Interfaces and Free Boundaries **8** (2006), 131–157

Second order phase field asymptotics for multi-component systems

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[Received 25 January 2005 and in revised form 8 September 2005]

We derive a phase field model which approximates a sharp interface model for solidification of a multicomponent alloy to second order in the interfacial thickness ε. Since in numerical computations for phase field models the spatial grid size has to be smaller than ε the new approach allows for considerably more accurate phase field computations than have been possible so far.

In the classical approach of matched asymptotic expansions the equations to lowest order in ε lead to the sharp interface problem. Considering the equations to the next order, a correction problem is derived. It turns out that, when taking a possibly non-constant correction term to a kinetic coefficient in the phase field model into account, the correction problem becomes trivial and the approximation of the sharp interface problem is of second order in ε. By numerical experiments, the better approximation property is well supported. The computational effort to obtain an error smaller than a given value is investigated, revealing an enormous efficiency gain.

2000 Mathematics Subject Classification: 82C26, 82C24, 35K55, 34E05, 35B25, 35B40, 65M06.

Keywords: Phase field models; sharp interface models; numerical simulations; matched asymptotic expansions.

1. Introduction

In sharp interface approaches to solidification, phase boundaries are modeled as hypersurfaces across which certain quantities jump. In the last two decades also the phase field method has become a powerful tool for modeling the microstructural evolution during solidification (see [7, 25, 11, 8] for reviews). Instead of explicitly tracking the solid-liquid interface an order parameter is used. It takes different values in the phases and changes smoothly in the interfacial regions, which leads to the notion of diffuse interface models. The typical thickness of the diffuse interface is related to a small parameter ε. In the limit as $\varepsilon \to 0$ sharp interface models are recovered.

The relation between the phase field model and the free boundary problem is established using the method of matched asymptotic expansions. It is assumed that the solution to the phase field model can be expanded in ε-series in the bulk regions occupied by the phases (outer expansion) and, using rescaled coordinates, in the interfacial regions (inner expansion). To leading order in ε, a sharp interface problem is obtained. If we consider the phase field system as an approximation of the sharp interface problem it would of course be desirable that phase field solutions converge fast with respect to ε to solutions to the sharp interface problem. This becomes even more important as in numerical computations the spatial grid size has to be chosen smaller than ε (see e.g. [13]). In

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this paper we are interested in phase field approximations of the sharp interface problem which are of second order, i.e., we aim for constructing phase field systems such that the first order correction in the ε-expansion vanishes. This would then lead to much more efficient numerical approaches for solidification.

The method is formal in the sense that, a posteriori, it is not controlled whether the asymptotic expansions really exist and converge. In the context of solidification it has been applied on models for pure substances [10, 26], alloys [30, 5], multi-phase systems [16], and systems with both multiple phases and components [15] in order to derive sharp interface limits (first order asymptotics). We remark that, in some cases, this ansatz has been verified by rigorously showing that, in the limit as $\varepsilon \to 0$, the sharp interface model is obtained from the diffuse interface model (see e.g. [1, 10, 24, 28]).

Our interest in the higher order approximation is motivated by the results obtained by Karma and Rappel [19] in the context of thin interface asymptotics where the interface thickness is small but remains finite. Their analysis led to a positive correction term in the kinetic coefficient of the phase field equation balancing undesirable $O(\varepsilon)$-terms in the Gibbs–Thomson condition and raising the stability bound of explicit numerical methods. Moreover, the better approximation allows for larger values of ε and, therefore, for coarser grids. In particular, it is possible to consider the limit of vanishing kinetic undercooling. Almgren [2] extended the analysis to the case of different diffusivities in the phases and discussed both classical asymptotics and thin interface asymptotics. By choosing different interpolation functions for free energy density and internal energy density, an approximation to second order can still be achieved but the gradient structure of the model and thermodynamical consistency are lost. Andersson [4] showed, based on the work of Almgren, that even an approximation of third order is possible by using high order polynomials for the interpolation. McFadden, Wheeler, and Anderson [23] used an approach based on an energy and an entropy functional providing more degrees of freedom to tackle the difficulties with unequal diffusivities in the phases while avoiding the loss of the thermodynamical consistency. Again, both classical and thin asymptotics are discussed as well as the limit of vanishing kinetic undercooling. In a more recent analysis Ramirez et al. [27] considered a binary alloy also involving different diffusivities in the phases and obtained a better approximation by adding a small additional term to the mass flux (antitrapping mass current, the ideas stem from [18]).

We aim to extend the results to general non-isothermal multi-component alloy systems allowing for arbitrary phase diagrams with two phases. The models studied in the literature usually use the free energy or the entropy as thermodynamical potentials (see e.g. [3, 26, 29, 30] and the discussion in [20]). It turns out that, in our context, the reduced grand canonical potential ψ (see [22]) is more appropriate for the analysis. To motivate this let us review some thermodynamics.

We will, for simplicity, consider a system with uniform density, which is in mechanical equilibrium throughout the evolution. Changes in pressure or volume are neglected. In this case, the Helmholtz free energy density f is an appropriate thermodynamical quantity to work with. It is conveniently written as a function of the absolute temperature T and the concentrations $\boldsymbol{c} = (c^{(1)}, \dots, c^{(N)}) \in \mathbb{R}^N$, its derivatives being the negative entropy density $-s$ and the chemical potentials $\boldsymbol{\mu} = (\mu^{(1)}, \dots, \mu^{(N)}) \in \mathbb{R}^N$,

$$\mathrm{d}f = -s\, \mathrm{d}T + \boldsymbol{\mu} \cdot \mathrm{d}\boldsymbol{c}.$$

Here, the central dot denotes the scalar product on $\mathbb{R}^N$. The internal energy density is $e = f + Ts$. For the reduced grand canonical potential $\psi = -g/T$, $g = f - \boldsymbol{\mu} \cdot \boldsymbol{c}$ being the grand canonical potential, we then obtain

$$\mathrm{d}\psi = \mathrm{d}\left(\frac{f - \boldsymbol{\mu}\cdot\boldsymbol{c}}{-T}\right) = e\,\mathrm{d}\left(\frac{-1}{T}\right) + \boldsymbol{c}\cdot\mathrm{d}\left(\frac{\boldsymbol{\mu}}{T}\right),$$

in particular $\boldsymbol{u} = (u^{(0)}, \tilde{\boldsymbol{u}}) = (-1/T, \boldsymbol{\mu}/T) \in \mathbb{R}^{N+1}$ are the variables conjugate to $(e, \boldsymbol{c}) \in \mathbb{R}^{N+1}$. Assuming local thermodynamical equilibrium the vector $\boldsymbol{u}$ is continuous across the free boundary in a sharp interface model. This will be important in the matched asymptotic expansions studied later and therefore we will state the problem from the beginning in these variables. We refer to Appendix A for more details on the thermodynamical background.

Next, we will briefly state a sharp interface problem for a liquid-solid phase change in a non-isothermal multi-component system (cf. [15] for more details). Let D^l and D^s be the domains occupied respectively by the liquid phase and the solid phase and let Γ be the interface separating the phases. In D^l and D^s, conservation of mass and energy is expressed by the balance equations

$$\partial_t \psi_{,u^{(i)}}(\boldsymbol{u}) = -\nabla\cdot J_i = -\nabla\cdot\sum_{j=0}^{N} L_{ij}\nabla(-u^{(j)}), \qquad 0 \leqslant i \leqslant N, \tag{1}$$

where $\psi_{,u^{(0)}} = e$ and $\psi_{,u^{(i)}} = c^{(i)}$ denote derivatives of ψ, the J_i are the fluxes, and $\underline{L} = (L_{ij})_{i,j}$ is a matrix of Onsager coefficients which may depend on $\boldsymbol{u}$. Constitutive relations between ψ, $\underline{L}$, and $\boldsymbol{u}$ may depend on the two phases s and l. On Γ we have

$$u^{(i)} \text{ is continuous}, \qquad 0 \leqslant i \leqslant N, \tag{2}$$

$$[-J_i]_s^l\cdot\nu = \left[-\sum_{j=0}^{N} L_{ij}\nabla u^{(j)}\right]_s^l\cdot\nu = v[\psi_{,u^{(i)}}(\boldsymbol{u})]_s^l, \qquad 0 \leqslant i \leqslant N, \tag{3}$$

$$\alpha v = \sigma\kappa - [\psi(\boldsymbol{u})]_s^l, \tag{4}$$

where ν is the unit normal on Γ pointing into D^l, v is the normal velocity in the direction ν, σ is the surface tension, κ the curvature, α a kinetic coefficient, and $[\cdot]_s^l$ denotes the jump of the quantity in the brackets, for example $[\psi(\boldsymbol{u})]_s^l = \psi_l(\boldsymbol{u}) - \psi_s(\boldsymbol{u})$. Equations (2) and (3) are also due to conservation of mass and energy. The Gibbs–Thomson condition (4) couples the motion of the phase boundaries to the thermodynamical quantities of the adjacent phases such that, locally, entropy production is non-negative. For the case of a system involving multiple phases this is shown in [15].

The above stated sharp interface model will be approximated by a phase field model of the form

$$\omega\partial_t\varphi = \sigma\Delta\varphi - \sigma\frac{1}{\varepsilon^2}w'(\varphi) + \frac{1}{2\varepsilon}h'(\varphi)(\psi_l(\boldsymbol{u}) - \psi_s(\boldsymbol{u})), \tag{5}$$

$$\partial_t\psi_{,u^{(i)}}(\boldsymbol{u},\varphi) = \nabla\cdot\sum_{j=0}^{N} L_{ij}\nabla u^{(j)}, \qquad 0 \leqslant i \leqslant N. \tag{6}$$

Here, φ is the phase field variable. We have $\varphi = 1$ in the liquid phase and $\varphi = 0$ in the solid phase. The function w is a double-well potential with minima at 0 and 1 corresponding to the values of φ in the pure phases. The reduced grand canonical potentials ψ_l and ψ_s of the pure phases are interpolated to obtain the system potential $\psi(\boldsymbol{u},\varphi)$. For this purpose, interpolation functions between 0 and 1 like $h(\varphi)$ in the above equation are used.

The approximation of the sharp interface model has to be understood in the following sense: Assume that solutions $(\boldsymbol{u}, \varphi)$ to (5) and (6) can be expanded in ε-series of the form

$$\boldsymbol{u} = \boldsymbol{u}_0 + \varepsilon \boldsymbol{u}_1 + \cdots , \qquad \varphi = \varphi_0 + \varepsilon \varphi_1 + \cdots ,$$

and similarly in the interfacial regions using coordinates which are partially rescaled in ε (the expansions are precisely stated in Section 2, as is the following matching procedure). After matching the expansions, $\boldsymbol{u}_0$ and φ_0 solve (1)–(4) where $D^l = \{\varphi_0 = 1\}$, $D^s = \{\varphi_0 = 0\}$, Γ is the set where φ_0 jumps, and α is related to ω.

As long as the first order correction terms $(\boldsymbol{u}_1, \varphi_1)$ do not vanish the approximation of the sharp interface model by the phase field model is said to be *of order one*. Otherwise it is (at least) *of order two*. To see whether this is the case one has to derive and analyze the equations satisfied by $(\boldsymbol{u}_1, \varphi_1)$. Our result now reads as follows:

MAIN RESULT. *Consider a two-phase multi-component system with arbitrary phase diagram. Then there is a possibly non-constant correction term to the kinetic coefficient* ω *such that the sharp interface model* (1)-(4) *is approximated by the phase field model* (5), (6) *to second order. The kinetic coefficient has the structure* $\omega = \omega_0 + \varepsilon \omega_1(\boldsymbol{u})$ *where*

$$\omega_1(\boldsymbol{u}) = [\psi_{,\boldsymbol{u}}(\boldsymbol{u})]_s^l \cdot \underline{L}^{-1} [\psi_{,\boldsymbol{u}}(\boldsymbol{u})]_s^l C$$

with some constant C *depending on the interpolation function* h.

A new feature compared to the existing results in [2, 4, 19] is that, in general, this correction term depends on $\boldsymbol{u}$, i.e. on temperature and chemical potentials. Indeed, up to some numerical constants, the latent heat appears in the correction term obtained by Karma and Rappel [19]. Analogously, the equilibrium jump in the concentrations enters the correction term when an isothermal binary alloy is investigated. But from realistic phase diagrams it can be seen that this jump depends on the temperature leading to a temperature dependent correction term in the non-isothermal case.

Our model will be described in Section 2. In Section 3 we will apply matched asymptotic expansions to deduce a linear parabolic $O(\varepsilon)$-correction problem. Given appropriate initial and boundary conditions, zero is a solution to the correction problem. By numerical simulations of suitable test problems we investigate the gain in efficiency due to the better approximation. For this purpose, numerical approximations of solutions to the phase field model with and without the correction term are compared in Section 4.

2. Phase field model for multi-component systems

Let $D \subset \mathbb{R}^d$, $d = 1, 2, 3$, be a spatial domain with Lipschitz boundary which is occupied by an alloy and let $I = [0, t_{\max}]$ be a time interval. Further, let $N \in \mathbb{N}$ be the number of components in the system.

CONVENTION. Throughout this article, partial derivatives are sometimes denoted by subscripts after a comma. For example, $\psi_{,\boldsymbol{u}\varphi}(\boldsymbol{u}, \varphi)$ denotes the second order mixed derivative of $\psi(\boldsymbol{u}, \varphi)$ with $\boldsymbol{u}$ and φ. Vectors of size $N + 1$ are printed in bold face except for the derivatives of ψ, ψ_s, and ψ_l with respect to $\boldsymbol{u}$. Tensors of size $(N + 1) \times (N + 1)$ are underlined.

