + \sum_{i \ge 1} \varepsilon^i X_i(S,Z,t)$  where  $X^0(S,t) \in \Gamma_t^0$  is independent of Z and  $X_i$  is independent of  $\varepsilon$ . It then follows that we can

<sup>&</sup>lt;sup>1</sup> As pointed out by the referee, one can replace  $d^{\varepsilon}$  by d, the signed distance to the limit interface  $\Gamma^0$ , so that the change of variables is independent of  $\varepsilon$ . This will significantly simplify the calculation. On the other hand, one has to replace the form or inner expansion by  $\varphi^{\varepsilon} \sim \theta_0(Z - h(s)) + \varepsilon \Sigma_{i \ge 0} \varepsilon^i \varphi_i(S, Z, t)$ , where h(s) is a function to be determined; see elsewhere [42] for more details.

write the outer expansions as

$$\begin{split} \varphi &\sim \pm 1 + \varepsilon \sum_{i \ge 0} \varepsilon^i \varphi^i_{\pm} \Big( X_0 + \Sigma_{j \ge 1} \varepsilon^j X_j \Big) \\ &\sim \pm 1 + \varepsilon \sum_{i \ge 0} \sum_{\alpha \ge 0} \frac{D^{\alpha} \varphi^i_{\pm} (X_0)}{\alpha!} (\sum_{j \ge 1} \varepsilon^j X_j)^{\alpha} \\ &=: \pm 1 + \varepsilon \sum_{i \ge 0} \varepsilon^i \varphi^i_{\pm} (S, Z, t) \end{split}$$

where  $\psi_{\pm}^{i}$  depends upon the derivatives of  $\varphi_{\pm}^{j}$   $(j \leq i)$  on  $\Gamma^{0}$  and  $X_{j}$   $(j \leq i)$ . Thus, for the inner and outer expansion to match, one needs

$$\lim_{Z \to \pm \infty} \left[ \psi^i_{\pm}(S, Z, t) - \varphi(S, Z, t) \right] = 0, \quad \forall (S, t).$$

The above matching conditions, as well as solvability conditions for inner equations, will lead to exactly the number of supplementary conditions for solving uniquely the inner and outer equations. In this traditional approach, we find that the computation may be very tedious. One needs to use many differential geometry tools to perform the calculation. One notices that, as  $X_1(S, Z, t)$  grows linearly in Z,  $\psi^i_{\pm}$  grows in  $Z^i$ . Hence, the inner expansion  $\varphi_i(S, Z, t)$  grows in  $Z^i$  so it is unbounded, and it is very complicated to simplify the matching conditions.<sup>2</sup> Nevertheless, the leading order computation is quite easy.

Here we shall modify this traditional matched asymptotic expansion approach by using a multiscale expansion technique, another traditional tool frequently used in asymptotic expansions; see, for example, Lardner [43] in the study of fine structure of shock waves, and Markowich [44] in the study of semiconductors.

Instead of using the change of variables  $x \to (S, Z)$  in the inner expansion, we simply take Z as an extra independent variable, besides the original variables (x, t). More precisely, writing Z as z to distinguish it from the traditional approach, we look for functions  $\tilde{\varphi}^{\varepsilon}(x, z, t)$  such that  $\varphi^{\varepsilon}(x, t) = \tilde{\varphi}(x, z, t)|_{z=d^{\varepsilon}(x,t)/\varepsilon}$ . With this new independent variable added, the phase field equations can be written as differential equations in  $(x, z, t) \in \Omega \times \mathbb{R} \times (0, \infty)$ . One notices that, for the original phase field equations to be valid, we only need  $(\tilde{\varphi}^{\varepsilon}(x, z, t), \tilde{u}^{\varepsilon}(x, z, t))$  to satisfy the new differential equations on the hypersurface  $\{(x, z, t) \mid z = d^{\varepsilon}(x, t)/\varepsilon\} \subset \mathbb{R}^{N+2}$ . That is, we have freedom in defining the equations satisfied by  $(\tilde{\varphi}^{\varepsilon}, \tilde{u}^{\varepsilon})$  in the complement of the hypersurface.

As  $\varphi^{\varepsilon}(x,t) = \tilde{\varphi}^{\varepsilon}(x,z,t)|_{z=d^{\varepsilon}/\varepsilon}$  in a thin neighbourhood of the interface, for the inner and outer expansions to match, it is sufficient to require

$$\lim_{z \to \infty} (\varphi_+(x,t) - \tilde{\varphi}_i(x,z,t)) = 0$$

for all x in  $Q^0_+$  and x is in a thin neighbourhood of  $\Gamma^0$ . (An analogous matching is needed for  $z \to -\infty$ .) In fact, to make our calculation easier and presentation clearer, we extend the outer expansions into the domain  $\Gamma^0(\delta)$ , a  $\delta$ -neighbourhood of  $\Gamma^0$ , and require the

<sup>&</sup>lt;sup>2</sup> In [42], an inner expansion of the form  $\varphi^{\varepsilon} = \frac{1}{2}[1 + \zeta(Z)]\varphi^{\varepsilon}_{+} + \frac{1}{2}[1 - \zeta(Z)]\varphi^{\varepsilon}_{-} + \varphi^{\varepsilon}_{In}$  was used, where  $\phi^{\varepsilon}_{\pm}$  is the outer expansion, and  $\zeta$  is any fixed smooth function having the property that  $\zeta(\pm \infty) = 1$ . The matching conditions then become  $\lim_{|Z| \to \infty} \varphi_{In} = 0$ .

following matching

$$\tilde{\varphi}_i(x, z, t) = \varphi^i_+(x, t) + O(e^{-\beta|z|}) \text{ as } z \to \pm \infty$$

for all  $(x,t) \in \Gamma^0(\delta)$ . With this new requirement, restrictions on the definitions of the inner expansion equations off the hypersurface are imposed. Though they seem more complicated, all the computations are straightforward.

In summary, the traditional approach leads to a unique expansion but the calculation may be tedious and involves a great deal of differential geometry tools, whereas our approach involves a minimum number of differential geometry tools and leads to very neat matching conditions. Generally speaking, the choice is matter of taste. If one is concerned only with the leading order expansion, then the traditional one is clearly preferable.

## 4.1 Asymptotic expansion and matching conditions

Let  $(\varphi^{\varepsilon}, u^{\varepsilon})$  be the unique solution of the phase field equations (1.1) with smooth initial and Dirichlet boundary conditions  $\varphi^{\varepsilon} = \varphi_0^{\varepsilon}$  and  $u^{\varepsilon} = u_0^{\varepsilon}$  on  $\partial_p \Omega_T$ . Let  $\Gamma^{\varepsilon}$  be the zero level set of  $\varphi^{\varepsilon}, Q_{\pm}^{\varepsilon}$  be the set where  $\pm \varphi^{\varepsilon}$  is positive, and  $d^{\varepsilon}(x, t)$  be the signed distance to  $\Gamma^{\varepsilon}$  so that  $\pm d^{\varepsilon} > 0$  in  $Q_{\pm}^{\varepsilon}$ . Using the classical notation for asymptotic expansions [45], we seek asymptotic expansions for  $d^{\varepsilon}, \varphi^{\varepsilon}$ , and  $u^{\varepsilon}$  as  $\varepsilon \to 0$ :

$$\begin{cases} d^{\varepsilon}(x,t) \sim \sum_{i=0}^{\infty} \varepsilon^{i} d^{i}(x,t) & \text{ in } \Gamma^{0}(\delta), \\ \varphi^{\varepsilon}(x,t) \sim \pm 1 + \sum_{i=0}^{\infty} \varepsilon^{i+1} \varphi^{i}_{\pm}(x,t) & \text{ in } Q^{0}_{\pm} \setminus \Gamma^{0}(\delta/4), \\ u^{\varepsilon}(x,t) \sim \sum_{i=0}^{\infty} \varepsilon^{i} u^{i}_{\pm}(x,t) & \text{ in } Q^{0}_{\pm} \setminus \Gamma^{0}(\delta/4), \\ \varphi^{\varepsilon}(x,t) \sim \theta_{0}(z) + \sum_{i=0}^{\infty} \varepsilon^{i+1} \varphi_{i}(z,x,t)|_{z=\frac{d^{\varepsilon}(x,t)}{\varepsilon}} & \text{ in } \Gamma^{0}(\delta), \\ u^{\varepsilon}(x,t) \sim \sum_{i=0}^{\infty} \varepsilon^{i} u_{i}(z,x,t)|_{z=\frac{d^{\varepsilon}(x,t)}{\varepsilon}} & \text{ in } \Gamma^{0}(\delta), \end{cases}$$

where  $\delta$  is a small positive constant independent of  $\varepsilon$ ,  $\Gamma^0 \equiv \{(x,t) \in \Omega_T | d^0(x,t) = 0\}$ ,  $\Gamma^0(\delta) \equiv \{(x,t) \in \Omega_T | | d^0(x,t) | < \delta\}$ ,  $Q^0_{\pm} \equiv \{(x,t) \in \Omega_T | \pm d^0(x,t) > 0\}$ .

