



Second order phase field asymptotics
for multi-component systems

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SECOND ORDER PHASE FIELD ASYMPTOTICS FOR MULTI-COMPONENT SYSTEMS

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ABSTRACT. An asymptotic analysis of a phase field model for solidification in multi-component alloy systems is presented. In the limit of vanishing interface thickness the related sharp interface model is approximated to second order by taking a non-constant kinetic correction term into account. In numerical experiments the approximation properties of the phase field model as well as the gain in computational effort due to the correction are investigated.

1. INTRODUCTION

The phase field method has become a powerful tool for modelling the microstructural evolution during solidification (see [6, 20, 10, 7] 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 $\varepsilon \rightarrow 0$ a model with moving boundaries is recovered. This relation can be established by matched asymptotic expansions. We are interested in the quality of this approximation in terms of ε , namely, in an approximation to second order.

First results in the above direction have been obtained by Karma and Rappel [16] in the context of thin interface asymptotics. 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. Besides, 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 thermodynamic consistency are lost. In a more recent analysis Ramirez et al. [22] 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 [15]). 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.

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

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are usually use the free energy or the entropy as thermodynamic potentials (see e.g. [3, 21, 24, 25] and the discussion in [17]). It turns out that in our context the reduced grand canonical potential ψ (see [19]) 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. In this case the free energy f is conveniently written as a function of the absolute temperature T and the concentrations $c = (c^{(1)}, \dots, c^{(N)})$. Now we define the entropy and the chemical potentials via

$$df = -sdT + \mu \cdot dc$$

and the internal energy as $e = f + Ts$. For the reduced grand canonical potential $\psi = -\frac{g}{T}$, $g = f - \mu \cdot c$ being the grand canonical potential, we then obtain

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

in particular $u = (u^{(0)}, \tilde{u}) = (\frac{-1}{T}, \frac{\mu}{T})$ are the to (e, c) conjugate variables. Assuming local thermodynamical equilibrium the vector u will be 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 thermodynamic background.

Next we will formulate the sharp interface problem for a liquid-solid phase change in a non-isothermal multi-component system. 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 there holds

$$\partial_t \psi_{,u}(u) = -\nabla \cdot L \nabla(-u)$$

where $\psi_{,u^{(0)}} = e$ and $\psi_{,\tilde{u}} = c$ and L is a matrix of Onsager coefficients. On Γ it holds

$$\begin{aligned} u &\text{ is continuous,} \\ [-L \nabla u]_s^l \cdot \nu &= v[(e, c)^\perp]_s^l, \\ \alpha v &= \sigma \kappa - [\psi(u)]_s^l, \end{aligned}$$

where ν is the unit normal on Γ pointing into D^l , v is the normal velocity into 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.

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

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

$$\partial_t \psi_{,u}(u, \varphi) = \nabla \cdot L \nabla u. \quad (2)$$

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 in 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 $\psi(u, \varphi)$. For this purpose, interpolation functions between 0 and 1 like $h(\varphi)$ in the above equation are used. The relation to the sharp interface model is established using the method of formally matched asymptotic expansions ([8] contains a careful discussion of several limits in the case of pure substances).

In this paper we show that it is possible to derive a phase field model that approximates the sharp interface model to higher order in ε . More precisely, we obtain the following

Main result: *For two phase multi-component systems with arbitrary phase diagrams we find a correction term to the kinetic coefficient such that the model with moving boundaries is approximated to second order.*

A new feature compared to the existing results in [2, 4, 16] is that, in general, this correction term depends on 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 [16]. 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 formally 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 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.

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 a 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 these 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 thermodynamic quantities can be modeled.

The above differential equation is coupled to balance equations for energy and mass. The thermodynamic potentials are postulated to be the derivatives of the entropy density (see [13]) and for the fluxes we postulate linear combinations of the corresponding thermodynamic forces, hence with Onsager coefficients L_{ij} we obtain

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

where T is the temperature and $c = (c^{(1)}, \dots, c^{(N)})$ a vector of concentrations, $c^{(i)}$ describing the presence of component i . Given the free energy density $f = f(T, c)$, 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.