2.1 *Motivation*

The Allen–Cahn equation

$$\omega_0 \partial_t \varphi = \Delta\varphi - \frac{1}{\varepsilon^2} w'(\varphi)$$

models the motion of an interface between two phases; here, φ is a phase field variable. It describes the presence of one of the phases. In the regions occupied by pure phases, φ takes values close to 0 or 1. These values are the absolute minima of the double-well potential w. In transition regions connecting the regions occupied by the pure phases, φ varies smoothly between 0 and 1 due to the diffusion term $\Delta\varphi$. The transition region will turn out to have a thickness of order ε. By adding further terms a dependence of the interface motion on thermodynamical quantities can be modeled.

The above differential equation is coupled to balance equations for energy and mass. The thermodynamical potentials are postulated to be the derivatives of the entropy density (see [15]), and for the fluxes we postulate linear combinations of the corresponding thermodynamical forces, hence with Onsager coefficients L_{ij} we obtain

$$\begin{aligned}
\partial_t e &= -\nabla \cdot \left(L_{00}(T, \boldsymbol{c}, \varphi)\nabla \frac{1}{T} + \sum_{j=1}^{N} L_{0j}(T, \boldsymbol{c}, \varphi)\nabla \frac{-\mu^{(j)}}{T} \right), \\
\partial_t c^{(i)} &= -\nabla \cdot \left(L_{i0}(T, \boldsymbol{c}, \varphi)\nabla \frac{1}{T} + \sum_{j=1}^{N} L_{ij}(T, \boldsymbol{c}, \varphi)\nabla \frac{-\mu^{(j)}}{T} \right),
\end{aligned}$$

where T is the temperature and $\boldsymbol{c} = (c^{(1)}, \dots, c^{(N)})$ a vector of concentrations, $c^{(i)}$ describing the presence of component i. Given the free energy density $f = f(T, \boldsymbol{c})$, the chemical potential corresponding to component i is the derivative of f with respect to $c^{(i)}$, i.e. $\mu^{(i)} = f_{,c^{(i)}}$. The internal energy density is $e = f + sT$, $s = -f_{,T}$ being the entropy density.

2.2 *Model and assumptions*

It turns out to be more appropriate to write down the above conservation laws in terms of the variables $\boldsymbol{u} = (-1/T, \boldsymbol{\mu}/T)$ and to use the reduced grand canonical potential as the thermodynamical potential (see Appendix A for the thermodynamical relations). We define the set

$$\Sigma^N := \left\{ \boldsymbol{c} = (c^{(1)}, \dots, c^{(N)}) \in \mathbb{R}^N : \sum_{i=1}^{N} c^{(i)} = 1 \right\},$$

and identify its tangent space at every point $\boldsymbol{c}$ with

$$T\Sigma^N := \left\{ \tilde{\boldsymbol{u}} = (u^{(1)}, \dots, u^{(N)}) \in \mathbb{R}^N : \sum_{i=1}^{N} u^{(i)} = 0 \right\}.$$

Moreover, we define $Y := \mathbb{R} \times T\Sigma^N$. The problem then consists in finding smooth functions

$$\varphi : I \times D \to \mathbb{R}, \qquad \boldsymbol{u} = (u^{(0)}, \dots, u^{(N)}) : I \times D \to Y$$

that solve the partial differential equations

$$(\omega_0 + \varepsilon\omega_1(\boldsymbol{u}))\partial_t\varphi = \varDelta\varphi - \frac{1}{\varepsilon^2}w'(\varphi) + \frac{1}{2\varepsilon}h'(\varphi)\varPsi(\boldsymbol{u}), \tag{7}$$

$$\partial_t\psi_{,u^{(i)}}(\boldsymbol{u},\varphi) = \nabla\cdot\sum_{j=0}^{N}L_{ij}\nabla u^{(j)}, \qquad 0 \leqslant i \leqslant N. \tag{8}$$

The first equation is a forced Allen–Cahn equation for the phase field variable φ. The coupling to the thermodynamical quantities via the last term in that equation will be clarified below. We are interested in the limit $\varepsilon \to 0$. The function $\omega_1 : Y \to \mathbb{R}$ is some correction term in order to obtain quadratic convergence and will be determined later. The derivatives of the reduced grand canonical potential are the conserved quantities of energy $e = \psi_{,u^{(0)}}$ and concentrations $c^{(i)} = \psi_{,u^{(i)}}$, $1 \leqslant i \leqslant N$ (see Appendix A for the exact relation between $(e, \boldsymbol{c})$ and the derivatives of ψ with respect to $\boldsymbol{u}$). The equations in (7) are the balance equations for these conserved quantities. Concerning all the other functions and constants appearing in the above equations we make the following definitions and assumptions:

A. ω_0 is a positive constant.

B. $w : \mathbb{R} \to \mathbb{R}^+$ is some nonnegative smooth double-well potential which attains its global minima at 0 and 1; more precisely, we have

$$\begin{aligned}&w(\varphi) > 0 \quad \text{if } \varphi \notin \{0,1\},\\ &w(0) = w(1) = 0, \qquad w'(0) = w'(1) = 0, \qquad w''(0) = w''(1) > 0.\end{aligned}$$

Moreover, w is symmetric with respect to 1/2, i.e. $w(1/2 + \varphi) = w(1/2 - \varphi)$.

C. $h : \mathbb{R} \to \mathbb{R}$ is a monotone symmetric interpolation function between 0 and 1, i.e.

$$h(0) = 0, \qquad h(1) = 1, \qquad h(1/2 + \varphi) = 1 - h(1/2 - \varphi), \qquad h'(\varphi) \geqslant 0.$$

Furthermore, we require that $h'(0) = h'(1) = 0$.

D. $\psi : Y \times \mathbb{R} \to \mathbb{R}$ is smooth and given as interpolation between the reduced grand canonical potentials of the two possible phases s and l, i.e.

$$\psi(\boldsymbol{u},\varphi) = \psi_s(\boldsymbol{u}) + \tilde{h}(\varphi)(\psi_l(\boldsymbol{u}) - \psi_s(\boldsymbol{u}))$$

with a function $\tilde{h}$ satisfying Assumption C. Observe that in the case $\tilde{h} \neq h$ the model lacks thermodynamical consistency, i.e. an entropy inequality might not hold (see [26, 19, 2]). In (7) we used the abbreviation

$$\varPsi(\boldsymbol{u}) := \psi_l(\boldsymbol{u}) - \psi_s(\boldsymbol{u}).$$

The function ψ is convex in $\boldsymbol{u}$ so that (8) becomes parabolic. We will frequently use $\psi(\boldsymbol{u},\varphi)$, $\psi_s(\boldsymbol{u})$ and $\psi_l(\boldsymbol{u})$ as functions of arbitrary $\boldsymbol{u} \in \mathbb{R}^{N+1}$, which enables one to write down the partial derivative $\psi_{,u^{(k)}}(\boldsymbol{u},\varphi)$. But no results depend on the extension as only arguments $\boldsymbol{u} \in Y$ and derivatives along Y will be used.

E. The matrix $\underline{L} = (L_{ij})_{i,j=0}^{N}$ of Onsager coefficients is constant, symmetric, positive semi-definite, and the kernel is exactly $Y^\perp = \text{span}\{(0,1,\dots,1) \in \mathbb{R}^{N+1}\}$. Observe that then

$$\sum_{i=1}^{N}L_{ij} = 0,\ 0 \leqslant j \leqslant N \ \Rightarrow\ \partial_t\Big(\sum_{i=1}^{N}\psi_{,u^{(i)}}(\boldsymbol{u},\varphi)\Big) = 0 \ \Rightarrow\ \partial_t(\psi_{,\boldsymbol{u}}(\boldsymbol{u},\varphi)) \in Y.$$

Moreover, for each $v \in Y$ the linear system $\underline{L}\xi = v$ has exactly one solution $\xi \in Y$ which we will denote by $\xi = \underline{L}^{-1}v$.
The handling of dependence on $\boldsymbol{u}$ is straightforward (cf. the remark at the end of Subsection 3.5), and dependence of the diffusivities on the phase has already been considered in [2]. Therefore, the analysis is restricted to this simple case.

2.3 *Evolving curves*

To relate the diffuse interface model to a sharp interface model, the method of formally matched asymptotic expansions will be used. The procedure is outlined with great care in [14, 12]. Here, we will only sketch the main ideas for the two-dimensional case, i.e. $d = 2$.

For some $\varepsilon > 0$ we will denote a smooth solution to (7) and (8) by $(\boldsymbol{u}(t, x; \varepsilon), \varphi(t, x; \varepsilon))$. The family of curves

$$\Gamma(t; \varepsilon) := \{x \in D : \varphi(t, x; \varepsilon) = 1/2\}, \qquad \varepsilon > 0,\ t \in I, \tag{9}$$

is supposed to be a set of smooth curves in D. In addition, we assume that they are uniformly bounded away from ∂D and depend smoothly on (ε, t) so that as $\varepsilon \to 0$ some limiting curve $\Gamma(t; 0)$ is obtained. We denote by $D^l(t; \varepsilon)$ and $D^s(t; \varepsilon)$ the regions occupied by the liquid phase (where $\varphi(t, x; \varepsilon) > 1/2$) and the solid phase (where $\varphi(t, x; \varepsilon) < 1/2$) respectively.

Let $\gamma(t, s; 0)$ be a parametrization of $\Gamma(t; 0)$ by arc-length s for every $t \in I$. The vector $\nu(t, s; 0)$ denotes the unit normal on $\Gamma(t; 0)$ pointing into $D^l(t; 0)$, and $\tau(t, s; 0) := \partial_s \gamma(t, s; 0)$ denotes the unit tangent vector. The orientation is such that (ν, τ) is positively oriented.

We assume that the curves $\Gamma(t; \varepsilon)$ can be parametrized over $\Gamma(t; 0)$ using some distance function $d(t, s; \varepsilon)$ by

$$\gamma(t, s; \varepsilon) := \gamma(t, s; 0) + d(t, s; \varepsilon)\nu(t, s; 0). \tag{10}$$

Close to $\varepsilon = 0$ we assume that there is an expansion $d(t, s; \varepsilon) = d_0(t, s) + \varepsilon^1 d_1(t, s) + \varepsilon^2 d_2(t, s) + O(\varepsilon^3)$. As $d(t, s; 0) \equiv 0$ we conclude that $d_0(t, s) \equiv 0$.

Also the curvature $\kappa(t, s; \varepsilon)$ and the normal velocity $v(t, s; \varepsilon)$ of $\Gamma(t; \varepsilon)$ are smooth and can be expanded (see Appendix C). We get

$$\begin{aligned}
\kappa(t, s; \varepsilon) &= \kappa(t, s; 0) + \varepsilon(\kappa(t, s; 0)^2 d_1(t, s) + \partial_{ss} d_1(t, s)) + O(\varepsilon^2), \\
v(t, s; \varepsilon) &= \partial_t \gamma(t, s; \varepsilon) \cdot \nu(t, s; \varepsilon) = v(t, s; 0) + \varepsilon \partial^\circ d_1(t, s) + O(\varepsilon^2);
\end{aligned}$$

here, $\partial^\circ = \partial_t - v_\tau \partial_s$ denotes the (intrinsic) normal time derivative, $v_\tau = \partial_t \gamma \cdot \tau$ being the non-intrinsic tangential velocity (cf. Appendix B).

2.4 *Definition of outer variables*

We suppose that in each domain E whose closure $\overline{E}$ with respect to the topology on $\mathbb{R}^d$ satisfies $\overline{E} \subset D \backslash \Gamma(t; 0)$ the solution can be expanded in a series close to $\varepsilon = 0$ (outer expansion):

$$\boldsymbol{u}(t, x; \varepsilon) = \sum_{k=0}^{K} \varepsilon^k \boldsymbol{u}_k(t, x) + O(\varepsilon^{K+1}), \qquad \varphi(t, x; \varepsilon) = \sum_{k=0}^{K} \varepsilon^k \varphi_k(t, x) + O(\varepsilon^{K+1}). \tag{11}$$

Near $\Gamma(t;0)$, we can define the coordinates (s,r), r being the signed distance of x from $\Gamma(t;0)$ (positive in direction ν, i.e. if $x \in D^l(t;0)$). Hence, in a neighborhood of $\Gamma(t;0)$ we can write, for $r \neq 0$,

$$\hat{\boldsymbol{u}}(t,s,r;\varepsilon) = \boldsymbol{u}(t,x;\varepsilon), \qquad \hat{\varphi}(t,s,r;\varepsilon) = \varphi(t,x;\varepsilon). \tag{12}$$

2.5 *Definition of inner variables*

Let z be the $1/\varepsilon$-scaled signed distance of x from $\Gamma(t;0)$, i.e. $z = r/\varepsilon$, and let $\boldsymbol{U}(t,s,z;\varepsilon) := \hat{\boldsymbol{u}}(t,s,r;\varepsilon)$, $\Phi(t,s,z;\varepsilon) := \hat{\varphi}(t,s,r;\varepsilon)$. We now suppose that we can expand $\boldsymbol{U}$ and Φ in these new variables as follows:

$$\boldsymbol{U}(t,s,z;\varepsilon) = \sum_{k=0}^{K} \varepsilon^k \boldsymbol{U}_k(t,s,z) + O(\varepsilon^{K+1}), \tag{13}$$

$$\Phi(t,s,z;\varepsilon) = \sum_{k=0}^{K} \varepsilon^k \Phi_k(t,s,z) + O(\varepsilon^{K+1}). \tag{14}$$

2.6 *Matching conditions*

For the two expansions for $\boldsymbol{u}$ to match in the limit as $\varepsilon \to 0$, certain conditions are necessary (see Appendix D for the derivation): as $z \to \pm\infty$ for all $i \in \{0,\dots,N\}$,

$$\boldsymbol{U}_0^{(i)}(z) \approx \boldsymbol{u}_0^{(i)}(0^\pm), \tag{15}$$

$$\boldsymbol{U}_1^{(i)}(z) \approx \boldsymbol{u}_1^{(i)}(0^\pm) + (\nabla \boldsymbol{u}_0^{(i)}(0^\pm)\cdot\nu)z, \tag{16}$$

$$\partial_z \boldsymbol{U}_1^{(i)}(z) \approx \nabla \boldsymbol{u}_0^{(i)}(0^\pm)\cdot\nu, \tag{17}$$

$$\partial_z \boldsymbol{U}_2^{(i)}(z) \approx \nabla \boldsymbol{u}_1^{(i)}(0^\pm)\cdot\nu + ((\nu\cdot\nabla)(\nu\cdot\nabla)\boldsymbol{u}_0^{(i)}(0^\pm))z \tag{18}$$

and analogously for Φ and φ. Here, for a function $g(t,x) = \hat{g}(t,s,r)$,

$$g(0^+) := \lim_{r\searrow 0} \hat{g}(t,s,r), \qquad g(0^-) := \lim_{r\nearrow 0} \hat{g}(t,s,r),$$

where $r = \mathrm{dist}(x,\Gamma(t;0))$. Remember that $r > 0$ if and only if $x \in D^l(t;0)$, and that $r < 0$ if and only if $x \in D^s(t;0)$.