We note that the function  $d^0(x,t)$  and the constant  $d^0$  in (1.3) are totally unrelated. Though we frequently write  $d^0(x,t)$  as  $d^0$ , the meaning is evident from the context. In the sequel, we denote  $\varphi_{\pm}^{-1} = \pm 1, \varphi_{-1} = \theta_0(\cdot)$ . Also we use the convention that  $\sum_{i=i_1}^{i_2} = 0$  if  $i_2 < i_1$ , that  $a_i b^0 + a_0 b^i = a_0 b^0$  if i = 0, and that  $\varphi_{-2} = u_{\pm}^{-2} = u_{\pm}^{-1} = u_{-2} = u_{-1} = 0$ .

The prototype  $\varphi^{\varepsilon} = \pm 1 + O(\varepsilon)$  in the outer region and  $\varphi^{\varepsilon} = \theta_0(d^{\varepsilon}/\varepsilon)$  in  $\Gamma^0(\delta)$  can be understood as a basic assumption, which can also be derived from the -1 order expansion.

The heuristic rationale for the expansion is that the inner expansion (4.1d),(4.1e) must match the outer expansion (4.1b), (4.1c) in their overlap region. This is achieved through the following *matching conditions*:

$$\begin{cases} D_x^m D_t^n D_z^l(u_i(\pm z, x, t) - u_{\pm}^i(x, t)) = O(e^{-\beta z}) & \text{in } \Gamma^0(\delta) \\ D_x^m D_t^n D_z^l(\varphi_i(\pm z, x, t) - \varphi_{\pm}^i(x, t)) = O(e^{-\beta z}) & \text{in } \Gamma^0(\delta) \end{cases} \quad \text{as } z \to \infty$$
(4.2)

for all  $m, n, l, i \ge 0$ , and  $\beta = \frac{1}{2} \min\{\sqrt{f'(1)}, \sqrt{f'(-1)}\}$ . Since  $\theta_0$  is the solution to (2.5), the matching condition is automatically satisfied for  $\varphi_{\pm}^{-1}$  and  $\varphi_{-1}$ .

Note that the matching condition is imposed in  $\Gamma^{\overline{0}}(\delta)$ . This requires the well-definedness of the outer expansion terms  $(\varphi_{\pm}^{i}, u_{\pm}^{i})$  in the set larger than its original definition in (4.1b), (4.1c). Hence, one has to extend  $(\varphi_{\pm}^{i}, u_{\pm}^{i})$  to  $\Gamma^{0}(\delta)$  by artificial smooth extensions. More details will be given in the next section.

## 4.2 Expansion equations and solvability conditions

Since  $d^{\varepsilon}$  is a distance function,  $|\nabla d^{\varepsilon}|^2 = 1$ , so that for each nonnegative integer *i*,  $d^i$  needs to satisfy the following *distance equation*:

$$\nabla d^0 \nabla d^i = \begin{cases} 1 & \text{if } i = 0\\ -\frac{1}{2} \sum_{j=1}^{i-1} \nabla d^{j-i} \nabla d^j & \text{if } i \ge 1 \end{cases} \quad \text{in } \Gamma^0(\delta). \tag{4.3}$$

Similarly, substituting the outer expansions (4.1b,c) into the phase field equations (1.2) and equating the  $\varepsilon^i$  terms yields the following *outer expansion* equations, for each non-negative integer *i*:

$$\begin{cases} (c^{0}\partial_{t} - \varDelta)u_{\pm}^{i} = A_{\pm}^{i-1} & \text{in } Q_{0}^{\pm}, \\ \varphi_{\pm}^{i} = s^{0}u_{\pm}^{i}/f'(\pm 1) + B_{\pm}^{i-1} & \text{in } Q_{0}^{\pm}, \\ u_{\pm}^{i} = \delta_{i0}g & \text{on } \partial_{p}\Omega_{T} \cap \overline{Q_{\pm}^{0}} \end{cases}$$
(4.4)

where  $\delta_{i0} = 1$  if i = 0 and = 0 if  $i \ge 1$ ,  $A_{\pm}^{i-1} = -(\varphi_{\pm}^{i-1})_t, B_{\pm}^{i-1} = \frac{1}{f'(\pm 1)} [\Delta \varphi^{i-2} - \alpha^0 \varphi_{\pm t}^{i-2} - f^{i-1}(\pm 1, \varphi_{\pm}^0, \cdots, \varphi_{\pm}^{i-1})]$  and  $f^{i-1}$  is defined by the expansion equation

$$f\left(a_{-1} + \sum_{i=0}^{\infty} a_i \varepsilon^{i+1}\right) = f(a_{-1}) + \sum_{i=0}^{\infty} \left[f'(a_{-1})a_i + f^{i-1}(a_{-1}, a_0, \cdots, a_{i-1})\right] \varepsilon^{i+1}.$$
 (4.5)

Also, we have implicitly assumed that  $\Gamma^0$  is strictly contained in  $\Omega$ .

Note that, for each  $i \ge 0$ , the outer expansion equations (4.5) form a complete system provided that the boundary values of  $u_{\pm}^i$  on  $\Gamma^0$  are prescribed. These boundary values will be obtained, in a coupled manner, through the inner expansion and matching conditions.

Note also that no boundary values of  $\varphi_{\pm}^{i}$  on  $\partial_{p}\Omega_{T}$  can be assigned in (4.4). Therefore, to enforce a particular boundary value  $\varphi^{\varepsilon} \sim 1 + \sum_{i=0}^{\infty} \varepsilon^{i+1} \varphi_{0}^{i}(x,t)$  on  $\partial \Omega \times [0,T]$ , one has to use boundary layer expansions. We shall briefly discuss this in the last part of this section.

Once the outer expansion equations have been solved, we obtain the values of  $(\varphi_{\pm}^i, u_{\pm}^i)$ in  $Q_{\pm}^0$ . The values of  $(\varphi_{\pm}^i, u_{\pm}^i)$  in  $\Gamma^0(\delta) \setminus Q_{\pm}^0$  can be obtained, for example, as follows. Define  $u_{\pm}^i(x,t) = \sum_{j=0}^J C_{ij}^{\pm}(S^0(x,t),t)(d^0(x,t))^j$  in  $\Gamma^0(\delta) \setminus Q_{\pm}^0$ , where J is a large integer depending on the order of the approximate solution needed,  $S^0(x,t)$  is the projection of x onto  $\Gamma^0$  along the normal of  $\Gamma^0$ , and  $C_{ij}(s,t), (s,t) \in \Gamma^0$ , are coefficients uniquely determined by requiring the extended function to be in  $C^J(Q_0^{\pm} \cup \Gamma^0(\delta))$ . Though there are other theoretically better methods of extending smooth (but not analytic) functions over domains having smooth boundaries, for definiteness, we shall use one of these extensions,

such as that just mentioned. Once we have the extension of  $u_{\pm}^i$ , the extension of  $\varphi_{\pm}^i$  is then defined by the outer expansion equation (4.4b) in  $\Gamma^0(\delta) \cup Q_{\pm}^0$ .

Since the extended functions may not satisfy the outer expansion equation (4.4a) in the domain where extensions are made, we introduce the discrepancy function

$$\begin{cases} R^{i}_{\pm}(x,t) \equiv c^{0}u^{i}_{\pm,t} - \Delta u^{i}_{\pm} + (\varphi^{\pm}_{i-1})_{t} \\ R^{\varepsilon}_{\pm}(x,t) \sim \sum_{i=0}^{\infty} \varepsilon^{i}R^{i}_{\pm}(x,t) & \text{ in } \Gamma^{0}(\delta). \end{cases}$$

Clearly,  $R_+^i \equiv 0$  in  $Q_+^0$ , and  $R_+^i$  is in  $C^J(\Gamma^0(\delta))$ , where J can be arbitrarily large.