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

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

and its tangential space

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

Moreover we define

$$Y := \mathbb{R} \times T\Sigma^N.$$

The problem then consists of finding smooth functions

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

that solve the partial differential equations

$$(\omega_0 + \varepsilon\omega_1(u))\partial_t\varphi = \Delta\varphi - \frac{1}{\varepsilon^2}w'(\varphi) + \frac{1}{2\varepsilon}h'(\varphi)\Psi(u), \quad (3)$$

$$\partial_t\psi_{,u^{(i)}}(u, \varphi) = \nabla \cdot \sum_{j=0}^N L_{ij}\nabla u^{(j)}, \quad 0 \leq i \leq N. \quad (4)$$

The first equation is a forced Allen-Cahn equation for the phase field variable φ . The coupling to the thermodynamic quantities via the last term in that equation will be clarified below. We are interested in the limit $\varepsilon \rightarrow 0$. The function $\omega_1 : Y \rightarrow \mathbb{R}$ 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 energy $e = \psi_{,u^{(0)}}$ and concentrations $c^{(i)} = \psi_{,u^{(i)}}$, $1 \leq i \leq N$ (see the Appendix A for the exact relation between (e, c) and the derivatives of ψ with respect to u). The equations in (3) 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. $w : \mathbb{R} \rightarrow \mathbb{R}^+$ is some nonnegative smooth double well potential which attains its global minima in 0 and 1, more precisely we have

$$\begin{aligned} w(\varphi) &> 0 && \text{if } \varphi \notin \{0, 1\}, \\ w(0) = w(1) &= 0, && w'(0) = w'(1) = 0, \quad w''(0) = w''(1) > 0. \end{aligned} \quad (5)$$

Besides w is symmetric with respect to $\frac{1}{2}$, i.e. $w(\frac{1}{2} + \varphi) = w(\frac{1}{2} - \varphi)$.

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

$$h(0) = 0, \quad h(1) = 1, \quad h(\frac{1}{2} + \varphi) = 1 - h(\frac{1}{2} - \varphi), \quad h'(\varphi) \geq 0. \quad (6)$$

Furthermore we require that

$$h'(0) = h'(1) = 0. \quad (7)$$

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

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

with a function \tilde{h} satisfying Assumption C. Observe that in the case $\tilde{h} \neq h$ the model lacks thermodynamic consistency, i.e. an entropy inequality might not hold (see [21, 16, 2]). In (3) we used the abbreviation

$$\Psi(u) := \psi_l(u) - \psi_s(u).$$

The function ψ is convex in u so that (4) becomes parabolic. We will frequently use $\psi(u, \varphi)$, $\psi_s(u)$ and $\psi_l(u)$ as a function for arbitrary $u \in \mathbb{R}^{N+1}$ which motivates to write down the partial derivative $\psi_{,u^{(k)}}(u, \varphi)$. But all the results do not depend on the extension as only arguments $u \in Y$ and derivatives along Y will be used.

E. The matrix $L = (L_{ij})_{i,j=0}^N$ of Onsager coefficients is 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

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

Besides for each $v \in Y$ the linear system $L\xi = v$ has exactly one solution $\xi \in Y$ which we will denote with $\xi = L^{-1}v$.

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 [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 (3) and (4) with $(u(t, x; \varepsilon), \varphi(t, x; \varepsilon))$. The family of curves

$$\Gamma(t; \varepsilon) := \left\{ x \in D : \varphi(t, x; \varepsilon) = \frac{1}{2} \right\}, \quad \varepsilon > 0, t \in I, \quad (8)$$

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) such that if $\varepsilon \rightarrow 0$ some limiting curve $\Gamma(t; 0)$ is obtained. With $D^l(t; \varepsilon)$ and $D^s(t; \varepsilon)$ we denote the regions occupied by the liquid phase (where $\varphi(t, x; \varepsilon) > \frac{1}{2}$) and the solid phase (where $\varphi(t, x; \varepsilon) < \frac{1}{2}$) respectively.

Let $\gamma(t, s; 0)$ be a parametrization of $\Gamma(t; 0)$ by arc-length s for every $t \in I$. $\nu(t, s; 0)$ 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 tangential vector. The orientation is such that (ν, τ) ist 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

$$\gamma(t, s; \varepsilon) := \gamma(t, s; 0) + d(t, s; \varepsilon)\nu(t, s; 0). \quad (9)$$

Close to $\varepsilon = 0$ we assume that there is the 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 $d_0(t, s) \equiv 0$.