3. Asymptotic analysis

3.1 *Outer solutions*

In the region away from $\Gamma(t;0)$ we plug the expansions (11) into the differential equations (7) and (8). All terms that appear are expanded in ε.

To leading order $O(\varepsilon^{-2})$ we obtain from (7) the identity $0 = -w'(\varphi_0)$. But the only stable solutions to this equation are the minima of w, hence $\varphi_0 \equiv 0$ or $\varphi_0 \equiv 1$. We define $D^s(t;0)$ as the set of all points with $\varphi_0 = 0$ and similarly $D^l(t;0)$ with $\varphi_0 = 1$.

To the next order $O(\varepsilon^{-1})$ we obtain

$$0 = -w''(\varphi_0)\varphi_1 + \tfrac{1}{2}h'(\varphi_0)\Psi(\boldsymbol{u}_0). \tag{19}$$

As $\varphi_0 = 0$ or $= 1$, using Assumptions B and C we obtain $\varphi_1 \equiv 0$ as the only solution.

To leading order $O(\varepsilon^0)$ we obtain from (8), written as a vectorial equation,

$$\partial_t(\psi_{,\boldsymbol{u}}(\boldsymbol{u}_0, \varphi_0)) = \underline{L}\Delta \boldsymbol{u}_0. \tag{20}$$

Depending on φ_0 we have $\psi_{,\boldsymbol{u}}(\boldsymbol{u}_0, \varphi_0) = (\psi_l)_{,\boldsymbol{u}}(\boldsymbol{u}_0)$ or $\psi_{,\boldsymbol{u}}(\boldsymbol{u}_0, \varphi_0) = (\psi_s)_{,\boldsymbol{u}}(\boldsymbol{u}_0)$. In both cases (20) is a parabolic equation for $\boldsymbol{u}_0$ by Assumption D.

To order $O(\varepsilon^1)$ we obtain

$$\partial_t((\underline{\psi_{,\boldsymbol{uu}}})(\boldsymbol{u}_0, \varphi_0)\boldsymbol{u}_1) = \underline{L}\Delta \boldsymbol{u}_1 \tag{21}$$

where we have already made use of $\varphi_1 \equiv 0$. Assumption D states that ψ is convex so that (21) is a linear parabolic equation for $\boldsymbol{u}_1$.

To determine boundary conditions for (20) and (21) on $\Gamma(t; 0)$ we plug the expansions (13) and (14) into the differential equations.

3.2 *Inner solutions to leading order*

In Appendix B we describe how the derivatives with respect to (t, x) transform into derivatives with respect to (t, s, z). To leading order $O(\varepsilon^{-2})$ we get from (7)

$$0 = \partial_{zz}\Phi_0 - w'(\Phi_0). \tag{22}$$

By (9) and the assumption that (14) holds true for $\varepsilon = 0$ we have $\Phi_0(0) = 1/2$. The matching conditions (15) imply

$$\begin{aligned} \Phi_0(t, s, z) &\to \varphi(t, s; 0^+) = 1 \quad \text{as } z \to \infty, \\ \Phi_0(t, s, z) &\to \varphi(t, s; 0^-) = 0 \quad \text{as } z \to -\infty. \end{aligned}$$

Therefore $\Phi_0(z)$ only depends on z. Furthermore Φ_0 is monotone, approximates the values at $\pm\infty$ exponentially fast and satisfies $\Phi_0(-z) = 1 - \Phi_0(z)$.

For the conserved variables we get from (8)

$$\boldsymbol{0} = \underline{L}\partial_{zz}\boldsymbol{U}_0. \tag{23}$$

Using Assumption E we have $\partial_{zz}\boldsymbol{U}_0 = \underline{L}^{-1}\boldsymbol{0} = \boldsymbol{0}$ in Y so that $\boldsymbol{U}_0$ is affine linear in z. By the matching conditions (15), $\boldsymbol{U}_0$ has to be bounded as $z \to \pm\infty$, hence we see that $\boldsymbol{U}_0$ must be constant in z, which means $\boldsymbol{U}_0 = \boldsymbol{U}_0(t, s)$. The matching condition (15) implies that $\boldsymbol{U}_0(t, s)$ is exactly the value of $\boldsymbol{u}_0$ at the point $\gamma(t, s; 0) \in \Gamma(t; 0)$ from both sides of the interface. In particular,

$$\boldsymbol{u}_0 \text{ is continuous across the interface } \Gamma(t; 0). \tag{24}$$

3.3 *Inner solutions to first order*

To order $O(\varepsilon^{-1})$ equation (7) yields

$$-\omega_0 v\partial_z\Phi_0 = \partial_{zz}\Phi_1 - \kappa\partial_z\Phi_0 - w''(\Phi_0)\Phi_1 + \tfrac{1}{2}h'(\Phi_0)\Psi(\boldsymbol{U}_0). \tag{25}$$

From the solution to (19) we get $\varphi_1(t, s, 0^\pm) = 0$. Moreover, $\nabla\varphi_0(t, s, 0^\pm) \cdot \nu = 0$ as φ_0 is constant. Due to the matching conditions (16) we have $\Phi_1 \to 0$ as $z \to \pm\infty$. The operator $\mathcal{L}(\Phi_0)b =$

$\partial_{zz} b - w''(\Phi_0) b$ is symmetric with respect to the L^2-product over $\mathbb{R}$. Differentiating (22) with respect to z we see that $\partial_z \Phi_0$ lies in the kernel of $\mathcal{L}(\Phi_0)$. Since $\Phi_0(-z) = 1 - \Phi_0(z)$ we find with the help of Assumption C that $\partial_z \Phi_0$ and $h'(\Phi_0)$ are even, hence (25) allows for an even solution and in the following we will assume that Φ_1 is even.

We can deduce a solvability condition by multiplying the equation with $\partial_z \Phi_0$ and integrating over $\mathbb{R}$ with respect to z:

$$0 = \int_{\mathbb{R}} ((\kappa - \omega_0 v)(\partial_z \Phi_0(z))^2 - \tfrac{1}{2} \Psi(\boldsymbol{U}_0) h'(\Phi_0(z)) \partial_z \Phi_0(z))\, \mathrm{d}z = (\kappa - \omega_0 v) I - \tfrac{1}{2} \Psi(\boldsymbol{U}_0) \tag{26}$$

where

$$I = \int_{\mathbb{R}} (\partial_z \Phi_0)^2 \, \mathrm{d}z.$$

The system (8) becomes, to order $O(\varepsilon^{-1})$,

$$-v \partial_z \psi_{,\boldsymbol{u}}(\boldsymbol{U}_0, \Phi_0) = -v \partial_z ((\psi_s)_{,\boldsymbol{u}}(\boldsymbol{U}_0) + \tilde{h}(\Phi_0) \Psi_{,\boldsymbol{u}}(\boldsymbol{U}_0)) = \underline{L} \partial_{zz} \boldsymbol{U}_1.$$

As $\boldsymbol{U}_0 = \boldsymbol{U}_0(t,s)$ we obtain $\Psi_{,\boldsymbol{u}}(\boldsymbol{U}_0) = [\psi_{,\boldsymbol{u}}(\boldsymbol{u}_0)]_s^l = (\psi_l)_{,\boldsymbol{u}}(\boldsymbol{u}_0) - (\psi_s)_{,\boldsymbol{u}}(\boldsymbol{u}_0)$ for all z. We integrate two times with respect to z and get

$$\begin{aligned} \boldsymbol{U}_1 &= -\underline{L}^{-1}\left(v \int_0^z \psi_{,\boldsymbol{u}}(\boldsymbol{U}_0, \Phi_0)\, \mathrm{d}z' - \boldsymbol{A} z \right) + \bar{\boldsymbol{u}} \\ &\sim -\underline{L}^{-1}(v(\psi_l)_{,\boldsymbol{u}}(\boldsymbol{U}_0) z - \boldsymbol{A} z - v[\psi_{,\boldsymbol{u}}(\boldsymbol{u}_0)]_s^l \tilde{H}) + \bar{\boldsymbol{u}} \quad \text{as } z \to \infty \\ &\sim -\underline{L}^{-1}(v(\psi_s)_{,\boldsymbol{u}}(\boldsymbol{U}_0) z - \boldsymbol{A} z - v[\psi_{,\boldsymbol{u}}(\boldsymbol{u}_0)]_s^l \tilde{H}) + \bar{\boldsymbol{u}} \quad \text{as } z \to -\infty \end{aligned} \tag{27}$$

where $\boldsymbol{A} \in \mathbb{R} \times \Sigma^N$ (observe that then $v\psi_{,\boldsymbol{u}} - \boldsymbol{A} \in Y$, which allowed us to use Assumption E to invert $\underline{L}$) and $\bar{\boldsymbol{u}} \in Y$ are two integration constants and

$$\tilde{H} = \int_0^\infty (1 - \tilde{h}(\Phi_0(z)))\, \mathrm{d}z = \int_{-\infty}^0 \tilde{h}(\Phi_0(z))\, \mathrm{d}z.$$

Here, we used the fact that Φ_0 converges to constants exponentially fast, so that the integral $\int_0^z$ has been replaced by $\int_0^\infty$ while the linear terms remain. Using (16) we derive

$$\boldsymbol{u}_1(t, s, 0^\pm) = \bar{\boldsymbol{u}} + v \underline{L}^{-1} [\psi_{,\boldsymbol{u}}(\boldsymbol{u}_0)]_s^l \tilde{H}, \tag{28}$$

which means, in particular, that

$$\boldsymbol{u}_1 \text{ is continuous across } \Gamma(t; 0). \tag{29}$$

By (17) the following jump condition is obtained at the interface:

$$\begin{aligned} [-\underline{L} \nabla \boldsymbol{u}_0]_s^l \cdot \nu &:= -\underline{L} \nabla \boldsymbol{u}_0(t, s, 0^+) \cdot \nu + \underline{L} \nabla \boldsymbol{u}_0(t, s, 0^-) \cdot \nu \\ &= (v(\psi_l)_{,\boldsymbol{u}}(\boldsymbol{u}_0) - \boldsymbol{A}) - (v(\psi_s)_{,\boldsymbol{u}}(\boldsymbol{u}_0) - \boldsymbol{A}) \\ &= v[\psi_{,\boldsymbol{u}}(\boldsymbol{u}_0)]_s^l. \end{aligned} \tag{30}$$

3.4 *Inner solutions to second order*

Using the fact that Φ_0 only depends on z the phase field equation to order $O(\varepsilon^0)$ gives

$$\begin{aligned}
&-\omega_0 v\partial_z\Phi_1 - \omega_1(\boldsymbol{u}_0)v\partial_z\Phi_0 - \omega_0(\partial^\circ d_1)\partial_z\Phi_0 \\
&\quad = \partial_{zz}\Phi_2 - w''(\Phi_0)\Phi_2 + (\partial_s d_1)^2\partial_{zz}\Phi_0 - \kappa^2(z+d_1)\partial_z\Phi_0 - \partial_{ss}d_1\partial_z\Phi_0 \\
&\qquad - \kappa\partial_z\Phi_1 - \tfrac{1}{2}w'''(\Phi_0)(\Phi_1)^2 + \tfrac{1}{2}\Psi(\boldsymbol{U}_0)h''(\Phi_0)\Phi_1 + \tfrac{1}{2}\Psi_{,\boldsymbol{u}}(\boldsymbol{U}_0)\cdot\boldsymbol{U}_1 h'(\Phi_0).
\end{aligned}$$