Before we present the inner expansion equations, we give a brief rationale. If a function of independent variables z, x, and t is evaluated at  $z = \frac{d^{\varepsilon}(x,t)}{\varepsilon}$  to a function of variables xand t, then one has  $\partial_t = \varepsilon^{-1} d_t^{\varepsilon} \partial_z + \partial/\partial_t$  and  $\Delta_x = \varepsilon^{-2} \partial_{zz}^2 + \varepsilon^{-1} (\Delta d^{\varepsilon} \partial_z + 2\nabla d^{\varepsilon} \nabla \partial_z) + \Delta$ , where  $\partial/\partial_t$  and  $\Delta$  on the right-hand sides are the partial derivatives which involve fixed z. Hence substituting the inner expansions (4.1d,e) into the phase field equations and equating the  $\varepsilon^i$  terms leads to second order linear ordinary differential equations, in z, for each  $\varphi_i$ and  $u_i$ . As will be seen later, the linear differential operators are independent of i, and have eigenvectors with zero eigenvalue. This amounts to imposing solvability conditions for the inhomogeneous term with dependence only on expansions of lower order terms. The requirements of the solvability conditions for the next order expansion then yields the extra condition needed to obtain a complete system for inner-outer expansions. For  $(x,t) \in \Gamma^0$ , this provides exactly the number of conditions needed for (4.4) and the determination of the motion of  $\Gamma^{\varepsilon}$ . However, when  $(x, t) \notin \Gamma^{0}$ , no extra conditions can be imposed. (This displays the advantage of taking z as the dependent variable mentioned at the beginning of this section.) To resolve this dilemma, recall that the ordinary differential equations for z are only required at a single point  $z = \frac{d^{e}(x,t)}{d^{e}(x,t)}$ . Hence, we can modify the equation, for z, off the hypersurface  $\{(z, x, t) \in \mathbb{R}^1 \times \Gamma^0(\delta) ; z = d^{\varepsilon}(x, t)/\varepsilon\}$ , in any way that we choose. Hence, we shall add terms which vanish on  $\{\varepsilon z = d^{\varepsilon}\}$  to the inner expansion equations. For this purpose, let  $\eta(z)$  be a fixed smooth function having the following properties:

$$\eta(z) = 0$$
 if  $z < -1$ ,  $\eta(z) = 1$  if  $z > 1$ ,  $\eta'(z) > 0$  in  $(-1, 1)$ ,  $\int_{\mathbf{R}^1} z \eta'(z) dz = 0$ .

Also, let  $M_1 \equiv ||d^1||_{C^0(\Gamma^0(\delta))} + 1$  be a constant obtained after the first order expansion. We add a term

$$g^{\varepsilon}(x,t)\eta'(z)(d^{\varepsilon}-\varepsilon z)\sim\left(\sum_{i=0}^{\infty}g_{i}(x,t)\varepsilon^{i}\right)\eta'(z)\left(\sum_{i=0}^{\infty}d^{i}(x,t)\varepsilon^{i}-\varepsilon z\right)$$

to the ordinary differential equation (in z) for  $\varphi^{\varepsilon}$  and a term

$$\begin{split} \varepsilon^{-2}[h^{\varepsilon}(x,t)\eta''(z) + \varepsilon L^{\varepsilon}(x,t)\eta'(z)](d^{\varepsilon} - \varepsilon z) + [\eta(M_1 + z)R^{\varepsilon}_+(x,t) + \eta(-M_1 - z)R^{\varepsilon}_-(x,t)] \\ &= \varepsilon^{-2} \left[ \eta''(z) \sum_{i=0}^{\infty} h_i(x,t)\varepsilon^i + \eta'(z) \sum_{i=0}^{\infty} l_i(x,t)\varepsilon^{i+1} \right] \left[ \sum_{i=0}^{\infty} d^i(x,t)\varepsilon^i - \varepsilon z \right] \\ &- \sum_{i=0}^{\infty} \varepsilon^i \left[ R^i_+(x,t)\eta(M_1 + z) + R^i_-(x,t)\eta(-M_1 - z) \right] \end{split}$$

to the ordinary differential equation (in z) for  $u^{\varepsilon}$ . Here the functions  $g_i, h_i$  and  $l_i$  are to be determined along with  $(u^i_{\pm}, u_i, \varphi^i_{\pm}, \varphi_i)$ . Note that the terms  $R^{\varepsilon}_{\pm}$  added only affect the expansions of order no less than 1; in particular, it does not affect  $d^1(x, t)$ , so that  $M_1 \equiv \|d^1\|_{C^0(\Gamma^0(\delta))} + 2$  can be taken arbitrarily. Since  $R^{\varepsilon}_{\pm} \equiv 0$  in  $Q^0_{\pm}$ , the terms  $\eta(M_1 + z)R^{\varepsilon}_{+} + \eta(-M_1 - z)R^{\varepsilon}_{-}$  vanishes when  $z = d^{\varepsilon}/\varepsilon$ ,  $(x, t) \in \Gamma^0(\delta)$ . In fact, if  $(x, t) \in Q^0_+$  and  $z = \frac{d^{\varepsilon}}{\varepsilon}$ , then  $R^{\varepsilon}_{+} = 0$  and  $d^0 > 0$  so that  $z > d^1 + O(\varepsilon)$ , and consequently  $\eta(-M_1 - z) = 0$ . A similar analysis also applies to the case when  $(x, t) \in Q^0_-$ .

Now substituting the inner expansions (4.1d,e) into the phase field equations, adding the terms mentioned above, and equating the  $\varepsilon^i$  terms, we obtain the following inner equations, for each  $i = 0, 1, 2, \cdots$ ,

$$\begin{cases} \left[ u_{i} - \sum_{j=0}^{i} h_{i} d^{i-j} \eta \right]'' = A_{i-1} + \hat{A}_{i-2} & \text{in } \mathbb{R}^{1} \times \Gamma^{0}(\delta) \\ -\varphi_{i}'' + f'(\theta_{0})\varphi_{i} = B_{i} + \tilde{B}_{i-1} \end{cases}$$
(4.6)

where prime denotes  $\frac{\partial}{\partial z}$  and

$$\begin{cases} A_{i-1} = d_{t}^{i-1}\theta_{0}' + (c^{0}d_{t}^{0} - \varDelta d^{0})u_{i-1}' + (c^{0}d_{t}^{i-1} - \varDelta d^{i-1})u_{0}' - 2(\nabla d^{0}\nabla u_{i-1}' + \nabla d^{i-1}\nabla u_{0}') \\ + (l_{i-1}d^{0} + l_{0}d^{i-1})\eta' - h_{i-1}z\eta'', \end{cases}$$

$$\hat{A}_{i-2} = \sum_{j=1}^{i-2} \{d_{t}^{j}\varphi_{i-1-j}' + (c^{0}d_{t}^{j} - \varDelta d^{j})u_{i-1-j}' - 2\nabla d^{j}\nabla u_{i-1-j}' + d^{j}l_{i-1-j}\eta'\} - l_{i-2}z\eta'' \\ + [c^{0}u_{i-2,t} - \varDelta u_{i-2} + \varphi_{i-2,t} - \eta(M+z)R_{+}^{i-2} - \eta(-M_{1}-z)R_{-}^{i-2}], \qquad (4.7)$$

$$B_{i} = s^{0}u_{i} + (\varDelta d^{i} - \alpha^{0}d_{t}^{i})\theta_{0}' + (g_{i}d^{0} + g^{0}d^{i})\eta', \\ \hat{B}_{i-1} = \sum_{j=0}^{i-1} [(\varDelta d^{j} - \alpha^{0}d_{t}^{j})\varphi_{i-1-j}' + 2\nabla d^{j}\nabla\varphi_{i-1-j}] + \sum_{j=1}^{i-1} d^{j}g_{i-j}\eta' \\ - f^{i-1}(\theta_{0}, \varphi_{0}, \cdots, \varphi_{i-1}) + \varDelta \varphi_{i-2} - \alpha^{0}\varphi_{i-2,t} - g_{i-1}z\eta'$$

where  $f^{i-1}(\theta_0, \varphi_0, \cdots, \varphi_{i-1})$  is defined as in (4.5).