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

$$\kappa(t, s; \varepsilon) = \kappa(t, s; 0) + \varepsilon(\kappa(t, s; 0)^2 d_1(t, s) + \partial_{ss} d_1(t, s)) + O(\varepsilon^2), \quad (10)$$

$$v(t, s; \varepsilon) = \partial_t \gamma(t, s; \varepsilon) \cdot \nu(t, s; \varepsilon) = v(t, s; 0) + \varepsilon \partial^\circ d_1(t, s) + O(\varepsilon^2); \quad (11)$$

here, ∂° denotes the (intrinsic) normal time derivative (see Appendix B).

We suppose that in each domain $\tilde{D} \subset\subset D \setminus \Gamma(t; 0)$ the solution can be expanded in a series close to $\varepsilon = 0$ (outer expansion):

$$u(t, x; \varepsilon) = \sum_{k=0}^K \varepsilon^k u_k(t, x) + O(\varepsilon^{K+1}), \quad \varphi(t, x; \varepsilon) = \sum_{k=0}^K \varepsilon^k \varphi_k(t, x) + O(\varepsilon^{K+1}). \quad (12)$$

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

$$\hat{u}(t, s, r; \varepsilon) = u(t, x; \varepsilon), \quad \hat{\varphi}(t, s, r; \varepsilon) = \varphi(t, x; \varepsilon). \quad (13)$$

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

$$U(t, s, z; \varepsilon) = \sum_{k=0}^K \varepsilon^k U_k(t, s, z) + O(\varepsilon^{K+1}), \quad (14)$$

$$\Phi(t, s, z; \varepsilon) = \sum_{k=0}^K \varepsilon^k \Phi_k(t, s, z) + O(\varepsilon^{K+1}). \quad (15)$$

We remark that, in some cases, this ansatz has been verified by rigorously showing that, in the limit as $\varepsilon \rightarrow 0$, the sharp interface model is obtained from the diffuse interface model (see e.g. [1, 9, 11, 23]).

For the two expansions for u to match in the limit as $\varepsilon \rightarrow 0$ there are certain conditions (see Appendix D for the derivation): As $z \rightarrow \pm\infty$

$$U_0(z) \approx u_0(0^\pm), \quad (16)$$

$$U_1(z) \approx u_1(0^\pm) + (\nabla u_0(0^\pm) \cdot \nu)z, \quad (17)$$

$$\partial_z U_1(z) \approx \nabla u_0(0^\pm) \cdot \nu, \quad (18)$$

$$\partial_z U_2(z) \approx \nabla u_1(0^\pm) \cdot \nu + (\nu \cdot D^2 u_0(0^\pm) \nu)z \quad (19)$$

and analogously for Φ and φ . For a function $g(t, x)$, $g(0^+)$ denotes the limit of $g(t, x)$ if $r(x) = \text{dist}(x, \Gamma(t; 0)) \rightarrow 0$ and if $x \in D^l(t; 0)$ (which is equivalent to $r > 0$); analogously we define $g(0^-)$ considering $x \in D^s(t; 0)$.

3. ASYMPTOTIC ANALYSIS

3.1. Outer solutions. In the region away from $\Gamma(t; 0)$ we plug the expansions (12) into the differential equations (3) and (4). All terms that appear are expanded in ε .

To leading order $O(\varepsilon^{-2})$ we obtain from (3) 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

$$0 = -w''(\varphi_0)\varphi_1 + \frac{1}{2}h'(\varphi_0)\Psi(u_0). \quad (20)$$

As φ_0 is already known, using the Assumptions B and C, we obtain $\varphi_1 \equiv 0$ as the only solution.

To leading order $O(\varepsilon^0)$ we obtain from (4), written as vectorial equation,

$$\partial_t(\psi_{,u}(u_0, \varphi_0)) = L\Delta u_0. \quad (21)$$

Depending on φ_0 we have $\psi_{,u}(u_0, \varphi_0) = (\psi_l)_{,u}(u_0)$ or $\psi_{,u}(u_0, \varphi_0) = (\psi_s)_{,u}(u_0)$. In both cases (21) is a parabolic equation for u_0 by Assumption D.

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

$$\partial_t((\psi_{,uu})(u_0, \varphi_0)u_1) = L\Delta u_1 \quad (22)$$

where we already made use of $\varphi_1 \equiv 0$. Assumption D states that ψ is convex so that (22) is a linear parabolic equation for u_1 .