To guarantee that Φ_2 exists there is again a solvability condition which is obtained by multiplying with $\partial_z\Phi_0$ and integrating over $\mathbb{R}$ with respect to z. The Φ_1-terms in this condition vanish as can be seen as follows:

$$\begin{aligned}
&\int_{\mathbb{R}} ((\kappa - \omega_0 v)\partial_z\Phi_1 + \tfrac{1}{2}w'''(\Phi_0)(\Phi_1)^2 - \tfrac{1}{2}\Psi(\boldsymbol{U}_0)h''(\Phi_0)\Phi_1)\partial_z\Phi_0\,\mathrm{d}z \\
&\quad = \int_{\mathbb{R}} ((\kappa - \omega_0 v)\partial_z\Phi_1\partial_z\Phi_0 - w''(\Phi_0)\Phi_1\partial_z\Phi_1 + \tfrac{1}{2}\Psi(\boldsymbol{U}_0)h'(\Phi_0)\partial_z\Phi_1)\,\mathrm{d}z \\
&\quad = 2(\kappa - \omega_0 v)\int_{\mathbb{R}} \partial_z\Phi_1\partial_z\Phi_0\,\mathrm{d}z - \int_{\mathbb{R}} \partial_{zz}\Phi_1\partial_z\Phi_1\,\mathrm{d}z
\end{aligned}$$

where we used (25) to obtain the last identity. Since $\partial_z\Phi_1\cdot\partial_z\Phi_0$ and $\partial_{zz}\Phi_1\cdot\partial_z\Phi_1$ are odd the integrals in the last line vanish. Defining the constants

$$\begin{aligned}
H &:= \int_0^\infty z\partial_z(h\circ\Phi_0)(z)\,\mathrm{d}z = -\int_{-\infty}^0 z\partial_z(h\circ\Phi_0)(z)\,\mathrm{d}z, \\
J &:= \int_0^\infty \partial_z(h\circ\Phi_0)(z)\int_0^z (1-(\tilde{h}\circ\Phi_0)(z'))\,\mathrm{d}z'\,\mathrm{d}z \\
&= \int_{-\infty}^0 \partial_z(h\circ\Phi_0)(z)\int_z^0 (\tilde{h}\circ\Phi_0)(z')\,\mathrm{d}z'\,\mathrm{d}z
\end{aligned}$$

and using (27) for the remaining $\boldsymbol{U}_1$-term, a short calculation shows

$$\begin{aligned}
&-\int_{\mathbb{R}} \tfrac{1}{2}\Psi_{,\boldsymbol{u}}(\boldsymbol{U}_0)\cdot\boldsymbol{U}_1\partial_z(h\circ\Phi_0)\,\mathrm{d}z \\
&\quad = -\tfrac{1}{2}[\psi_{,\boldsymbol{u}}(\boldsymbol{u}_0)]_s^l\cdot(\bar{\boldsymbol{u}} - \underline{L}^{-1}[\psi_{,\boldsymbol{u}}(\boldsymbol{u}_0)]_s^l H + \underline{L}^{-1}[\psi_{,\boldsymbol{u}}(\boldsymbol{u}_0)]_s^l 2J) \\
&\quad = -\tfrac{1}{2}[\psi_{,\boldsymbol{u}}(\boldsymbol{u}_0)]_s^l\cdot\boldsymbol{u}_1 + v[\psi_{,\boldsymbol{u}}(\boldsymbol{u}_0)]_s^l\cdot\underline{L}^{-1}[\psi_{,\boldsymbol{u}}(\boldsymbol{u}_0)]_s^l(H+\tilde{H}-2J)/2
\end{aligned}$$

where we used (28) to get the last equality.

The whole solvability condition then becomes

$$\begin{aligned}
0 &= (-\omega_0\partial^\circ + \partial_{ss} + \kappa^2)d_1 I - \tfrac{1}{2}[\psi_{,\boldsymbol{u}}(\boldsymbol{u}_0)]_s^l\boldsymbol{u}_1 \\
&\quad + v(-\omega_1(\boldsymbol{u}_0)I + [\psi_{,\boldsymbol{u}}(\boldsymbol{u}_0)]_s^l\cdot\underline{L}^{-1}[\psi_{,\boldsymbol{u}}(\boldsymbol{u}_0)]_s^l(H+\tilde{H}-2J)/2). \qquad (31)
\end{aligned}$$

We remark that $\partial^\circ d_1$ and $(\partial_{ss}+\kappa^2)d_1$ are the first order corrections of the normal velocity and the curvature of $\Gamma(t,s;\varepsilon)$ (see Appendix C).

In the following, whenever we will evaluate ψ and its derivatives at $(\boldsymbol{U}_0, \Phi_0)$ this will be denoted by a superscript ^{0}. The conservation laws (8) yield, to order $O(\varepsilon^0)$,

$$-v\partial_z(\underline{\psi^0_{,\boldsymbol{uu}}}\boldsymbol{U}_1 + \psi^0_{,\boldsymbol{u}\varphi}\Phi_1) + \partial^\circ\psi^0_{,\boldsymbol{u}} - (\partial^\circ d_1)\partial_z\psi^0_{,\boldsymbol{u}} = \underline{L}\,(\partial_{zz}\boldsymbol{U}_2 - \kappa\partial_z\boldsymbol{U}_1 + \partial_{ss}\boldsymbol{U}_0) \tag{32}$$

where we used the fact that $\boldsymbol{U}_0$ does not depend on z. Integrating once with respect to z leads to

$$\begin{aligned} -\underline{L}\partial_z\boldsymbol{U}_2 = {} & \underbrace{v\partial_z(\underline{\psi^0_{,\boldsymbol{uu}}}\boldsymbol{U}_1 + \psi^0_{,\boldsymbol{u}\varphi}\Phi_1) - \boldsymbol{B}}_{\text{(i)}} \\ & + \underbrace{\int_0^z ((\partial^\circ d_1)\partial_z\psi^0_{,\boldsymbol{u}} - \partial^\circ\psi^0_{,\boldsymbol{u}})\,\mathrm{d}z'}_{\text{(ii)}} - \underbrace{\kappa\underline{L}\boldsymbol{U}_1}_{\text{(iii)}} + \underline{L}\partial_{ss}\boldsymbol{U}_0 z \end{aligned} \tag{33}$$

where $\boldsymbol{B} \in Y$ is an integration constant. We want to derive a correction to the jump condition (30), i.e. a jump condition for $\boldsymbol{u}_1$. Therefore we are interested in the terms contributing to $\nabla\boldsymbol{u}_1 \cdot \nu$ in (18). Applying (16) to $\Phi_1, \boldsymbol{U}_1$ and using the fact that $\tilde{h}'(0) = \tilde{h}'(1) = 0$ we see that

$$\begin{aligned} \text{(i)} &\sim v\underline{(\psi_l)_{,\boldsymbol{uu}}}(\boldsymbol{u}_0)\boldsymbol{u}_1 - \boldsymbol{B} + (\dots)z \quad \text{as } z \to \infty, \\ &\sim v\underline{(\psi_s)_{,\boldsymbol{uu}}}(\boldsymbol{u}_0)\boldsymbol{u}_1 - \boldsymbol{B} + (\dots)z \quad \text{as } z \to -\infty. \end{aligned}$$

Furthermore,

$$\begin{aligned} \text{(ii)} &= (\partial^\circ d_1)(\psi^0_{,\boldsymbol{u}}|_0^z) - \int_0^z [\partial^\circ((\psi_s)^0_{,\boldsymbol{u}}) + (\partial^\circ\Psi^0_{,\boldsymbol{u}})(\tilde{h}\circ\Phi_0)(z')]\,\mathrm{d}z' \\ &\sim \tfrac{1}{2}(\partial^\circ d_1)[\psi_{,\boldsymbol{u}}(\boldsymbol{u}_0)]_s^l - (\partial^\circ(\psi_l)_{,\boldsymbol{u}}(\boldsymbol{u}_0))z + \partial^\circ[\psi_{,\boldsymbol{u}}(\boldsymbol{u}_0)]_s^l\tilde{H} \qquad \text{as } z \to \infty, \\ &\sim -\tfrac{1}{2}(\partial^\circ d_1)[\psi_{,\boldsymbol{u}}(\boldsymbol{u}_0)]_s^l - (\partial^\circ(\psi_s)_{,\boldsymbol{u}}(\boldsymbol{u}_0))z + \partial^\circ[\psi_{,\boldsymbol{u}}(\boldsymbol{u}_0)]_s^l\tilde{H} \qquad \text{as } z \to -\infty \end{aligned}$$

where for the first term the symmetry of $\tilde{h}$ in Assumption C has been used. In (iii) we use (28) again to obtain

$$\text{(iii)} = \kappa\underline{L}\boldsymbol{u}_1(t,s,0) + (\dots)z \qquad \text{as } z \to \pm\infty.$$

Finally, by (29), the first order correction of the jump condition (30) at the interface is

$$[-\underline{L}\nabla\boldsymbol{u}_1]_s^l \cdot \nu = v[\underline{\psi_{,\boldsymbol{uu}}}(\boldsymbol{u}_0)]_s^l \cdot \boldsymbol{u}_1 + (\partial^\circ d_1)[\psi_{,\boldsymbol{u}}(\boldsymbol{u}_0)]_s^l. \tag{34}$$

3.5 *Summary of the leading order problem and the correction problem*

The problem to leading order consists of the bulk equation (20) which is coupled to the conditions (24), (30) and (26) on $\Gamma(t;0)$:

(LOP) Find a function $\boldsymbol{u}_0 : I \times D \to Y$ and a family of curves $\{\Gamma(t;0)\}_{t\in I}$ separating D into two domains $D^l(t;0)$ and $D^s(t;0)$ such that

$$\begin{aligned} \partial_t((\psi_l)_{,\boldsymbol{u}}(\boldsymbol{u}_0)) &= \underline{L}\Delta\boldsymbol{u}_0 \quad \text{in } D^l(t;0),\ t \in I, \\ \partial_t((\psi_s)_{,\boldsymbol{u}}(\boldsymbol{u}_0)) &= \underline{L}\Delta\boldsymbol{u}_0 \quad \text{in } D^s(t;0),\ t \in I, \end{aligned}$$

and such that for all $t \in I$, on $\Gamma(t;0)$ we have:

$$\begin{gathered} \boldsymbol{u}_0 \text{ is continuous,} \\ [-\underline{L}\nabla \boldsymbol{u}_0]_s^l \cdot \nu = v[\psi_{,\boldsymbol{u}}(\boldsymbol{u}_0)]_s^l, \\ \omega_0 v = \kappa - \frac{1}{2I}[\psi(\boldsymbol{u}_0)]_s^l \end{gathered}$$

where ν is the unit normal to $\Gamma(t;0)$ pointing into $D^l(t;0)$.

If we choose

$$\omega_1 = \omega_1(\boldsymbol{u}_0) := [\psi_{,\boldsymbol{u}}(\boldsymbol{u}_0)]_s^l \cdot \underline{L}^{-1}[\psi_{,\boldsymbol{u}}(\boldsymbol{u}_0)]_s^l \frac{H + \tilde{H} - 2J}{2I} \tag{35}$$

then the correction problem consisting of (21), (29), (34) and (31) reads as follows:

(CP) Let $(\boldsymbol{u}_0, \{\Gamma(t;0)\}_t)$ be a solution to (LOP), let $l(t)$ be the length of $\Gamma(t;0)$ and set $S_I = \{(t,s) : t \in I, s \in [0, l(t))\}$. Find functions $\boldsymbol{u}_1 : I \times D \to Y$ and $d_1 : S_I \to \mathbb{R}$ such that

$$\begin{aligned} \partial_t(\underline{(\psi_l)_{,\boldsymbol{uu}}}(\boldsymbol{u}_0)\boldsymbol{u}_1) &= \underline{L}\Delta \boldsymbol{u}_1 \quad \text{in } D^l(t;0),\ t \in I, \\ \partial_t(\underline{(\psi_s)_{,\boldsymbol{uu}}}(\boldsymbol{u}_0)\boldsymbol{u}_1) &= \underline{L}\Delta \boldsymbol{u}_1 \quad \text{in } D^s(t;0),\ t \in I, \end{aligned}$$

and such that for all $t \in I$ on $\Gamma(t;0)$ we have:

$$\begin{gathered} \boldsymbol{u}_1 \text{ is continuous,} \\ [-\underline{L}\nabla \boldsymbol{u}_1]_s^l \cdot \nu = v[\underline{\psi_{,\boldsymbol{uu}}}(\boldsymbol{u}_0)]_s^l \boldsymbol{u}_1 + (\partial^\circ d_1)[\psi_{,\boldsymbol{u}}(\boldsymbol{u}_0)]_s^l, \\ \omega_0(\partial^\circ d_1) = (\partial_{ss} + \kappa^2)d_1 - \frac{1}{2I}[\psi_{,\boldsymbol{u}}(\boldsymbol{u}_0)]_s^l \cdot \boldsymbol{u}_1. \end{gathered}$$

Obviously, $(\boldsymbol{u}_1, d_1) \equiv 0$ is a solution given appropriate boundary conditions on ∂D. If this solution is unique then the leading order problem is approximated to second order in ε by the phase field model. The calculation in Appendix C shows that (CP) is in fact the linearization of (LOP). We point out that the choice (35) is crucial in order to guarantee that the undesired terms in (31) vanish.