Since we assume that the set  $\Gamma^{\varepsilon} := \{(x,t) : d^{\varepsilon}(x,t) = 0\}$  is the zero level set of  $\varphi^{\varepsilon}$ , we impose the following sufficient condition:

$$\varphi^{i}(0, x, t) = 0 \qquad \forall (x, t) \in \Gamma^{0}(\delta), i = 1, 2, \cdots.$$

$$(4.8)$$

Clearly, to ensure that (4.6a) has a bounded solution, it is necessary that the lower order expansions satisfy the condition  $\int_{-\infty}^{\infty} (A_{i-1} + \hat{A}_{i-2})(z, x, t)dz = 0$ . This condition is also sufficient in the sense that if all the functions up to order i - 1 have the property that they approach their limits exponentially fast (in order of  $O(e^{-\beta z})$ ) as  $z \to \pm \infty$ , then there exists a bounded solution of  $u_i$ , unique up to an additive constant, which will also have the properties that it approaches their limits as  $z \to \pm \infty$  with speed  $O(e^{-\beta(z)})$ . In other words, in solving the  $i^{\text{th}}$  order expansion, we need  $\int_{-\infty}^{\infty} (A_i + \hat{A}_{i-1})(z, x, t)dz = 0$  so that the next order expansion equation (i.e. (4.6a) with *i* replaced by i + 1) is solvable. Hence, using the expression of  $A_i$  and  $\hat{A}_{i-1}$ , we need the following *compatibility* conditions:

$$2d_{t}^{i} + (c^{0}d_{t}^{0} - \Delta d^{0})[u_{i}] + [c^{0}d_{t}^{i} - \Delta d^{i}][u_{0}] -2(\nabla d^{0}[\nabla u_{i}] + \nabla d^{i}[\nabla u_{0}]) + (l_{i}d^{0} + l_{0}d^{i}) + h_{i} = a_{i-1} \text{ in } \Gamma^{0}(\delta)$$
(4.9)

where  $a_{i-1}$  is a function that depends only upon inner expansions of order less than *i*, and  $[u_i] = u_i(+\infty, x, t) - u_i(-\infty, x, t) (= u^+(x, t) - u_-^i(x, t))$  if we have the matching condition). Here we have used the fact that  $\int_{R^1} \theta'_0 = 2$ ,  $\int_{R^1} \eta' = 1$ ,  $\int_{R^1} z \eta'' dz = [z\eta' - \eta]|_{-\infty}^{\infty} = -1$ . Due to the term  $\eta(M_1 + z)R_+^{i-1} + \eta(-M_1 - z)R_-^{i-1}$  we added in $\hat{A}_{i-1}$ , the function  $\hat{A}_{i-1}$  approaches zero exponentially fast (in order of  $O(e^{-\beta t})$ ) as  $z \to \pm \infty$ , as long as all the expansions of order lower than *i* do so. Hence,  $a_{i-1}$  is bounded and approaches  $a_{i-1}(\pm\infty, x, t)$  exponentially fast (in order of  $O(e^{-\beta(z)})$ ) as  $z \to \pm \infty$ .

Similarly, since  $\theta'_0$  is a positive eigenfunction of the operator  $-\frac{d^2}{dz^2} + f'(\theta_0)$  corresponding to the zero eigenvalue, and since  $f'(\theta_0) \rightarrow f'(\pm 1) \ge 4\beta^2$  as  $z \rightarrow \pm \infty$ , (4.7b) and (4.8) has a unique solution if and only if  $\int_{R^1} (B_i + \hat{B}_{i-1})\theta'_0 = 0$ . Substituting the expression for  $B_i$  and  $\hat{B}_{i-1}$ , one has

$$\bar{u}_{i} = -\frac{m}{2s^{0}} \left[ \varDelta d^{i} - \alpha^{0} d^{i}_{t} \right] + \frac{m_{1}}{2} \left[ g_{i} d^{0} + g_{0} d^{i} \right] + b_{i-1} \quad \text{in } \Gamma^{0}(\delta)$$
(4.10)

where  $m = \int_{-\infty}^{\infty} (\theta'_0)^2 = \int_{-1}^{1} (2 \int_{-1}^{1} f(s) ds) du$  is the same *m* as in § 1,  $m_1 = \int_{-\infty}^{\infty} \eta'(z) \theta'_0(z) dz$ ,  $b_{i-1}$  is a function which depends only on expansions of order less than *i*, and

$$\bar{u}_i = \frac{\int_{-\infty}^{\infty} u_i(z, x, t) \theta'_0(z) dz}{\int_{-\infty}^{\infty} \theta'_0(z) dz} = \frac{1}{2} \int_{-\infty}^{\infty} u_i(z, x, t) \theta'_0(z) dz.$$

Note that (4.10) is different from (4.9) in the sense that it is not a condition used for the next order expansion. If (4.10) is satisfied, then there exists a unique bounded solution  $\varphi_i$ , and it satisfies

$$\varphi_{i} \to \lim_{z \to \pm \infty} \frac{1}{f'(\theta_{0})} [B_{i} + \hat{B}_{i-1}] \\= \frac{1}{f'(\pm 1)} [s^{0} u_{\pm}^{i} - f^{i-1}(\pm, \varphi_{\pm 1}^{0}, \cdots, \varphi_{\pm}^{i-1}) + \Delta \varphi_{\pm}^{i-2} - \alpha^{0} \varphi_{\pm}^{i-2}] = \varphi_{\pm}^{i}(x, t).$$
(4.11)

The limit is exponentially fast (in the order of  $O(e^{-\beta(z)})$ ) if all the lower order expansions and  $u_i$  are so.

In summary, we define the *i*th order inner-outer expansion problem as follows:

**Definition 4.1** Let  $i \ge 0$  be an integer. Assume that for all  $k \le i - 1$  the *k*th order expansion  $V_k \equiv \{u_{\pm}^k, u_k, \varphi_{\pm}^k, \varphi^k, d^k, h_k, l_k, g_k\}$  are all known and they satisfy the matching conditions in (4.2) and the compatibility condition (4.9) (with i = k). Then the *i*th order expansion problem is to find  $V_i = \{u_{\pm}^i, u_i, \varphi_{\pm}^i, \varphi_i, d^i, h_i, l_i, g_i\}$  such that the outer-expansion equations (4.4), the inner expansion equations (4.6) and (4.8), the matching conditions (4.2), the distance equations (4.3), and the compatibility condition (4.9) are all satisfied.

In the following two subsections, we shall solve the *i*th expansion problem for i = 0 and  $i \ge 1$ , respectively.

#### 4.3 The zero-th order expansion

**Lemma 4.1** Let  $u_0^0(x,t)$  be given, and assume that the free boundary problem (2.1) with  $d^0 = \frac{m}{2s^0}$  and  $g = u_0^0$  has a smooth solution  $(u, \Gamma^0)$ . Then the zero-th order expansion exists and the outer expansion  $u_{\pm}^0$  coincides with u in  $Q_{\pm}^0$ .

**Proof** Assume that  $d^0(x, t)$  is known. (For example, one can assume that it is the solution to the free boundary problem (2.1).)

Since the equation for  $u_0$  is  $(u_0 - h_0 d^0 \eta)'' = 0$ , there is a bounded solution and the general solution is given by

$$u_0(z, x, t) = \hat{u}(x, t) + h_0(x, t)d^0(x, t)\eta(z), \quad z \in \mathbf{R}^1, \quad (x, t) \in \Gamma^0(\delta)$$
(4.12)

where  $\hat{u}_0$  is an additive function. Since  $d^0 = 0$  on  $\Gamma^0$ ,  $u_0 = \hat{u}(x, t)$  on  $R^1 \times \Gamma^0$  so that one has  $\bar{u}_0(x, t) = \hat{u}_0(x, t)$  on  $\Gamma^0$ . For i = 0, equation (4.10) reads  $\bar{u}_0 = -\frac{m}{2s^0} [\alpha^0 d_t^0 - \Delta d^0]$  which, after translating to  $\hat{u}$  and then to  $u_0(z, x, t)$  yields

$$u_0(z, x, t) = \frac{m}{2s^0} (\alpha^0 d_t^0 - \Delta d^0) = -\frac{m}{2s^0} (\kappa_{\Gamma^0} - v_{\Gamma^0}) \text{ on } \mathbf{R}^1 \times \Gamma^0,$$

since  $d^0$  as a distance function implies that  $\Delta d^0 = \kappa_{\Gamma^0}$  is the sum of the principal curvatures,  $d_t =: v_{\Gamma^0}$  is the normal velocity of  $\Gamma^0$ . Consequently,  $u^0_{\pm}(x,t)|_{\Gamma^0} = u_0(\pm\infty, x,t) = -\frac{m}{2s^0}(\kappa_{\Gamma^0} - V_{\Gamma^0})$ . With this boundary value, we can uniquely solve  $u^0_{\pm}$  in  $Q^0_{\pm}$  via the outer expansion equation. As mentioned earlier, we extend  $u^0_{\pm}$  smoothly over  $\Gamma^0(\delta)$ .