To determine boundary conditions for (21) and (22) on $\Gamma(t; 0)$ we plug the expansions (14) and (15) into the differential equations.

3.2. Inner solutions. 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 (3)

$$0 = \partial_{zz}\Phi_0 - w'(\Phi_0). \quad (23)$$

By (8) and the assumption that (15) holds true for $\varepsilon = 0$ we have $\Phi_0(0) = \frac{1}{2}$. The matching conditions (16) imply

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

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

For the conserved variables we get from (4)

$$0 = L\partial_{zz}U_0. \quad (24)$$

Using Assumption E we have $\partial_{zz}U_0 = L^{-1}0 = 0$ in Y so that U_0 is affine linear in z . By the matching conditions (16), U_0 has to be bounded as $z \rightarrow \pm\infty$, hence we see that U_0 must be constant in z which means $U_0 = U_0(t, s)$. The matching condition (16) implies that $U_0(t, s)$ is exactly the value of u_0 in the point $\gamma(t, s; 0) \in \Gamma(t; 0)$ from both sides of the interface. In particular,

$$u_0 \text{ is continuous across the interface } \Gamma(t; 0). \quad (25)$$

To order $O(\varepsilon^{-1})$ equation (3) yields

$$-\omega_0 v \partial_z \Phi_0 = \partial_{zz}\Phi_1 - \kappa \partial_z \Phi_0 - w''(\Phi_0)\Phi_1 + \frac{1}{2}h'(\Phi_0)\Psi(U_0). \quad (26)$$

From the solution to (20) we get $\varphi_1(t, s, 0^\pm) = 0$. Besides $\nabla\varphi_0(t, s, 0^\pm) \cdot \nu = 0$ as φ_0 is constant. Due to the matching conditions (17) we have $\Phi_1 \rightarrow 0$ as $z \rightarrow \pm\infty$. The operator $\mathcal{L}(\Phi_0)b = \partial_{zz}b - w''(\Phi_0)b$ is self-adjoint with respect to the L^2 -product over \mathbb{R} . Differentiating (23) with respect to z we obtain that $\partial_z\Phi_0$ lies in the kernel of $\mathcal{L}(\Phi_0)$. Since $\Phi_0(-z) = 1 - \Phi_0(z)$ we get with the help of Assumption C that $\partial_z\Phi_0$ and $h'(\Phi_0)$ are even, hence (26) 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 :

$$0 = \int_{\mathbb{R}} ((\kappa - \omega_0 v)(\partial_z \Phi_0(z))^2 - \frac{1}{2} \Psi(U_0) h'(\Phi_0(z)) \partial_z \Phi_0(z)) dz = (\kappa - \omega_0 v) I - \frac{1}{2} \Psi(U_0) \quad (27)$$

where

$$I = \int_{\mathbb{R}} (\partial_z \Phi_0)^2 dz.$$

The system (4) becomes to the order $O(\varepsilon^{-1})$

$$-v \partial_z \psi_{,u}(U_0, \Phi_0) = -v \partial_z ((\psi_s)_{,u}(U_0) + \tilde{h}(\Phi_0) \Psi_{,u}(U_0)) = L \partial_{zz} U_1. \quad (28)$$

As $U_0 = U_0(t, s)$ we obtain $\Psi_{,u}(U_0) = [\psi_{,u}(u_0)]_s^l = (\psi_l)_{,u}(u_0) - (\psi_s)_{,u}(u_0)$ for all z . We integrate two times with respect to z and get

$$\begin{aligned} U_1 &= -L^{-1} \left(v \int_0^z \psi_{,u}(U_0, \Phi_0) dz' - Az \right) + \bar{u} \\ &\sim -L^{-1} \left(v(\psi_l)_{,u}(U_0) z - Az - v[\psi_{,u}(u_0)]_s^l \tilde{H} \right) + \bar{u} \text{ as } z \rightarrow \infty \\ &\sim -L^{-1} \left(v(\psi_s)_{,u}(U_0) z - Az - v[\psi_{,u}(u_0)]_s^l \tilde{H} \right) + \bar{u} \text{ as } z \rightarrow -\infty \end{aligned} \quad (29)$$