REMARK. If the diffusivity matrix $\underline{L}$ depends on $\boldsymbol{u}$ then equation (32) becomes

$$\begin{aligned} -v\partial_z(\underline{\psi_{,\boldsymbol{uu}}}^0 \boldsymbol{U}_1 + \psi^0_{,\boldsymbol{u}\varphi}\Phi_1) + \partial^\circ \psi^0_{,\boldsymbol{u}} - (\partial^\circ d_1)\partial_z \psi^0_{,\boldsymbol{u}} &= \underline{L}(\boldsymbol{U}_0)\partial_{zz}\boldsymbol{U}_2 \\ &+ \partial_z(\underline{L}_{,\boldsymbol{u}}(\boldsymbol{U}_0)\boldsymbol{U}_1\partial_z\boldsymbol{U}_1) + \underline{L}_{,\boldsymbol{u}}(\boldsymbol{U}_0)(\partial_s\boldsymbol{U}_0)^2 + \underline{L}(\boldsymbol{U}_0)\partial_{ss}\boldsymbol{U}_0 - \kappa\underline{L}(\boldsymbol{U}_0)\partial_z\boldsymbol{U}_1 \end{aligned}$$

resulting in

$$-\underline{L}\partial_z\boldsymbol{U}_2 = \text{(i)} + \text{(ii)} - \underbrace{\kappa\underline{L}(\boldsymbol{U}_0)\boldsymbol{U}_1}_{=\text{(iii)}} + \underbrace{\underline{L}_{,\boldsymbol{u}}(\boldsymbol{U}_0)\cdot\boldsymbol{U}_1\partial_z\boldsymbol{U}_1}_{=:\text{(iv)}} + (\underline{L}_{,\boldsymbol{u}}(\boldsymbol{U}_0)(\partial_s\boldsymbol{U}_0)^2 + \underline{L}(\boldsymbol{U}_0)\partial_{ss}\boldsymbol{U}_0)z$$

instead of (33). The matching conditions (15), (16) and (17) yield

$$\text{(iv)} = \underline{L}_{,\boldsymbol{u}}(\boldsymbol{u}_0)\cdot\boldsymbol{u}_1\nabla\boldsymbol{u}_0(0^\pm)\cdot\nu + (\ldots)z \qquad \text{as } z \to \pm\infty.$$

This leads to an additional term in the jump condition of the correction problem. The condition (34) now reads

$$[-\underline{L}(\boldsymbol{u}_0)\nabla\boldsymbol{u}_1 - \underline{L}_{,\boldsymbol{u}}(\boldsymbol{u}_0)\cdot\boldsymbol{u}_1\nabla\boldsymbol{u}_0]_s^l \cdot \nu = v[\underline{\psi_{,\boldsymbol{uu}}}(\boldsymbol{u}_0)]_s^l\boldsymbol{u}_1 + (\partial^\circ d_1)[\psi_{,\boldsymbol{u}}(\boldsymbol{u}_0)]_s^l,$$

but this is still consistent with the above statement that (CP) is the linearization of (LOP) as the additional term results from expanding $\underline{L}$ in a straightforward way.

4. Numerical simulations

Numerical simulations were performed in order to show that convergence to second order indicated by the analysis can really be obtained. For this purpose, we analyzed the ε-dependence of numerical solutions to the phase field system and compared the numerical solutions with analytical solutions to the sharp interface problem if available. The differential equations of the phase field system were discretized in space and time using finite differences on uniform grids with spatial mesh size Δx and time step Δt. The update in time was explicit, and to guarantee stability we chose $\Delta t \lesssim \Delta x^2$. If not otherwise stated we decreased the mesh size Δx until we were sure that the error due to the discretization became inessential.

The order of convergence can be estimated by the following procedure. Assume that the ε-dependence of the error can approximately be expressed by

$$\mathrm{Err}(\varepsilon) = \mathrm{err}\,\varepsilon^k + \text{higher order terms}$$

with a constant err and an exponent $k > 0$ which we are interested in. Given some $m > 1$ (we often used $m = \sqrt{2}$) one can derive up to higher order terms

$$\frac{\mathrm{Err}(\varepsilon) - \mathrm{Err}(\varepsilon/m)}{\mathrm{Err}(\varepsilon/m) - \mathrm{Err}(\varepsilon/m^2)} = \left(\frac{1}{m}\right)^{-k} = m^k \tag{36}$$

from which one can calculate k by inserting the measured values for $\mathrm{Err}(\varepsilon)$.

4.1 *Scalar case in 1D*

Let $d = 1$ and $N = 1$, i.e. we consider a pure material. We set $u = u^{(0)}$ and postulate the reduced grand canonical potential

$$\psi(u,\varphi) = \tfrac{1}{2}c_v u^2 + \lambda(u_m - u)(1 - h(\varphi)), \quad \text{i.e.} \quad \Psi(u) = \lambda(u - u_m),$$

where λ, u_m and c_v are constants. Choosing $w(\varphi) = \frac{9}{2}\varphi^2(1-\varphi)^2$ as double-well potential we obtain:

$$\varepsilon(\omega_0 + \varepsilon\omega_1)\partial_t\varphi = \varepsilon\sigma\partial_{xx}\varphi - \frac{9\sigma}{\varepsilon}\varphi(1-\varphi)(1-2\varphi) + \frac{1}{2}\lambda(u - u_m)h'(\varphi), \tag{37}$$

$$\partial_t\psi_{,\boldsymbol{u}} = \partial_t(c_v u - \lambda(1 - \tilde{h}(\varphi))) = K\partial_{xx}u. \tag{38}$$

This system differs from typical phase field systems (see e.g. [26]) by the term $\varepsilon\omega_1$. With these equations the following sharp interface problem is approximated:

$$\begin{aligned} c_v \partial_t u &= K \partial_{xx} u, && x \neq p(t), \\ &u \text{ is continuous}, && \\ \lambda p'(t) &= [-K\partial_x u]_s^l, && x = p(t), \\ \omega_0 p'(t) &= \lambda(u_m - u), && x = p(t), \end{aligned}$$

where $p(t)$ denotes the position of the interface at time t. Imposing the boundary condition $u \to u_\infty$ as $x \to \infty$ there is the following traveling wave solution: setting $u_i = c_v^{-1}\lambda + u_\infty$ we define

$$p(t) = vt = \omega_0^{-1}\lambda(u_m - u_i)t, \tag{39}$$

$$u = u_i, \qquad x \leqslant vt, \tag{40}$$

$$u = u_\infty + (u_i - u_\infty)\exp(-K^{-1}c_v v(x - vt)), \qquad x > vt. \tag{41}$$

Choosing $\tilde{h}(\varphi) = h(\varphi) = \varphi^2(3 - 2\varphi)$ we compute $I = 1/2$, $H + \tilde{H} - 2J = 19/90$. Furthermore, if

$$\lambda = 0.5, \quad u_m = -1.0, \quad u_\infty = -2.0, \quad c_v = 1.0, \quad \omega_0 = 0.25, \quad K = 1.0, \quad \sigma = 1.0$$

we obtain the velocity $v = 1.0$, the value $u_i = -1.5$ at the interface and by (35) the correction term $\omega_1 \approx 0.013194444$.

We solved the differential equations on the time interval $I = [0, 0.1]$ for several values of ε. We chose Dirichlet boundary conditions for u given by the traveling wave solution (40), (41) to the sharp interface model and homogeneous Neumann boundary conditions for φ. To initialize φ we set

$$\varphi(0, x) := \tfrac{1}{2}(1 + \tanh(\tfrac{3}{2}z)) = \Phi_0(z), \qquad z = (x - x_0)/\varepsilon, \tag{42}$$

with some suitable initial transition point x_0 such that the transition region (the set $\{\varphi \in (\delta, 1 - \delta)\}$ for some small δ, e.g. $\delta = 10^{-3}$) remains away from the outer boundary during the evolution. The function Φ_0 is the solution to (22) with the boundary conditions $\Phi_0(z) \to 0, 1$ as $z \to -\infty, +\infty$. Initial values for u were obtained by matching outer and inner solutions to leading and first order obtained from the asymptotic expansions (see e.g. [21])

$$u(0, x) = \boldsymbol{u}_0(0, x) + \varepsilon\boldsymbol{u}_1(0, x) + \boldsymbol{U}_0(0, z) + \varepsilon\boldsymbol{U}_1(0, z) - \text{common part.}$$

The function $\boldsymbol{u}_0(0, x)$ has the profile of the traveling wave solution:

$$\boldsymbol{u}_0(0, x) = \begin{cases} u_\infty + (u_i - u_\infty)\exp\left(-\dfrac{c_v}{K}v(x - x_0)\right), & x > x_0, \\ u_i, & x \leqslant x_0. \end{cases} \tag{43}$$

As we want $\boldsymbol{u}_1 \equiv 0$ to be a solution to the correction problem we chose $\boldsymbol{u}_1(0, x) = 0$. By equations (23) and (24), $\boldsymbol{U}_0 \equiv u_i$ is the interface value which is constant in the normal direction. Equation (17) implies $\partial_z \boldsymbol{U}_1(z) \to \nabla \cdot \boldsymbol{u}_0(x_0^-) = 0$ as $z \to -\infty$. As $\boldsymbol{u}_1(0, x) = 0$ we have $\bar{\boldsymbol{u}} = -(v/K)\lambda\tilde{H}$ by (28). By (27) we see that $\boldsymbol{A} = v(\psi_s)_{,\boldsymbol{u}}(\boldsymbol{U}_0)$, which yields

$$\boldsymbol{U}_1(0, z) = \frac{v}{K}\begin{cases} \lambda - z + \displaystyle\int_0^z (1 - \tilde{h} \circ \varphi_0)(z')\,\mathrm{d}z' - \tilde{H}, & z > 0, \\ \lambda \displaystyle\int_z^0 (\tilde{h} \circ \varphi_0)(z')\,\mathrm{d}z' - \tilde{H}, & z < 0. \end{cases}$$

The common part is $u_i - (v\lambda/K)z$ if $z > 0$ and u_i if $z < 0$.

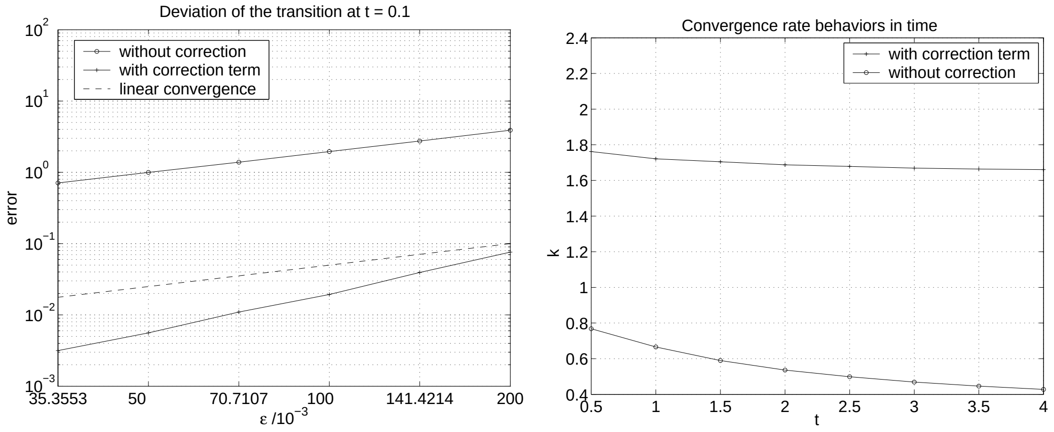

FIG. 1. Left: deviations of the phase boundaries measured from the exact interface position given by (39) over ε; the resolution of the transition region is very fine so that the error caused by the discretization is negligible; the dashed line corresponds to a linear convergence behavior in ε. Right: behavior of the numerically computed convergence rates (cf. (36)) in time for the angle $\beta = 15^\circ$ (see Section 4.2).

The phase boundaries $\{\varphi = 1/2\}$ were determined by linearly interpolating the values at the grid points. Subtracting from the computed transition point the exact position given by (39) we got, up to sign, the values in Figure 1 (left). We found that when considering the correction term the interface was too slow but the numerical results indicated a quadratic convergence. Without the correction term ω_1 the interface was too fast and larger errors occurred indicating only linear convergence in ε. Similar results concerning the order of convergence hold true if

$$u(0, x) = \boldsymbol{u}_0(0, x) \quad \text{or} \quad \varphi = \chi_{[x_0, \infty]}$$

was chosen as initial data instead of the above smooth functions. The only difference is that then the errors are larger.

In the above simulations, the transition regions were resolved by more than 100 grid points to determine the error and the convergence behavior accurately. In applications, such resolutions of the interface are much too costly. Therefore, we simulated the same problem over the larger time interval $I = [0, 8.0]$ with much less grid points in the interface. We found that the $\varepsilon/\Delta x$ ratio should be at least $5\sqrt{2}$. The deviations at $t = 8.0$ are given in the following table:

ε	0.4	$0.4/\sqrt{2}$	0.2	$0.2/\sqrt{2}$	0.1	$0.1/\sqrt{2}$	0.05
with correction	-0.0601	-0.0354	-0.0280				
without corr.	0.5867	0.4155	0.2867	0.2020	0.1355	0.0948	0.0502

Again the errors are much larger without the correction term. To get an error as obtained with the correction term we need to take ε and Δx eight times smaller. If explicit methods are used the expenditure becomes 8 times larger if the grid constant is halved due to the stability constraint $\Delta t \lesssim \Delta x^2$ for the time step. Hence, in our example, the costs without the correction term are $8^3 = 512$ times larger to obtain the same size of the error.

4.2 *Scalar case in 2D*

Now, let $N = 1$ and $d = 2$ and consider the same reduced grand canonical potential as in Subsection 4.1. Instead of the smooth double-well potential we used the obstacle potential

$$w_{\mathrm{ob}}(\varphi) = \begin{cases} \dfrac{8}{\pi^2}\varphi(1-\varphi), & 0 \leqslant \varphi \leqslant 1, \\ \infty, & \text{elsewhere.} \end{cases}$$

Then (37) has to be replaced by a variational inequality for φ but the asymptotic analysis can be done in a similar way (see [6]). The main advantage of such a potential is that the stable minima 0 and 1 of w are attained outside of the thin interfacial layer so that the phase field equations only have to be solved in a small tube around the approximated interface. The equation (38) for u remains the same except that ∂_{xx} is replaced by the Laplacian Δ.