Using the matching condition for  $(u_0, u_+^0)$  and the expression of  $u_0$  in (4.12), we have

$$\hat{u}^{0}(x,t) + h^{0}d^{0}\left(\frac{1}{2} \pm \frac{1}{2}\right) = u^{0}_{\pm}(x,t) \quad \text{in } \Gamma^{0}(\delta)$$

which implies that

$$\hat{u}^{0}(x,t) = \frac{1}{2}(u^{0}_{+}(x,t) + u^{0}_{-}(x,t)), \qquad h_{0}d^{0} = u^{+}_{0}(x,t) - u^{+}_{0}(x,t).$$
 (4.13)

Since  $u_0^{\pm}$  are smooth and  $u_+^0 = u_-^0$  on  $\Gamma^0$ ,  $h_0$  is well-defined on  $\Gamma^0$  and  $h_0|_{\Gamma_0} = \lim_{d^0 \to 0} \frac{1}{d^0} (u_0^+ - u_-^0) = \nabla u^0 \nabla d^0$ .

Observe that where i = 0, (4.9) reads  $2d_t^0 = -(c^0d_t^0 - \Delta d^0)[u^0] + 2\nabla d^0[\nabla u_0] - l_0d^0 - h_0$ . Since on  $\Gamma^0$ ,  $[u^0] = u_+^0 - u_-^0 = 0$ ,  $d^0 = 0$ , we obtain

$$d_t^0 = \frac{1}{2} [2\nabla d^0 [\nabla u_0] - h_0] = \frac{1}{2} \nabla d^0 [\nabla u_0] = -\frac{1}{2} \left( \frac{\partial u_+^0}{\partial n} - \frac{\partial u_-^0}{\partial n} \right)$$

since  $\nabla d^0 = -n|_{\Gamma^0}$ , the unit normal of  $\Gamma^0$  pointing to  $Q^0_+$ .

Now we can go backwards to solve the zero-th order expansion. Let  $(u, \Gamma^0)$  be the solution to the free boundary problem (2.1),  $d^0(x, t)$  be the signed distance function to  $\Gamma^0$ , and  $\delta$  be a small positive constant such that  $d^0(x, t)$  is smooth in  $\Gamma^0(2\delta)$ . Define  $(\hat{u}_0, h_0, u_0)$  by (4.13) and (4.12), and set  $u^0_{\pm} = u|_{Q^0_{\pm}}$ , then the outer expansion equation (4.4a), the inner expansion equation (4.6a), and the matching condition (4.2a) are satisfied. In addition, (4.9) and (4.10) are both valid on  $\Gamma^0$ .

Now define  $\varphi^0_+$  by (4.4b), and define  $g^0$  by

$$g_0 d^0 = \frac{2}{m_1} \{ \bar{u}_0(x,t) - \frac{m}{2s^0} (\Delta d^0 - \alpha^0 d^0 t) \}$$
 in  $\Gamma^0(\delta)$ .

(Observe that the right-hand side vanishes on  $\Gamma^0$ , so that  $g^0$  is well-defined and is smooth in  $\Gamma^0(\delta)$ .) Then (4.10) holds in  $\Gamma^0(\delta)$ , and consequently, one can solve (4.6b) with i = 0to obtain a unique solution  $\varphi_0$ , which, by utilizing (4.11), satisfies the matching condition (4.2b). Finally, defining  $l^0$  in a similar manner as for  $g^0$ , the compatibility condition (4.9) can be satisfied in  $\Gamma^0(\delta)$ . This completes the proof of the lemma.

## 4.4 Higher order expansions

Since  $V_0$ , along with  $d^0$ ,  $Q_{\pm}^0$ , and  $\delta$ , has been constructed, by mathematical induction, we only need to find, for each  $j \ge 1$ , the *j*th order expansion under the assumption that all the previous order expansions have been constructed.

First we assume that  $d^{j}(x,t), (x,t) \in \Gamma^{0}(\delta)$ , is known. We shall express all the *j*th order unknowns in terms of  $d^{j}$  and then solve for  $d^{j}$ .

To solve the inner expansion equations (4.6b) and (4.8) uniquely, it is necessary and sufficient, by (4.10), to take

$$\bar{u}_j = \frac{m}{2s^0} (\alpha^0 d_t^0 - \Delta d^j) - \frac{m_1}{2} (g_j d^0 + g_0 d^j) + b_{j-1} \quad \text{in } \Gamma^0(\delta).$$
(4.14)

Since, by induction, the solvability condition (4.9) (with i = j - 1) is satisfied, one can solve (4.6a) with i = j to

$$u_j(z, x, t) = (h_j d^0 + h_0 d^j)(\eta - \bar{\eta}) + \bar{u} + c^{j-1}(z, x, t)$$
(4.15)

where  $\bar{\eta} = \int_{R^1} \eta \theta'_0 / \int \theta'_0$ , and  $c^{j-1}$  is obtained by solving  $(c^{j-1})'' = A_{j-1} + \tilde{A}_{j-2}$ ,  $\int c^{j-1} \theta'_0 = 0$ , so that  $c^{j-1}$  depends only upon the previous order expansions.

Substituting (4.14) into (4.15) and sending  $z \to \pm \infty$ , we then obtain

$$u_{j}(\pm\infty, x, t) = (h_{j}d^{0} + h_{0}d^{j})(\frac{1}{2} \pm \frac{1}{2} - \bar{\eta}) + \frac{m}{2s^{0}}(\alpha^{0}d_{t}^{j} - \Delta d^{j}) -\frac{m_{1}}{2}(g_{j}d^{0} + g_{0}d^{j}) + b_{j-1} + c^{j-1}(\pm\infty, x, t).$$
(4.16)

In particular, on  $\Gamma^0$ ,

$$u_{j}(\pm\infty,\cdot) = \left(h_{0}(\frac{1}{2}\pm\frac{1}{2}-\bar{\eta})-\frac{m_{1}}{2}g_{0}\right)d^{j} + \frac{m}{2s^{0}}(\alpha^{0}d^{j}_{\pm}-\Delta d^{j}) + b_{j-1} + c^{j-1}(\pm\infty,\cdot) \text{ on } \Gamma^{0}.$$
(4.17)

Noting that the right-hand side depends only upon  $d^j$  and known quantities, we can use this as the boundary value of  $u_{\pm}^j$  to solve the outer expansion equation (4.2a), using the matching condition, to obtain  $u_{\pm}^j$  in  $Q_{\pm}^0$ . (Then we extend them smoothly into  $\Gamma^0(\delta)$ .) We can consider  $u_{\pm}^j$  as functional of  $d^j$ .

Obtaining  $u_{\pm}^{j}$  in this way only satisfies the matching condition for  $u_{j}$  and  $u_{\pm}^{j}$  on  $\Gamma^{0}$ . To guarantee the matching of  $u_{j}$  and  $u_{\pm}^{j}$  in the full neighbourhood of  $\Gamma^{0}(\delta)$ , it is necessary and sufficient, by (4.16), to define  $h_{j}$  and  $g_{j}$  by

$$d^{0}h_{j} = c_{1}^{j-1}(\infty, x, t) - c^{j-1}(-\infty, x, t) - h_{0}d^{j} \text{ on } \Gamma^{0}(\delta) \setminus \Gamma^{0},$$

$$d_{0}g_{j} = (1 - \bar{\eta})u_{-}^{j} + \bar{\eta}u_{+}^{j} + \frac{m}{2\Omega}(\alpha^{0}d_{+}^{j} - \Delta d^{j}) - \frac{m_{1}}{2}g_{0}d^{j} + b_{j-1}$$
(4.18)

Since both of the right-hand sides vanish on  $\Gamma^0$  (by the definition of  $u_{\pm}^j$ ),  $h_j$  and  $g_j$  are smooth functionals of  $d^j$  in  $\Gamma^0(\delta)$ . To enforce (4.9), one only needs to take

$$2d_{t}^{j} = -[c^{0}d_{t}^{0} - \Delta d^{0}][u_{j}] + 2\nabla d^{0}[\nabla u_{j}] + 2\nabla d^{j}[\nabla u_{0}] - l_{0}d^{j} - h_{j} + a_{j-1} \text{ on } \Gamma^{0}$$
(4.20)  
$$d^{0}l^{j} = -2d_{t}^{j} - [c^{0}d_{t}^{0} - \Delta d^{0}][u_{j}] + 2\nabla d^{0}[\nabla u_{j}] + 2\nabla u^{j}[\nabla u_{0}] - l_{0}d^{j} - h_{j} + a_{j-1} \text{ in } \Gamma^{0}(\delta)$$
(4.21)

since  $[u_0]_{\Gamma^0} = 0$ . Clearly, once the first equation is satisfied,  $l^j$  is a smooth function. Using