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

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

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^∞ while the linear terms remain. Using (17) we derive

$$u_1(t, s, 0^\pm) = \bar{u} + vL^{-1} [\psi_{,u}(u_0)]_s^l \tilde{H} \quad (30)$$

which means, in particular, that

$$u_1 \text{ is continuous across } \Gamma(t; 0). \quad (31)$$

With (18) the following jump condition is obtained at the interface:

$$\begin{aligned} [-L \nabla u_0]_s^l \cdot \nu &:= -L \nabla u_0(t, s, 0^+) \cdot \nu + L \nabla u_0(t, s, 0^-) \cdot \nu \\ &= \left(v(\psi_l)_{,u}(u_0) - A \right) - \left(v(\psi_s)_{,u}(u_0) - A \right) \\ &= v[\psi_{,u}(u_0)]_s^l. \end{aligned} \quad (32)$$

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

$$\begin{aligned} & -\omega_0 v \partial_z \Phi_1 - \omega_1(u_0) v \partial_z \Phi_0 - \omega_0 (\partial^\circ d_1) \partial_z \Phi_0 \\ &= \partial_{zz} \Phi_2 - w''(\Phi_0) \Phi_2 + (\partial_s d_1)^2 \partial_{zz} \Phi_0 - \kappa^2 (z + d_1) \partial_z \Phi_0 - \partial_{ss} d_1 \partial_z \Phi_0 + \\ & - \kappa \partial_z \Phi_1 - \frac{1}{2} w'''(\Phi_0) (\Phi_1)^2 + \frac{1}{2} \Psi(U_0) h''(\Phi_0) \Phi_1 + \frac{1}{2} \Psi_{,u}(U_0) \cdot U_1 h'(\Phi_0). \end{aligned}$$

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:

$$\begin{aligned}
& \int_{\mathbb{R}} \left((\kappa - \omega_0 v) \partial_z \Phi_1 + \frac{1}{2} w'''(\Phi_0) (\Phi_1)^2 - \frac{1}{2} \Psi(U_0) h''(\Phi_0) \Phi_1 \right) \partial_z \Phi_0 dz \\
&= \int_{\mathbb{R}} \left((\kappa - \omega_0 v) \partial_z \Phi_1 \partial_z \Phi_0 - w''(\Phi_0) \Phi_1 \partial_z \Phi_1 + \frac{1}{2} \Psi(U_0) h'(\Phi_0) \partial_z \Phi_1 \right) dz \\
&= 2(\kappa - \omega_0 v) \int_{\mathbb{R}} \partial_z \Phi_1 \partial_z \Phi_0 dz - \int_{\mathbb{R}} \partial_{zz} \Phi_1 \partial_z \Phi_1 dz
\end{aligned}$$

where we used (26) 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

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

and using (29) for the remaining U_1 -term, a short calculation shows

$$\begin{aligned}
& - \int_{\mathbb{R}} \frac{1}{2} \Psi(U_0) \cdot U_1 \partial_z (h \circ \Phi_0) dz \\
&= - \frac{1}{2} [\psi_{,u}(u_0)]_s^l \cdot \left(\bar{u} - L^{-1} [\psi_{,u}(u_0)]_s^l H + L^{-1} [\psi_{,u}(u_0)]_s^l 2J \right) \\
&= - \frac{1}{2} [\psi_{,u}(u_0)]_s^l \cdot u_1 + v [\psi_{,u}(u_0)]_s^l \cdot L^{-1} [\psi_{,u}(u_0)]_s^l \frac{(H + \tilde{H} - 2J)}{2}
\end{aligned}$$

where we used (30) to get the last equality.

The whole solvability condition then becomes

$$\begin{aligned}
0 &= [-\omega_0 \partial^\circ + \partial_{ss} + \kappa^2] d_1 I - \frac{1}{2} [\psi_{,u}(u_0)]_s^l u_1 \\
&\quad + v \left(-\omega_1(u_0) I + [\psi_{,u}(u_0)]_s^l \cdot L^{-1} [\psi_{,u}(u_0)]_s^l \frac{H + \tilde{H} - 2J}{2} \right). \tag{33}
\end{aligned}$$