We chose the following constants:

$$\lambda = 0.5, \quad u_m = 2.0, \quad c_v = 1.0, \quad \omega_0 = 0.25, \quad K = 0.1, \quad \sigma = 0.1.$$

We simulated the evolution of a radial interface. Initially, for φ we used the profile

$$\varphi(0,x) = \begin{cases} 0, & -\infty < z \leqslant -\pi^2/8, \\ \frac{1}{2}(1+\sin(4z/\pi)), & -\pi^2/8 \leqslant z \leqslant \pi^2/8, \\ 1, & \pi^2/8 \leqslant z < \infty, \end{cases} \qquad z = \frac{r-r_0}{\varepsilon},$$

which is the solution to the variational inequality corresponding to (22) when restricted to a radial direction. Here, $r = \sqrt{x^2+y^2}$ is the radius and we chose $r_0 = 0.8$. For $\tilde{h}(\varphi) = h(\varphi) = \varphi^2(3-2\varphi)$ we get the constants $I = \frac{1}{2}$, $H + \tilde{H} - 2J = 23\pi^2/1024$ and hence

$$\omega_1 = \frac{\lambda^2}{K}\frac{H+\tilde{H}-2J}{2I} \approx 0.554201419.$$

For u initially the 1D profile (43) of the traveling wave solution in Subsection 4.1 in the radial direction was used. As in the 1D case, $u_i = -1.5$, $v = (\omega_0/\lambda)(u_m - u_i) = 0.25$ and $u_\infty = -2.0$.

We considered the domain $D = [0,8]^2$ and chose the grid constant $\Delta x = 0.02$. At different times we measured the distance of the level set $\varphi = 1/2$ from the origin depending on the angle β with the x-direction. Again, the values at the grid points were linearly interpolated. At $t = 1.5$ we obtain the following results:

	without correction			with correction		
	$\beta = 20°$	$\beta = 15°$	$\beta = 0°$	$\beta = 20°$	$\beta = 15°$	$\beta = 0°$
$\varepsilon = 0.2$	2.398226	2.398924	2.399661	1.851693	1.852492	1.853469
$\varepsilon = 0.14$	2.277925	2.278367	2.278668	1.889131	1.889779	1.890377
$\varepsilon = 0.1$	2.180093	2.180095	2.179580	1.910175	1.910433	1.910311
k	0.596551	0.589719	0.576271	1.662103	1.704448	1.777240

The distances as well as the order of convergence (cf. the procedure around equation (36) for its derivation) do not essentially depend on the angle. The order of convergence is much better if the correction term is taken into account. Moreover, the change in the radius when changing ε is much smaller if a correction ω_1 is considered. In Figure 1 the time behavior of the convergence rates is shown indicating a slight decrease.

4.3 *Binary isothermal systems*

To model phase transformations in systems with non-trivial, non-linearized phase diagrams (see e.g. Figure 2) we need to introduce a $\boldsymbol{u}$-dependent correction term. In this subsection we will demonstrate that our approach in fact makes it possible to obtain a superior approximation behavior also in this case.

Since $\tilde{\boldsymbol{u}} = (u^{(1)}, u^{(2)}) \in T\Sigma^2$ it is sufficient to consider $u^{(1)}$. We postulate the reduced grand canonical potential

$$\psi(u^{(0)}, u^{(1)}, \varphi) = \tfrac{1}{2}((u^{(0)})^2 + (u^{(1)})^2) + (\lambda(u^{(0)} - u_m) + G(u^{(1)})^2(3 - 2u^{(1)}))(1 - \tilde{h}(\varphi))$$

with constants $u_m = -1.0$, $\lambda = G = 0.1$. The two phases l and s are in equilibrium if $[\psi(u)]_s^l = 0$ (see Appendix A). Here, the equilibrium condition reads

$$u^{(0)} = u_m - \frac{G}{\lambda}(u^{(1)})^2(3 - 2u^{(1)}) \tag{44}$$

from which we can construct the phase diagram in Figure 2 by the relations $T = -1/u^{(0)}$ and $c = \psi_{,u^{(1)}} = u^{(1)} - 6Gh_s(\varphi)u^{(1)}(1 - u^{(1)})$ where $h_s(\varphi) := 1 - \tilde{h}(\varphi)$. Moreover, we get

$$[c(u^{(1)})]_s^l = 6Gu^{(1)}(1 - u^{(1)}).$$

For the isothermal case, i.e. $u^{(0)}$ is constant, we solved (7) and

$$\partial_t c(u^{(1)}) = \partial_t \psi_{,u^{(1)}}(u^{(1)}) = d\partial_{xx}u^{(1)}$$

in the domain $D = [0, 28]$ for $t \in [0, 40]$ numerically. We imposed homogeneous Neumann boundary conditions and set $d = 0.4$. Initially we chose for $u^{(1)}$ a profile as in (43) for $u^{(0)}$,

$$u^{(1)}(0, x) = \begin{cases} u_\infty^{(1)} + (u_i - u_\infty^{(1)}) \exp(-\frac{1}{d}v(x - x_0)), & x > x_0, \\ u_i^{(1)}, & x \leqslant x_0. \end{cases} \tag{45}$$

Writing $u^{(1)}$ as a function in c we get

$$u^{(1)} = \begin{cases} c, & h_s(\varphi) = 0, \\ \dfrac{1}{12Gh_s(\varphi)}(6Gh_s(\varphi) - 1 + \sqrt{(6Gh_s(\varphi) - 1)^2 + 24Gh_s(\varphi)c}), & h_s(\varphi) > 0. \end{cases}$$

Due to the fraction this is numerically unstable as $h_s(\varphi) \to 0$. Defining $\beta = 6Gh_s(\varphi)$ we set $u^{(1)} = c$ if $\beta \leqslant 10^{-4}$, but checks were done with different cut off values. The following results do not essentially depend on the cut off value.

Choosing $u_i^{(1)} = 0.6$ for the interface value, the equilibrium concentrations are $c^{(l)} = 0.6$ and $c^{(s)} = 0.456$. To model the solidification of an alloy of concentration 0.456, we let $c^{(l)}$ decay and $u^{(1)}$ exponentially to this value by setting $u_\infty^{(1)} = 0.456$. For $u^{(1)} = u_i^{(1)} = 0.6$ we obtain at equilibrium $u_{\text{eq}}^{(0)} \approx -1.648$ and an equilibrium temperature of $T_{\text{eq}} \approx 0.6067$. To make the front move we initialized with an undercooling of $T = 0.55$, i.e. $u^{(0)} \equiv -1/0.55$. Formula (39) yields an estimation of the initial velocity of the front: for $\omega_0 = 0.08$ we have $v \approx (\lambda/\omega_0)(u_{\text{eq}}^{(0)} - u^{(0)}) \approx 0.2$. The initial position of the front $x_0 = 8.0$ was appropriately chosen so that there were not much interaction with the external boundary. Initial values for φ were again defined as in (42). By (35),

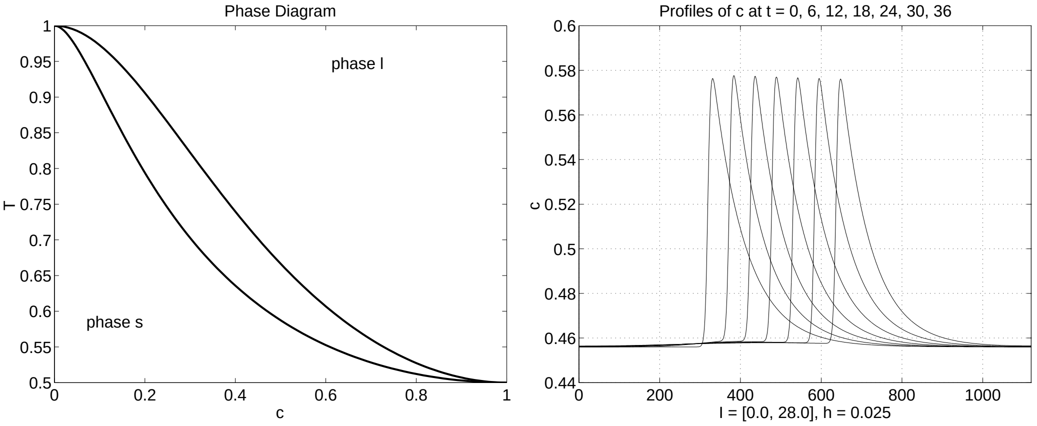

FIG. 2. Left: phase diagram for a binary mixture computed from (44). Right: profiles of the solution c for the binary system in Section 4.3 during the evolution, $\varepsilon = 0.4$; the figure indicates already that there is only a negligible influence of the boundary conditions on the evolution as gradients of c do not vanish only in the transition region. But simulations on domains with different lengths were performed to verify this conjecture.

the correction term is (h and $\tilde{h}$ are chosen as before)

$$\omega_1(u^{(1)}) = \frac{([c(u^{(1)})]_s^l)^2}{d} \frac{H + \tilde{H} + J}{2I}.$$

Equation (45) does not describe the profile of a traveling wave solution, but a nearly traveling wave solution can be observed (see Figure 2). We computed the following transition points of φ at $t = 20.0$:

	without correction				with correction			
ε	0.4	$\frac{0.4}{\sqrt{2}}$	0.2	$\frac{0.2}{\sqrt{2}}$	0.4	$\frac{0.4}{\sqrt{2}}$	0.2	$\frac{0.2}{\sqrt{2}}$
transition	12.3923	12.3369	12.2945	12.2589	12.1928	12.1976	12.1971	12.1907

Without the correction term, the changes in the interface position when changing ε are much larger than with the correction term. For example, comparing the positions for $\varepsilon = 0.4$ and 0.2, there is a change of $\approx 10^{-1}$ without the correction term but only of $\approx 5 \cdot 10^{-3}$ with it. An explicit solution to the corresponding sharp interface model to compare with is not known. But this behavior in ε indicates that the approximation of the sharp interface solution is improved thanks to the correction term. A convergence rate of the interface position for simulations with the correction term could not be computed because of the oscillations in the positions (the position does not behave monotonically in ε). Simulations on several slightly finer grids indicated that the numerical error is of the same size of about 10^{-3} which explains these oscillations.

4.4 *Binary non-isothermal case*

Now we will demonstrate that a better convergence behavior can also be observed if several conserved quantities are considered. We postulate the following reduced grand canonical potential:

$$\psi(u^{(0)}, u^{(1)}, \varphi) = \tfrac{1}{2}((u^{(0)})^2 + (u^{(1)})^2) + (\lambda(u^{(0)} - u_m) + G(u^{(1)} - u_e))(1 - \tilde{h}(\varphi))$$

with constants $u_m = -1.0$, $u_e = 0.6$, $\lambda = G = 0.2$. For the energy $e = \psi_{,u^{(0)}}$ we postulate the flux $K\nabla u^{(0)}$ with $K = 4.0$ and for the concentration $c = \psi_{,u^{(1)}}$ we postulate $d\nabla u^{(1)}$ with $d = 0.1$, i.e. there are no cross effects between mass and energy diffusion. As $[c(\boldsymbol{u})]_s^l = G$ and $[e(\boldsymbol{u})]_s^l = \lambda$ are independent of $\boldsymbol{u}$ we obtain a constant correction term (h and $\tilde{h}$ are chosen as above) $\omega_1 = (\frac{\lambda^2}{K} + \frac{G^2}{d})\frac{H+\tilde{H}-2J}{2I} \approx 0.8655555$. Usually temperature diffusivity is much faster than mass diffusivity so that the influence of the concentration part on the correction term is much larger.

At equilibrium (see Appendix A for the conditions) we have the linear relation $u_{\text{eq}}^{(1)} - u_e = u_{\text{eq}}^{(0)} - u_m$. For $u^{(1)} = u_e = 0.6$ and $u^{(0)} = u_m = -1.0$ ($\rightsquigarrow T^{(0)} = T_m = 1.0$) the equilibrium concentrations are $c^{(l)} = u^{(1)} = 0.6$ and $c^{(s)} = u^{(1)} - G = 0.4$.

We solved the differential equations for $x \in D = [0.0, 1.4]$ and $t \in I = [0.0, 0.5]$ numerically. Initial values for φ were again defined as in (42) with an interface located at $x_0 = 0.6$ away from the boundaries. Setting $u^{(1)}(t = 0) \equiv 0.6$ and $u^{(0)}(t = 0) \equiv -1.0$ we got initial values for c and e from ψ. For φ and $u^{(1)}$ we imposed homogeneous Neumann boundary conditions. We took the same boundary condition for $u^{(0)}$ at $x = 1.4$, but at the other boundary point we imposed the Dirichlet boundary condition $u^{(0)}(x = 0.0) = -1.25$ which corresponds to an undercooling of $1/5$ and made the transition point move to the right. We chose $\omega_0 = 0.08$ and $\sigma = 1.0$. At $t = 0.4$ we measured the interface and we obtained the following results (varying Δx in the column and ε in the line):

	$\Delta x \backslash \varepsilon$	$0.4/\sqrt{2}$	0.2	$0.2/\sqrt{2}$	0.1	$0.1/\sqrt{2}$
with correction	0.002	0.704470	0.708335	0.710319		
	0.001			0.710339	0.711441	0.712032
without correction	0.002	0.730569	0.726796	0.723258		
	0.001			0.723281	0.720480	0.718347

The computations for $\varepsilon = 0.2/\sqrt{2}$ reveal that the error due to the grid is small compared to the deviation due to the different values for ε. Computing numerically the order of convergence (see (36)) we obtained values of $k \approx 1.78$ with the correction term and $k \approx 0.57$ without the correction term when the runs for $\varepsilon \in \{0.4/\sqrt{2}, 0.2/\sqrt{2}, 0.1/\sqrt{2}\}$ are compared. Similar results were obtained at time $t = 0.5$.

5. Conclusions

The asymptotic analysis of a phase field model for solidification in multi-component alloy systems has been carried out using matched asymptotic expansions. In addition to the leading order problem a linear correction problem has been derived. If a certain small correction term to the kinetic coefficient in the phase field equation is taken into account the zero function solves this correction problem. Hence, there is no linear correction and our model approximates the related sharp interface problem to second order.