the expression for  $h_j$  in (4.18), equation (4.20) can be written as

$$2d_t^j = -[c^0 d_t^0 - \Delta d^0][u_j] + 2\nabla d^0 [\nabla u_j] + 2\nabla d^j [\nabla u_0] - l_0 d^j -\nabla d^0 [\nabla u_j] - \nabla d^0 \nabla h_0 d^j - h_0 \nabla d^0 \nabla d^j + \nabla d^0 [\nabla c^{j-1}] + a_{j-1} = -(c^0 d_t^0 - \Delta d^0)(h_0 d_j) + \nabla d^0 [\nabla u_j] + \nabla d^j h_0 \nabla d^0 - l_0 d^j + \hat{a}_{j-1} \text{ on } \Gamma^0$$

since  $[u_j]|_{\Gamma^0} = h_0 d^j + [c^{j-1}]$  and  $[\nabla u_0] = h_0 \nabla d^0$ . Note that the right-hand side depends also upon  $[u_j] = u_+^j - u_-^j$ . Hence, we have to solve  $(d^j, u_+^j, u_-^j)$  together. After replacing  $\nabla d^0 \nabla d^j = -\frac{1}{2} \sum_{i=1}^{j-1} \nabla d^{j-i} \nabla d^i$ , we obtain the following linear system for  $(d^j, u_+^j, u_-^j)$ :

$$\begin{cases} d_{t}^{j} = -\frac{1}{2} \left[ \frac{\partial}{\partial n} u_{\pm}^{j} - \frac{\partial}{\partial n} u_{-}^{j} \right] + e_{1}^{j-1} d^{j} + e_{2}^{j-1} \quad \text{on } \Gamma^{0}, \\ c^{0} u_{\pm t}^{j} - \Delta u_{\pm}^{j} = e_{3}^{j-1} \qquad \text{in } Q_{\pm}^{0}, \\ \frac{j}{\pm} = \frac{m}{2s_{0}} (\alpha^{0} d_{t}^{j} - \Delta d^{j}) + e_{4\pm}^{j-1} d^{j} + e_{5\pm}^{j-1} \qquad \text{on } \Gamma^{0}, \\ \nabla d^{0} \nabla d^{j} = e_{6}^{j-1} \qquad \text{in } \Gamma^{0}(\delta), \\ u_{\pm}^{j} = 0 \qquad \qquad \text{on } \partial_{p} \Omega_{T}, \\ d^{j}(\cdot, 0) = 0 \qquad \qquad \text{on } \Gamma^{0}(\delta). \end{cases}$$

$$(4.22)$$

Existence of a unique solution to (4.22) can be proved in a manner similar to (but much simpler than) that of the existence of the free boundary problem (2.1). For example, one can show the well-posedness of (4.22) as follows: Given  $d \in C^{2+\alpha,1+\alpha/2}(\Gamma^0(\delta))$ , solve  $u^j$ from (4.22a,b,e) with  $d^j = d$ . If we denote the solution by u, then from parabolic estimates, one obtains  $u \in C^{3+\alpha,(3+\alpha)/2}(\Gamma^0)$ . We then solve  $d^j$  from (4.15c,d,f) with  $u^j$  replaced by u. If we denote the solution by  $\tilde{d}$ , then by PDE estimates,  $\tilde{d} \in C^{3+\alpha,(3+\alpha)/2}(\Gamma^0(\delta))$ . One can easily show that the mapping from d to  $\tilde{d}$  is a contraction and maps a certain ball of the function space  $C^{2+\alpha,1+\alpha}(\Gamma(\delta) \cap \Omega \times [0, T_1])$  into itself, provided that one takes  $T_1$  sufficiently small. Hence by a fixed point theorem, the mapping from d to  $\tilde{d}$  has a unique fixed point, which yields a solution of (4.22) in time interval  $[0, T_1]$ . Noting that problem (4.22) is linear, step-by-step, one can show that (4.15) has a unique solution  $d^j$ in time interval [0, T]. Regularity follows from a boot-strap argument. For more details, see elsewhere [28], where existence of a solution to (2.1) is proved by first studying the well-posedness of a linearized problem similar to (4.22).

In summary, we can construct the *j*th order expansion as follows: First, let  $(d^j, u^j_{\pm})$  be the unique classical solution of (4.22). By the third equation in (4.22), the right-hand sides of (4.18) and (4.19) vanish on  $\Gamma^0$  so that we can define unique smooth functions  $h_j$  and  $g_j$  by (4.18) and (4.19), respectively. After that, we define  $\bar{u}_j$  by (4.14) and  $u_j$  by (4.15). Then the outer expansion equations for  $u^j_{\pm}$ , the inner expansion equations for  $u^j$ , the matching conditions for  $u^j_{\pm}$  and  $u_j$ , and the compatibility condition (4.9) (with i = j) are all satisfied. Next, define  $\varphi^j_{\pm}$  by the outer expansion equations. By (4.14), (4.10) (with i = j) holds, so that we can solve the inner expansion equation (4.6b) (with i = j) to obtain a unique bounded  $\varphi_j$ . In addition, by (4.11),  $(\varphi^j_{\pm}, \varphi_j)$ satisfies the matching condition. Finally, defining  $l_j$  by (4.21) completes the construction of the *j*th order expansion. Hence we have the following:

**Lemma 4.2** Assume that (2.2) has a smooth solution. Then for all non-negative integers *j*, there exists a *j*th order expansion.

## 4.5 Approximate solutions

In this subsection we 'glue' the inner and outer expansions to construct approximate solutions. Let  $K \ge 2$  be an arbitrary fixed integer, and let  $V^0, \dots, V^K$  be the expansions up to order K which are given in the previous subsections. In the sequel, all O's are in the  $C^0$  norm, although estimates on  $C^m$   $(m \ge 1)$  norm can be similarly obtained.

Define

$$d_{\varepsilon}^{K}(x,t) = \sum_{i=0}^{K} \varepsilon^{i} d^{i}(x,t) \qquad \forall (x,t) \in \Gamma^{0}(\delta),$$
$$\Gamma_{\varepsilon}^{K} = \{(x,t) \in \Gamma^{0}(\delta) \mid d_{\varepsilon}^{K} = 0\}.$$

Then by the equations satisfied by  $d^j$  in (4.3),  $d^K_{\varepsilon}$  is a Kth order approximate distance function to  $\Gamma^K_{\varepsilon}$ , in the sense that  $d^K_{\varepsilon}$  vanishes on  $\Gamma^K_{\varepsilon}$  and

$$|\nabla d_{\varepsilon}^{K}|^{2} = 1 + \sum_{1 \leq i, j \leq K, i+j \geq K+1} \varepsilon^{i+j} \nabla d^{j} \nabla d^{i} = 1 + O(\varepsilon^{K+1}). \qquad \forall (x,t) \in \Gamma^{0}(\delta).$$

Next we define the inner approximate solution  $(u_I^K, \varphi_I^K)$  by

$$\begin{split} u_{I}^{K}(x,t) &= \sum_{i=0}^{K} \varepsilon^{i} u^{i}(z,x,t) \Big|_{z = \frac{d_{\varepsilon}^{K}(x,t)}{\varepsilon}} \qquad \forall (x,t) \in \Gamma^{0}(\delta), \\ \varphi_{I}^{K}(x,t) &= \sum_{i=0}^{K} \varepsilon^{i} \varphi^{i}(z,x,t) \Big|_{z = \frac{d_{\varepsilon}^{K}(x,t)}{\varepsilon}} \qquad \forall (x,t) \in \Gamma^{0}(\delta). \end{split}$$

Note that, when  $\varepsilon$  is small enough,  $|\frac{d_{\varepsilon}^{K}}{\varepsilon} - \frac{d^{0} + \varepsilon d^{1}}{\varepsilon}| = |\sum_{i=2}^{K} \varepsilon^{i-1} d^{i}| \leq 1$ , and hence the term  $\eta(M_{1} + z)R_{+}^{\varepsilon} + \eta(-M_{1} - z)R_{-}^{\varepsilon}$  vanishes when  $z = d_{\varepsilon}^{K}/\varepsilon$ . From the equations satisfied by  $(u^{j}, \varphi^{j}), j = 0, \dots, K$ , and the fact that we are evaluating  $u^{j}$  and  $\varphi^{j}$  at  $z = d_{\varepsilon}^{K}/\varepsilon$ , it follows that

$$c^{0}(u_{I}^{K})_{t} + \Delta u_{I}^{K} + (\varphi_{I}^{K})_{t} = O(\varepsilon^{K-1})$$
  
$$\alpha^{0}\varepsilon(\varphi_{I}^{K})_{t} - \varepsilon\Delta\varphi_{I}^{K} + \varepsilon^{-1}f(\varphi_{I}^{K}) - s^{0}u_{I}^{K} = O(\varepsilon^{K}) \qquad \forall (x,t) \in \Gamma(\delta).$$