Numerical simulations in one and two space dimensions and for several conserved quantities were performed with and without the correction term. In all cases the convergence behavior turned out to be superior when the correction term was considered. Whenever a comparison with an explicit solution to the sharp interface model was possible a quadratic convergence could be observed while a linear convergence was observed without correction.

Acknowledgements

The authors gratefully acknowledge the financial support provided by the DFG (German Research Foundation) within the priority research program (SPP) “Analysis, Modeling and Simulation of Multiscale Problems” 1095 under Grant No. Ga 695/1-2.

Appendix A. Remarks on thermodynamics

To model solidification in alloy systems, often the free energy density f is taken as thermodynamical potential. We assume that pressure and mass density are constant. Then the free energy is a function of temperature and concentrations,

$$f : \mathbb{R} \times \Sigma^N \to \mathbb{R}, \qquad (T, \boldsymbol{c}) \mapsto f(T, \boldsymbol{c}).$$

Here, T is the temperature and $\boldsymbol{c} = (c^{(1)}, \dots, c^{(N)})$ is a vector of concentrations, i.e. $c^{(i)}$ describes the concentration of component i. The free energy f is supposed to be concave in T and convex in $\boldsymbol{c}$. Its derivative operates on the tangent space of the domain, i.e. on $\mathbb{R} \times T\Sigma^N \subset \mathbb{R}^{N+1}$, and its gradient can be naturally interpreted as a vector in $\mathbb{R} \times T\Sigma^N$, hence

$$Df : \mathbb{R} \times \Sigma^N \to \mathbb{R} \times T\Sigma^N, \qquad (T, \boldsymbol{c}) \mapsto Df(T, \boldsymbol{c}) = (\partial_T f, \partial_{\boldsymbol{c}} f) =: (-s, \boldsymbol{\mu}).$$

The quantity $s = -\frac{\partial}{\partial T} f$ is the entropy density and $\boldsymbol{\mu} = \frac{\partial}{\partial \boldsymbol{c}} f$ are generalized chemical potential differences. In the language of differential forms we have

$$\mathrm{d}f = -s\, \mathrm{d}T + \boldsymbol{\mu} \cdot \mathrm{d}\boldsymbol{c}.$$

The internal energy e is the Legendre transform of $-f$ with respect to T, i.e. $e(s) = (-f)^*(s) = sT(s) + f(T(s))$. As f is concave in T, e is concave in s. We have

$$\mathrm{d}e = \mathrm{d}f + s\, \mathrm{d}T + T\, \mathrm{d}s = T\, \mathrm{d}s + \boldsymbol{\mu} \cdot d\boldsymbol{c}$$

leading to

$$\mathrm{d}s = \frac{1}{T}\, \mathrm{d}e - \frac{\boldsymbol{\mu}}{T} \cdot \mathrm{d}\boldsymbol{c} =: -u^{(0)}\, \mathrm{d}e - \tilde{\boldsymbol{u}} \cdot \mathrm{d}\boldsymbol{c}.$$

In the following we will write $e = c^{(0)}$, $\bar{\boldsymbol{c}} = (c^{(0)}, c^{(1)}, \dots, c^{(N)})$ and $\boldsymbol{u} = (u_0, \tilde{u})$. We have

$$-s : \mathbb{R} \times \Sigma^N \to \mathbb{R}, \qquad \bar{\boldsymbol{c}} \mapsto -s(\bar{\boldsymbol{c}}),$$

and assume that $-s$ is strictly convex in $\bar{\boldsymbol{c}}$. This already implies that

$$D(-s) : \mathbb{R} \times \Sigma^N \to \mathbb{R} \times T\Sigma^N, \qquad \bar{\boldsymbol{c}} \mapsto D(-s)(\bar{\boldsymbol{c}}) = \boldsymbol{u},$$

can be locally inverted. We assume the inversion can even be done globally and that $\bar{\boldsymbol{c}}$ can be written as a function of $\boldsymbol{u}$, $\bar{\boldsymbol{c}}(\boldsymbol{u}) = (-Ds)^{-1}(\boldsymbol{u})$. The reduced grand canonical potential is then defined to be the Legendre transform of $-s$, i.e.

$$\psi := (-s)^* : \mathbb{R} \times T\Sigma^N \to \mathbb{R}, \qquad \boldsymbol{u} \mapsto \psi(\boldsymbol{u}) := \bar{\boldsymbol{c}}(\boldsymbol{u}) \cdot \boldsymbol{u} + s(\bar{\boldsymbol{c}}(\boldsymbol{u})).$$

One would naturally identify its derivative $D\psi(\boldsymbol{u})$ with a vector in $\mathbb{R}\times T\Sigma^N$. But using $\bar{\boldsymbol{c}}(\boldsymbol{u}) = (-Ds)^{-1}(\boldsymbol{u})$ we can derive the derivative of ψ in $\boldsymbol{u}$ in direction $\boldsymbol{v}\in\mathbb{R}\times T\Sigma^N$ to be

$$\begin{aligned}\langle D\psi(\boldsymbol{u}),\boldsymbol{v}\rangle &= \frac{\mathrm{d}}{\mathrm{d}\delta}((\boldsymbol{u}+\delta\boldsymbol{v})\cdot\bar{\boldsymbol{c}}(\boldsymbol{u}+\delta\boldsymbol{v}) + s(\bar{\boldsymbol{c}}(u+\delta\boldsymbol{v})))\Big|_{\delta=0}\\ &= \boldsymbol{u}\cdot(D\bar{\boldsymbol{c}}(\boldsymbol{u})\boldsymbol{v}) + \boldsymbol{v}\cdot\bar{\boldsymbol{c}}(\boldsymbol{u}) + Ds(\bar{\boldsymbol{c}}(\boldsymbol{u}))\cdot(D\bar{\boldsymbol{c}}(\boldsymbol{u})\boldsymbol{v})\\ &= \boldsymbol{v}\cdot\bar{\boldsymbol{c}}(\boldsymbol{u}).\end{aligned}$$

This motivates identifying $D\psi(\boldsymbol{u})$ with $\bar{\boldsymbol{c}}(\boldsymbol{u})$ and writing

$$D\psi:\mathbb{R}\times T\Sigma^N\to\mathbb{R}\times\Sigma^N,\qquad \boldsymbol{u}\mapsto D\psi(\boldsymbol{u}) = \bar{\boldsymbol{c}}(\boldsymbol{u}) = (-Ds)^{-1}(\boldsymbol{u}).$$

In particular, we see that

$$\frac{\mathrm{d}}{\mathrm{d}u^{(0)}}\psi(\boldsymbol{u}) = e(\boldsymbol{u}),\qquad \frac{\mathrm{d}}{\mathrm{d}\tilde{\boldsymbol{u}}}\psi(\boldsymbol{u}) = (c^{(1)},\dots,c^{(N)})(\boldsymbol{u}).$$

One can think of f, s and ψ as being extended to all of $\mathbb{R}^{N+1}$ whenever partial differentials of the functions appear. But only the definition on the domains and only derivatives in tangential direction as mentioned above enter the equations in Sections 2, 3 and 4.

Appendix B. Transformation of derivatives near the interface

For the following computations compare also [12]. Let $\varepsilon_0 > 0$. Near the interface $\Gamma(t;0)$ we consider the diffeomorphism

$$F_\varepsilon(t,s,z) := (t,\gamma(t,s;0) + (\varepsilon z + d(t,s;\varepsilon))\nu(t,s)),$$

which, for each $t\in I$ and $\varepsilon\in(0,\varepsilon_0)$, maps an open set $V(t;\varepsilon)\subset\mathbb{R}^2$ onto an open tube $B(t)$ around $\Gamma(t;0)$. The parameter s is the arc-length of $\Gamma(t;0)$ and ν and γ are as in Section 2. The coordinates (t,s,z) are such that the interface is given by the set $\{F_\varepsilon(t,s,z) : z=0\}$. It is supposed that, uniformly in t, s and ε, the tube $B(t)$ is large enough so that the values for z lying in a fixed interval around zero are allowed as arguments for z. We are interested in the inverse of the derivative of F_ε to obtain $\nabla_{(t,x)}z(t,x)$ and $\nabla_{(t,x)}s(t,x)$.

Let $\kappa := \kappa(t,s;0)$ be the curvature of $\Gamma(t;0)$ defined by $\partial_s\tau = \kappa\nu$ or, equivalently, by $\partial_s\nu = -\kappa\tau$. Furthermore, let

$$\begin{aligned} v &= v(t,s;0) = \partial_t\gamma(t,s;0)\cdot\nu(t,s;0) && \text{(normal velocity, intrinsic)},\\ v_\tau &= v_\tau(t,s;0) = \partial_t\gamma(t,s;0)\cdot\tau(t,s;0) && \text{(tangential velocity, non-intrinsic)}.\end{aligned}$$

Hence, writing $d_\varepsilon = d(t,s;\varepsilon)$ we get

$$\begin{aligned} DF_\varepsilon(t,s,z) &= \begin{pmatrix}\partial_t t(t,s,z) & \partial_s t(t,s,z) & \partial_z t(t,s,z)\\ \partial_t x(t,s,z) & \partial_s x(t,s,z) & \partial_z x(t,s,z)\end{pmatrix}\\ &= \begin{pmatrix} 1 & 0 & 0\\ \partial_t\gamma + (\varepsilon z + d_\varepsilon)\partial_t\nu + (\partial_t d_\varepsilon)\nu & \tau - (\varepsilon z + d_\varepsilon)\kappa\tau + (\partial_s d_\varepsilon)\nu & \varepsilon\nu\end{pmatrix}\end{aligned}$$

and

$$D(F_\varepsilon^{-1})(t,x) = (DF_\varepsilon)^{-1}(t,x) = \begin{pmatrix} \partial_t t(t,x) & \nabla_x t(t,x) \\ \partial_t s(t,x) & \nabla_x s(t,x) \\ \partial_t z(t,x) & \nabla_x z(t,x) \end{pmatrix}$$

$$= \begin{pmatrix} 1 & (0,0) \\ -\frac{1}{1-\kappa(\varepsilon z+d_\varepsilon)}(v_\tau + (\varepsilon z + d_\varepsilon)\tau \cdot \partial_t \nu) & \frac{1}{1-\kappa(\varepsilon z+d_\varepsilon)}\tau^\perp \\ \frac{1}{\varepsilon}(-\partial_t d_\varepsilon + \frac{\partial_s d_\varepsilon(\varepsilon z+d_\varepsilon)}{1-\kappa(\varepsilon z+d_\varepsilon)}\tau \cdot \partial_t \nu + \frac{\partial_s d_\varepsilon}{1-\kappa(\varepsilon z+d_\varepsilon)} v_\tau - v) & \frac{1}{\varepsilon}\nu^\perp - \frac{\partial_s d_\varepsilon}{\varepsilon(1-\kappa(\varepsilon z+d_\varepsilon))}\tau^\perp \end{pmatrix}$$

where $\partial_t \gamma$, ν, τ, κ and $\partial_t \nu$ are evaluated at $(t,s;0)$.

Inserting the ansatz $d_\varepsilon = \varepsilon d_1(t,s) + \varepsilon^2 d_2(t,s) + \cdots$ we obtain, for a function $b(t,s,z)$ and for a vector field $\vec{b}(t,s,z)$,

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t} b &= -\frac{1}{\varepsilon} v \partial_z b + \partial^\circ b - (\partial^\circ d_1)\partial_z b + O(\varepsilon), \\
\nabla_x b &= \frac{1}{\varepsilon}\partial_z b \nu + (\partial_s b - \partial_s d_1 \partial_z b)\tau \\
&\quad + \varepsilon(\kappa(z+d_1)\partial_s b - (\partial_s d_2 + \partial_s d_1 \kappa(z+d_1))\partial_z b)\tau + O(\varepsilon^2), \\
\nabla_x \cdot \vec{b} &= \frac{1}{\varepsilon}\partial_z \vec{b} \cdot \nu + (\partial_s \vec{b} - \partial_s d_1 \partial_z \vec{b}) \cdot \tau \\
&\quad + \varepsilon(\kappa(z+d_1)\partial_s \vec{b} - (\partial_s d_2 + \partial_s d_1 \kappa(z+d_1))\partial_z \vec{b}) \cdot \tau + O(\varepsilon^2), \\
\Delta_x b &= \frac{1}{\varepsilon^2}\partial_{zz} b - \frac{1}{\varepsilon}\kappa \partial_z b \\
&\quad + (\partial_s d_1)^2 \partial_{zz} b - 2\partial_s d_1 \partial_{sz} b - \kappa^2 (z+d_1)\partial_z b - \partial_{ss} d_1 \partial_z b + \partial_{ss} b + O(\varepsilon),
\end{aligned}$$

where $\partial^\circ = \partial_t - v_\tau \partial_s$ is the (intrinsic) normal time derivative (see e.g. [17]).

Appendix C. Expansions of interfacial normal velocity and curvature

Let us assume that the normal velocity and the curvature of $\Gamma(t;\varepsilon)$ can be expanded in ε-series, i.e.

$$\begin{aligned}
v(t,s;\varepsilon) &= v_0(t,s;0) + \varepsilon v_1(t,s;0) + \varepsilon^2 v_2(t,s;0) + \cdots, \\
\kappa(t,s;\varepsilon) &= \kappa_0(t,s;0) + \varepsilon \kappa_1(t,s;0) + \varepsilon^2 \kappa_2(t,s;0) + \cdots.
\end{aligned}$$

By (10) and the following paragraph, the interfaces $\Gamma(t;\varepsilon)$ are parametrized by $\gamma_\varepsilon := \gamma(t,s;\varepsilon) = \gamma(t,s;0) + d_\varepsilon \nu(t,s;0)$ where $d_\varepsilon = d(t,s;\varepsilon) = \varepsilon d_1(t,s) + \varepsilon^2 d_2(t,s) + \cdots$. We want to identify the functions v_i, κ_i in terms of the functions $d_i(t,s)$, $i = 1,2,\ldots$, $v := v(t,s;0)$ and $\kappa := \kappa(t,s;0)$.