Define the outer approximate solution  $(u_0, \varphi_0)$  by

$$u_{\mathcal{O}}^{K}(x,t) = \sum_{i=0}^{K} \varepsilon^{i} u_{i}^{+}(x,t) \chi_{\overline{\mathcal{Q}_{0}^{+}}} + \sum_{i=0}^{K} \varepsilon^{i} u_{i}^{-}(x,t) \chi_{\overline{\mathcal{Q}_{0}^{-}}} \qquad \forall (x,t) \in \Omega_{T},$$
$$\varphi_{\mathcal{O}}^{K}(x,t) = \sum_{i=0}^{K} \varepsilon^{i} \varphi_{i}^{+}(x,t) \chi_{\overline{\mathcal{Q}_{0}^{+}}} + \sum_{i=0}^{K} \varepsilon^{i} \varphi_{i}^{-}(x,t) \chi_{\overline{\mathcal{Q}_{0}^{-}}} \qquad \forall (x,t) \in \Omega_{T}.$$

Then by using the outer expansion equations, one can easily show that

$$c^{0}(u_{\mathrm{O}}^{K})_{t} + \Delta u_{\mathrm{O}}^{K} + (\varphi_{\mathrm{O}}^{K})_{t} = O(\varepsilon^{K}), \qquad \forall (x,t) \in \Omega_{T} \setminus \Gamma^{0},$$
  
$$\alpha^{0} \varepsilon \varphi_{\mathrm{O}}^{K} - \varepsilon \Delta \varphi_{\mathrm{O}}^{K} + \varepsilon^{-1} f(\varphi_{\mathrm{O}}^{K}) - s^{0} u_{\mathrm{O}}^{K} = O(\varepsilon^{K}), \qquad \forall (x,t) \in \Omega_{T} \setminus \Gamma^{0}.$$

Now we 'glue' the inner approximate solution  $(u_I^K, \varphi_I^k)$  and the outer approximate

solution  $(u_{\mathcal{O}}^{K}, v_{\mathcal{O}}^{K})$ . To do this, let  $\zeta(s) \in C_{0}^{\infty}(\mathbb{R})$  be a cut-off function as in (2.4) and define

$$u_A^K = \begin{cases} u_O^K & \text{in } \Omega_T \setminus \Gamma^0(\delta), \\ u_I^K \zeta(d^0/\delta) + (1 - \zeta(d^0/\delta))u_O^K & \text{in } \Gamma(\delta) \setminus \Gamma^0(\delta/2), \\ u_I^K & \text{in } \Gamma^0(\delta/2). \end{cases}$$

and similarly define  $\varphi_A^K$ . By the properties of the cut-off function  $\zeta$ , we know that  $(u_A^K, \varphi_A^K)$  is smooth in  $\overline{\Omega_T}$ . When  $z \in \Gamma^0(\delta) \setminus \Gamma^0(\delta/2)$ ,  $|d^0| \in [\delta/2, \delta)$ , so that  $d_{\varepsilon}^K \equiv d^0 + \sum_{i=1}^K \varepsilon^i d^i$  satisfies, when  $\varepsilon$  is small enough,  $|d_{\varepsilon}^k| \ge \delta/4$  for all  $(x, t) \in \Gamma^0(\delta) \setminus \Gamma^0(\delta/2)$ . Consequently, by the matching conditions, we get

$$\|u_A^K - u_O^K\|_{C^2(\Gamma^0(\delta) \setminus \Gamma^0(\delta/2))} = O(\varepsilon^{-2} e^{-\alpha \delta/(4\varepsilon)})$$

and a similar relation also holds for  $\varphi_A^K$  and  $\varphi_Q^K$ .

Hence, by the equations satisfied by  $(u_I^K, \varphi_I^K)$  and  $(u_O^K, \varphi_O^K)$ , we have

$$c^{0}(u_{A}^{K})_{t} - \Delta u_{A}^{K} + (\varphi_{A}^{K})_{t} =: e_{K}(x, t) = O(\varepsilon^{K-1}), \quad \text{in } \Omega_{T},$$
  
$$\alpha^{0} \varepsilon \varphi_{A}^{K} - \varepsilon \Delta \varphi_{A}^{K} + \varepsilon^{-1} f(\varphi_{A}^{K})_{s}^{0} u_{A}^{K} = O(\varepsilon^{K-1}) \quad \text{in } \Omega_{T}.$$

Finally, making a modification on  $u_A^K$ , of order  $O(\varepsilon^{K-1})$ , we can have that  $c^0(u_K^\varepsilon)_t - \Delta u_K^\varepsilon + (\varphi_A^K)_t = 0$  in  $\Omega_T$ , whereasthe equation for  $\varphi_A^K$  remains unchanged. In summary, we have the following lemma:

**Lemma 4.3** Assume that (2.2) admits a smooth solution. Then, for every positive integer K, there exists  $(\varphi_A^{\varepsilon}, u_A^{\varepsilon})$  such that

$$\begin{cases} \alpha^{0}\varepsilon\varphi_{At}^{\varepsilon} - \varepsilon\Delta\varphi_{A}^{\varepsilon} + \varepsilon^{-1}f(\varphi_{A}^{\varepsilon}) = s^{0}u_{A}^{\varepsilon} + \delta_{A}^{\varepsilon} & \text{in } \Omega_{T}, \\ c^{0}u_{At}^{\varepsilon} - \Delta u_{A}^{\varepsilon} = -(\varphi_{A}^{\varepsilon})_{t} \text{ in } \Omega_{T} & \text{in } \Omega_{T}, \\ \varphi_{A}^{\varepsilon} = \pm 1 + O(\varepsilon), \quad u_{A}^{\varepsilon} = g + O(\varepsilon) & \text{on } \partial_{p}\Omega_{T} \cap (\overline{\Omega_{0}^{\pm}} \times [0, T]) \end{cases}$$

$$(4.23)$$

where  $\delta^{\varepsilon}_A$  satisfies

$$\|\delta^{\varepsilon}_A\|_{C^0(\bar{\Omega}_T)} \leqslant \varepsilon^K$$

In addition, for every  $t \in [0, T]$ ,  $\varphi_A^{\varepsilon}(\cdot, t)$  is uniformly bounded and satisfies the assumption in *Proposition* 3.1.

## 4.6 Boundary layer expansion

From (4.4c), we see that we can let  $u_A^{\varepsilon} = g$  on  $\partial \Omega \times [0, T]$ . However, just using the innerouter expansion, we have  $\varphi_A^{\varepsilon} = 1 + O(\varepsilon)$  on  $\partial \Omega \times [0, T]$ , where the  $O(\varepsilon)$  term depends upon g and other known data. To ensure arbitrary 'compatible' boundary data, for example,  $\varphi_A^{\varepsilon} = 1$  on  $\partial \Omega \times [0, T]$ , we need to use a boundary layer expansion. Here we provide the main idea, and consider only the Dirichlet boundary condition

$$u^{\varepsilon} = g, \qquad \varphi^{\varepsilon} = 1 \qquad \text{on } \partial\Omega \times [0, T].$$

For more details, see [10].

Let  $d_B(x)$  be the distance from x to  $\partial \Omega$ . In a  $\delta$ -neighbourhood of  $\partial \Omega \times [0, T]$ , we seek

solutions of the form

$$u^{\varepsilon} = u^{\varepsilon}_{B}(z, x, t) \Big|_{z = \frac{d_{B}(x)}{\varepsilon}}, \qquad \varphi^{\varepsilon}(x, t) = \varphi^{\varepsilon}_{B}(z, x, t) \Big|_{z = \frac{d_{B}(x)}{\varepsilon}}$$

where

$$u_B^{\varepsilon}(z, x, t) \sim 1 + \sum_{i=0}^{\infty} \varepsilon^i u_B^i(z, x, t),$$
  
$$\varphi_B^{\varepsilon}(z, x, t) \sim \sum_{i=0}^{\infty} \varepsilon^{i+1} \varphi_B^i(z, x, t)$$

where  $z \in [0, \infty)$ ,  $t \in [0, T]$ , and  $x \in \partial \Omega(\delta) := \{x \in \overline{\Omega} : d_B(x) \in [0, \delta)\}$ . The outerboundary matching conditions are, for all  $x \in \partial \Omega(\delta), t \in [0, T]$ ,

$$\begin{cases} D_x^n D_t^m D_z^l(u_B^i(z, x, t) - u_+^i(x, t)) = O(e^{-\beta z}), & \text{as } z \to \infty, \\ D_x^n D_t^m D_z^l(\varphi_B^i(z, x, t) - \varphi_+^i(x, t)) = O(e^{-\beta z}), & \text{as } z \to \infty. \end{cases}$$
(4.24)

Similar to the inner expansion, the boundary layer equations are, for  $i = 0, 1, \dots$ ,

$$\begin{cases} u_{B,zz}^{i} = A_{B}^{i-1}, \\ -\varphi_{B,zz}^{i} + f'(1)\varphi_{k}^{i} = s^{0}u_{B}^{i} + B_{B}^{i-1} \end{cases}$$
(4.25)

where  $z \in (0, \infty)$ ,  $x \in \partial \Omega(\delta)$ ,  $t \in [0, T]$ , and  $A_B^{i-1} = A^{i-1}(z, x, t)$  and  $B_B^{i-1} = B_B^{i-1}(z, x, t)$  are functions depending only on the expansions of order not bigger than i - 1.