The unit tangent vector and the unit normal vector are

$$\begin{aligned}
\tau(t,s;\varepsilon) &= \frac{\partial_s \gamma_\varepsilon}{|\partial_s \gamma_\varepsilon|} = \frac{(1-\kappa d_\varepsilon)\tau + (\partial_s d_\varepsilon)\nu}{((1-\kappa d_\varepsilon)^2 + (\partial_s d_\varepsilon)^2)^{1/2}}, \\
\nu(t,s;\varepsilon) &= \frac{\partial_s \gamma_\varepsilon^\perp}{|\partial_s \gamma_\varepsilon|} = \frac{(1-\kappa d_\varepsilon)\nu - (\partial_s d_\varepsilon)\tau}{((1-\kappa d_\varepsilon)^2 + (\partial_s d_\varepsilon)^2)^{1/2}}.
\end{aligned}$$

Inserting the expansion for d_ε yields

$$((1-\kappa d_\varepsilon)^2+(\partial_s d_\varepsilon)^2)^{-1/2}=1+\varepsilon\kappa d_1(t,s)+O(\varepsilon^2)$$

and finally for $v(t,s;\varepsilon)$ the expansion

$$\begin{aligned}
v(t,s;\varepsilon) &= \partial_t\gamma_\varepsilon\cdot\nu(t,s;\varepsilon)\\
&= \frac{(\partial_t\gamma(t,s;0)+\partial_t d_\varepsilon\nu+d_\varepsilon\partial_t\nu)\cdot((1-\kappa d_\varepsilon)\nu-(\partial_s d_\varepsilon)\tau)}{((1-\kappa d_\varepsilon)^2+(\partial_s d_\varepsilon)^2)^{1/2}}\\
&= \frac{(1-\kappa d_\varepsilon)v+\partial_t d_\varepsilon(1-\kappa d_\varepsilon)-\partial_s d_\varepsilon v_\tau-d_\varepsilon\partial_s d_\varepsilon\partial_t\nu\cdot\tau}{((1-\kappa d_\varepsilon)^2+(\partial_s d_\varepsilon)^2)^{1/2}}\\
&= v+\varepsilon\partial^\circ d_1+O(\varepsilon^2)
\end{aligned}$$

where we used $\partial_t\nu\cdot\nu=\frac{1}{2}\partial_t|\nu|^2=0$. To compute the expansion of $\kappa(t,s;\varepsilon)$ we need

$$\partial_{ss}\gamma(t,s;\varepsilon)=-(2(\partial_s d_\varepsilon)\kappa+d_\varepsilon(\partial_s\kappa))\tau+(\kappa+\partial_{ss}d_\varepsilon-\kappa^2 d_\varepsilon)\nu.$$

Then

$$\det(\partial_s\gamma(t,s;\varepsilon),\partial_{ss}\gamma(t,s;\varepsilon))=-(1-\kappa d_\varepsilon)(\kappa+\partial_{ss}d_\varepsilon-\kappa^2 d_\varepsilon)-(\partial_s d_\varepsilon)(2(\partial_s d_\varepsilon)\kappa+d_\varepsilon(\partial_s\kappa)).$$

As

$$|\partial_s\gamma_\varepsilon|^{-3}=(1-2\kappa d_\varepsilon+\kappa^2 d_\varepsilon^2+(\partial_s d_\varepsilon^2))^{-3/2}=1+\varepsilon 3\kappa d_1+O(\varepsilon^2)$$

we obtain

$$\kappa(t,s;\varepsilon)=\frac{-\det(\partial_s\gamma_\varepsilon,\partial_{ss}\gamma_\varepsilon)}{|\partial_s\gamma_\varepsilon|^3}=\kappa+\varepsilon(\kappa^2 d_1+\partial_{ss}d_1)+O(\varepsilon^2).$$

Appendix D. Derivation of matching conditions

In this appendix we will derive the conditions (15)–(18) for $\boldsymbol{u}$. Analogous results can be obtained for φ.

By (11) and (12) the functions $\hat{\boldsymbol{u}}_k(t,s,r)=\boldsymbol{u}_k(t,x)$ are well defined in the neighborhood of $\Gamma(t;0)$ which we suppose to be a tube of radius δ_0. We assume that they can be smoothly and uniformly extended onto $\Gamma(t;0)$ from both sides as $r\searrow 0$ and $r\nearrow 0$ respectively. An expansion in Taylor series at $r=0$ yields

$$\begin{aligned}
\hat{\boldsymbol{u}}_k(t,s,r) &= \hat{\boldsymbol{u}}_k(t,s,0^+)+\partial_r\hat{\boldsymbol{u}}_k(t,s,0^+)r\\
&\quad+\tfrac{1}{2}\partial_{rr}\hat{\boldsymbol{u}}_k(t,s,0^+)r^2+O(r^3),\qquad r\in(0,\delta_0],
\end{aligned}\tag{46}$$

$$\begin{aligned}
\hat{\boldsymbol{u}}_k(t,s,r) &= \hat{\boldsymbol{u}}_k(t,s,0^-)+\partial_r\hat{\boldsymbol{u}}_k(t,s,0^-)r\\
&\quad+\tfrac{1}{2}\partial_{rr}\hat{\boldsymbol{u}}_k(t,s,0^-)r^2+O(r^3),\qquad r\in[-\delta_0,0).
\end{aligned}\tag{47}$$

Let $\alpha\in(0,1)$ and $l(t)$ be the length of $\Gamma(t;0)$. We assume that the expansion

$$\hat{\boldsymbol{u}}(t,s,r;\varepsilon)=\sum_{k=0}^{N}\varepsilon^k\hat{\boldsymbol{u}}_k(t,s,r)+O(\varepsilon^{N+1})\tag{48}$$

is valid uniformly on $\{(t,s,r;\varepsilon):t\in I,\ s\in[0,l(t)],\ r\in(\varepsilon^\alpha\delta_0/2,\ \delta_0],\ \varepsilon\in(0,\varepsilon_0]\}$.

We assume that the functions $\boldsymbol{U}_k(t,s,z)$ in (13) are defined for $t \in I$, $s \in [0, l(t)]$ and $z \in \mathbb{R}$ and that they approximate some polynomial in z uniformly in t, s for large z, i.e.

$$\boldsymbol{U}_k(t,s,z) \approx \boldsymbol{U}^{\pm}_{k,0}(t,s) + \boldsymbol{U}^{\pm}_{k,1}(t,s)z + \cdots + \boldsymbol{U}^{\pm}_{k,n_k}(t,s)z^{n_k}, \qquad z \to \pm\infty, \tag{49}$$

with $n_k \in \mathbb{N}$ for all k. Moreover, we assume that the expansion (13) is valid uniformly on $\{(t,s,z;\varepsilon) : t \in I,\ s \in [0,l(t)],\ z \in \varepsilon^{\alpha-1}[-\delta_0,\ \delta_0],\ \varepsilon \in (0,\varepsilon_0]\}$.

To derive the matching conditions let $\zeta \in (\delta_0/2, \delta_0)$ and $\varepsilon \in (0, \varepsilon_0]$ and consider the intermediate variable $\zeta\varepsilon^\alpha$. The expansion (48) is valid with $r = \zeta\varepsilon^\alpha$ for ε small enough. We can use (46) and get (dropping the uniform dependence on (t,s))

$$\begin{aligned}\hat{\boldsymbol{u}}(\zeta\varepsilon^\alpha;\varepsilon) = {} & \varepsilon^0\hat{\boldsymbol{u}}_0(0^+) + \varepsilon^\alpha\partial_r\hat{\boldsymbol{u}}_0(0^+)\zeta + \varepsilon^{2\alpha}\tfrac{1}{2}\partial_{rr}\hat{\boldsymbol{u}}_0(0^+)\zeta^2 + O(\varepsilon^{3\alpha})\\ & + \varepsilon^1\hat{\boldsymbol{u}}_1(0^+) + \varepsilon^{1+\alpha}\partial_r\hat{\boldsymbol{u}}_1(0^+)\zeta + \varepsilon^{1+2\alpha}\tfrac{1}{2}\partial_{rr}\hat{\boldsymbol{u}}_1(0^+)\zeta^2 + O(\varepsilon^{1+3\alpha})\\ & + \varepsilon^2\hat{\boldsymbol{u}}_2(0^+) + \varepsilon^{2+\alpha}\partial_r\hat{\boldsymbol{u}}_2(0^+)\zeta + \varepsilon^{2+2\alpha}\tfrac{1}{2}\partial_{rr}\hat{\boldsymbol{u}}_2(0^+)\zeta^2 + O(\varepsilon^{2+3\alpha})\\ & + O(\varepsilon^3 + \varepsilon^{4\alpha}).\end{aligned}$$

Using (47) the same can be written for $-\zeta \in (\delta_0/2, \delta_0)$ with 0^+ replaced by 0^-.

Now, for ζ positive, again (13) is valid for the choice $z = \zeta\varepsilon^{\alpha-1}$. Using (49) and again dropping the dependence on (t,s) we obtain

$$\begin{aligned}U(\zeta\varepsilon^{\alpha-1};\varepsilon) = {} & \varepsilon^0\boldsymbol{U}^+_{0,0} + \varepsilon^{\alpha-1}\boldsymbol{U}^+_{0,1}\zeta + \cdots + \varepsilon^{n_0(\alpha-1)}\boldsymbol{U}^+_{0,n_0}\zeta^{n_0}\\ & + \varepsilon^1\boldsymbol{U}^+_{1,0} + \varepsilon^{1+\alpha-1}\boldsymbol{U}^+_{1,1}\zeta + \cdots + \varepsilon^{1+n_1(\alpha-1)}\boldsymbol{U}^+_{1,n_1}\zeta^{n_1}\\ & + \varepsilon^2\boldsymbol{U}^+_{2,0} + \varepsilon^{2+\alpha-1}\boldsymbol{U}^+_{2,1}\zeta + \cdots + \varepsilon^{2+n_2(\alpha-1)}\boldsymbol{U}^+_{2,n_2}\zeta^{n_2} + \cdots.\end{aligned}$$

The same holds true for $-\zeta \in (\delta_0/2, \delta_0)$ with $\boldsymbol{U}^+$ replaced by $\boldsymbol{U}^-$.

The expansions of $\boldsymbol{U}$ and $\hat{\boldsymbol{u}}$ are said to match if, in the limit $\varepsilon \searrow 0$, the coefficients to every order in ε and ζ agree. Comparing the two series for $\boldsymbol{U}$ and $\hat{\boldsymbol{u}}$ yields the following relations between the coefficients $\boldsymbol{U}^+_{k,n}$ on the one hand and the derivatives $\partial_r^j\hat{\boldsymbol{u}}_l(0^+)$ on the other hand for $k \leqslant 2$:

$$\begin{array}{llll} \boldsymbol{U}^+_{0,0} = \hat{\boldsymbol{u}}_0(0^+), & & & \boldsymbol{U}^+_{0,i} = 0, \quad 1 \leqslant i \leqslant n_0,\\ \boldsymbol{U}^+_{1,0} = \hat{\boldsymbol{u}}_1(0^+), & \boldsymbol{U}^+_{1,1} = \partial_r\hat{\boldsymbol{u}}_0(0^+), & & \boldsymbol{U}^+_{1,i} = 0, \quad 2 \leqslant i \leqslant n_1,\\ \boldsymbol{U}^+_{2,0} = \hat{\boldsymbol{u}}_2(0^+), & \boldsymbol{U}^+_{2,1} = \partial_r\hat{\boldsymbol{u}}_1(0^+), & \boldsymbol{U}^+_{2,2} = \tfrac{1}{2}\partial_{rr}\hat{\boldsymbol{u}}_0(0^+), & \boldsymbol{U}^+_{2,i} = 0, \quad 3 \leqslant i \leqslant n_2.\end{array}$$

Obviously from the definition of r, a derivative of some function with respect to r corresponds to the derivative with respect to x in the direction $\nu = \nu(t, s(t,x); 0)$. Hence, we can replace $\partial_r\hat{\boldsymbol{u}}_k$ by $\nabla\boldsymbol{u}_k \cdot \nu$. As ν is independent of r we can also replace $\partial_{rr}\hat{\boldsymbol{u}}_k$ by $(\nu\cdot\nabla)(\nu\cdot\nabla)\boldsymbol{u}_k$. We use (49) again and obtain the following matching conditions (compare (15)–(18)): as $z \to \pm\infty$,

$$\begin{aligned}\boldsymbol{U}_0(z) &\approx \boldsymbol{u}_0(0^\pm),\\ \boldsymbol{U}_1(z) &\approx \boldsymbol{u}_1(0^\pm) + (\nabla\boldsymbol{u}_0(0^\pm)\cdot\nu)z,\\ \partial_z\boldsymbol{U}_1(z) &\approx \nabla\boldsymbol{u}_0(0^\pm)\cdot\nu,\\ \partial_z\boldsymbol{U}_2(z) &\approx \nabla\boldsymbol{u}_1(0^\pm)\cdot\nu + ((\nu\cdot\nabla)(\nu\cdot\nabla)\boldsymbol{u}_0(0^\pm)).\end{aligned}$$

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