Let the zero-th order inner-outer expansion be constructed as in § 4.3. We define

$$u_B^0(z, x, t) = u_+^0(x, t), \qquad \varphi^0(z, x, t) = \varphi_+^0(x, t).$$

for all  $z \in [0, \infty)$ ,  $x \in \partial \Omega(\delta), t \in [0, T]$ .

Assume that all the inner, outer and boundary expansions of order less than i ( $i \ge 1$ ) have been constructed. Assume also that as  $z \to \infty$ ,  $A_B^{i-1}(z, x, t)$  and  $B_B^{i-1}(z, x, t)$ , together with all its partial derivatives, exponentially approach  $A_B^{i-1}(\infty, x, t) \equiv 0$  and  $B^{i-1}(\infty, x, t)$ , respectively. We construct the *i*th order boundary, inner and outer expansion as follows:

Step 1. For each  $x \in \partial \Omega$ ,  $t \in [0, T]$ , solve (4.25) with boundary condition

$$u_B^i(0, x, t) = 0, \qquad \varphi_B^i(0, x, t) = 0.$$
 (4.26)

It is easy to see that there exists a unique *bounded* solution  $u_B^i(z, x, t)$  and  $\varphi_B^i(z, x, t)$ . Step 2. Take  $u_B^i(\infty, x, t)$ ,  $x \in \partial \Omega$ ,  $t \in [0, T]$ , as the boundary value of  $u_+^i$ . Proceeding with the inner-outer expansion process, we can obtain the *i*th order inner-outer expansion. In addition, since

$$\varphi_B^i(\infty, x, t) = s^0 u_B^i(\infty, x, t) / f'(1) + B_B^{i-1}(\infty, x, t) / f'(1),$$

by the actual expression of  $B_+^{i-1}$  and  $B_B^{i-1}$ , one can show that the outer-boundary matching condition (4.24) is satisfied for  $x \in \partial \Omega, t \in [0, T]$ .

Step 3. For all  $x \in \partial \Omega(\delta) \setminus \partial \Omega, t \in [0, T]$ , let  $u_B^i(z, x, t)$  and  $\varphi_B^i$  be the solution of (4.25) with the boundary condition

$$u_B^i(\infty, x, t) = u_+^i(x, t), \qquad \varphi^i(0, x, t) = 0,$$

one can obtain a unique bounded solution  $u_B^i$  and  $\varphi_B^i$ . In addition, one can show that the solution satisfies the outer-boundary matching condition. This completes the construction of the *i*-the expansion.

The 'glue' of inner, outer and boundary layer expansions is similar to that presented in the previous subsection, and is omitted. For more details, see [10].

## Remark 4.2

- (1) In step 3 (i.e. for  $x \in \partial\Omega(\delta) \setminus \partial\Omega$ ,  $t \in [0, T]$ ), the boundary condition  $u_B^i(\infty, x, t) = u_+^i(x, t)$  is mandatary, whereas the condition  $\varphi_B^i(0, x, t) = 0$  is not necessary. In fact, we can let  $\varphi_B^i(0, x, t)$  be any given smooth function  $\varphi_0^i(x, t)$  which satisfies  $\varphi_0^i(x, t) = 0$  on  $\partial\Omega \times [0, T]$ . Although this appears to create non-uniqueness, it will not interfere with the sum  $1 + \sum_{i=1}^{K} \varepsilon^{i+1} \varphi_B^i(\frac{d_B(x)}{\varepsilon}, x, t)$  in  $O(\varepsilon^{K+1})$  order, since all the arbitrariness will cancel in the later expansions, at the hypersurface  $z = \frac{d_B(x)}{\varepsilon}$ . This is the same idea as making smooth extension for the function  $u_+^i$  into  $\Gamma^0(\delta) \setminus Q^{\pm}(\delta)$ .
- (2) The reason that we cannot restrict ourself to considering only  $x \in \partial \Omega$  for the boundary expansion is that in the expression of  $A_B^{i-1}$  and  $B_B^{i-1}$ , there are terms involving the spatial derivatives of the boundary layer expansion terms.
- (3) Our analysis extends to the case when the boundary data  $u^{\varepsilon} = g$  and  $\varphi^{\varepsilon} = \varphi_0$  have the expansion

$$g = \sum_{i=0}^{\infty} \varepsilon^i g_i(x,t), \qquad h = 1 + \sum_{i=0}^{\infty} \varepsilon^{i+1} \varphi_0^i(x,t).$$

In fact, we need only modify the boundary condition for  $u_B^i$  and  $\varphi_B^i$  in Step 1 and the boundary condition for  $\varphi_B^i$  in Step 3.

(4) For Neumann or mixed boundary conditions, one can use the fact that  $\partial_n|_{\partial\Omega} = -\frac{1}{\varepsilon}\frac{\partial}{\partial z} - \nabla d_B \cdot \nabla_x$  and follow the same step to obtain boundary-inner-outer expansions, though it is more subtle and a little bit more complicated (see [10]).

## 5 Proof of the main theorems

**Proof of Theorem 2.1** The convergence of  $\varphi_A^{\varepsilon}$  to  $\varphi^{\varepsilon}$  in  $L^p$  follows from Theorem 3.1, Proposition 3.1 and Lemma 4.3. By Remark 3.1,  $\varphi_A^{\varepsilon} \to \varphi^{\varepsilon}$  in  $C^1$  if we construct higher order approximate solutions. Using the differential equations, we also know that  $u_A^{\varepsilon} \to u^{\varepsilon}$ in  $C^1$ . Since the leading order expansion of  $(u_A^{\varepsilon}, \varphi_A^{\varepsilon})$  coincides with the solution of the free boundary problem, we obtain the assertion of Theorem 2.1.

**Proof of Theorem 2.2** (1) Changing the boundary conditions will not affect the essential conclusions of Theorem 3.1, Proposition 3.1, and the construction of approximate solutions in § 4, so that the assertion of Theorem 2.1 holds if one replaces the boundary conditions.

(2)–(6). With the new  $\alpha(\varepsilon)$ ,  $s(\varepsilon)$ , and  $c(\varepsilon)$ , Theorem 3.1 and Proposition 3.1 remain valid, whereas in the construction of the approximation solutions, one only equates the terms of  $\varepsilon^i$  for the new system, which leads to the revised conclusion. The existence of a system similar to (4.22) can be proved in a manner similar to (but simpler than) the corresponding free boundary problem. In fact, (4.22) is a linearization of the corresponding free boundary problem.

## 6 Conclusion

We have proved that the solutions to the phase field equations converge to those of the corresponding sharp interface problems in each of the distinguished limits. Since there are no symmetry or other geometric assumptions on the domain other than regularity of the boundary, this general proof completes the rigorous foundation for the asymptotic analysis of the phase field equations. The sharp interface problems are defined within the context of classical (smooth) interfaces so that our basic assumption of the existence of such solutions is logically a natural limitation. When there is no smooth solution to the limiting sharp interface problem, the numerical studies confirm that the phase field equations still provide a reasonable physical description. However, the physically correct sharp interface problems have not been formulated in the case of self-intersections, and while the equilibrium conditions for intersections between the interface and external boundary are well understood, the dynamical conditions are a current research topic.

When  $\Gamma$  is not smooth, the sharp interface problems can be defined within the context of a particular mathematical regularization procedure that may or may not be the correct one physically. A more complete sharp interface problem can perhaps be obtained by a systematic derivation of interface conditions in each of the topological possibilities for the particular spatial dimension. Derivations from distinct perspectives including the phase field approach would be useful in understanding the range of validity of each avenue.

Remaining theoretical issues related to the convergence include the rate of the convergence and comparisons in convergence rates between different phase field models. These questions are particularly important to numerical studies where  $\varepsilon$  must be made significantly larger than its physically realistic (atomic) scale.

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