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 (U_0, Φ_0) this will be denoted by a superscript 0 . The conservation laws (4) yield to order $O(\varepsilon^0)$

$$-v \partial_z (\psi_{,uu}^0 U_1 + \psi_{,u\varphi}^0 \Phi_1) + \partial^\circ \psi_{,u}^0 - (\partial^\circ d_1) \partial_z \psi_{,u}^0 = L [\partial_{zz} U_2 - \kappa \partial_z U_1 + \partial_{ss} U_0]$$

where we used that U_0 does not dependent on z . Integrating once with respect to z leads to

$$-L \partial_z U_2 = \underbrace{v \partial_z (\psi_{,uu}^0 U_1 + \psi_{,u\varphi}^0 \Phi_1)}_{(i)} - B + \underbrace{\int_0^z ((\partial^\circ d_1) \partial_z \psi_{,u}^0 - \partial^\circ \psi_{,u}^0) dz'}_{(ii)} - \underbrace{\kappa L U_1}_{(iii)} + L \partial_{ss} U_0 z$$

where $B \in Y$ is an integration constant. We want to derive a correction to the jump condition (32), i.e. a jump condition for u_1 . Therefore we are interested in the terms

contributing to $\nabla u_1 \cdot \nu$ in (19). Applying (17) to Φ_1, U_1 and using the fact that $\tilde{h}'(0) = \tilde{h}'(1) = 0$ we see that

$$\begin{aligned} (i) &\sim v(\psi_l)_{,uu}(u_0)u_1 - B + (\dots)z && \text{as } z \rightarrow \infty, \\ &\sim v(\psi_s)_{,uu}(u_0)u_1 - B + (\dots)z && \text{as } z \rightarrow -\infty. \end{aligned}$$

Furthermore

$$\begin{aligned} (ii) &= (\partial^\circ d_1)(\psi_{,u}^0|_0^z) - \int_0^z [\partial^\circ((\psi_s)_{,u}^0) + (\partial^\circ \Psi_{,u}^0)(\tilde{h} \circ \Phi_0)(z')] dz' \\ &\sim \frac{1}{2}(\partial^\circ d_1)[\psi_{,u}(u_0)]_s^l - (\partial^\circ(\psi_l)_{,u}(u_0))z + \partial^\circ[\psi_{,u}(u_0)]_s^l \tilde{H} && \text{as } z \rightarrow \infty, \\ &\sim -\frac{1}{2}(\partial^\circ d_1)[\psi_{,u}(u_0)]_s^l - (\partial^\circ(\psi_s)_{,u}(u_0))z + \partial^\circ[\psi_{,u}(u_0)]_s^l \tilde{H} && \text{as } z \rightarrow -\infty \end{aligned}$$

where for the first term the symmetry of \tilde{h} in Assumption C has been used. In (iii) we use (30) again to obtain

$$(iii) = \kappa L u_1(t, s, 0) + (\dots)z \quad \text{as } z \rightarrow \pm\infty.$$

Finally we get for the first order correction of the jump condition (32) at the interface:

$$[-L\nabla u_1]_s^l \cdot \nu = v[\psi_{,uu}(u_0)]_s^l \cdot u_1 + (\partial^\circ d_1)[\psi_{,u}(u_0)]_s^l. \quad (34)$$

3.3. Summary of the leading order problem and the correction problem. The problem to leading order consists of the bulk equation (21) which is coupled to the conditions (25), (32) and (27) on $\Gamma(t; 0)$:

(LOP) Find a function $u_0 : I \times D \rightarrow Y$ 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

$$\partial_t((\psi_l)_{,u}(u_0)) = L\Delta u_0, \quad \text{in } D^l(t; 0), t \in I, \quad (35)$$

$$\partial_t((\psi_s)_{,u}(u_0)) = L\Delta u_0, \quad \text{in } D^s(t; 0), t \in I, \quad (36)$$

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

$$u_0 \text{ is continuous}, \quad (37)$$

$$[-L\nabla u_0]_s^l \cdot \nu = v[\psi_{,u}(u_0)]_s^l, \quad (38)$$

$$\omega_0 v = \kappa - \frac{1}{2I}[\psi(u_0)]_s^l \quad (39)$$

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

If we choose

$$\omega_1 = \omega_1(u_0) := [\psi_{,u}(u_0)]_s^l \cdot L^{-1}[\psi_{,u}(u_0)]_s^l \frac{H + \tilde{H} - 2J}{2I} \quad (40)$$

then the correction problem consisting of (22), (31), (34) and (33) reads as follows:

(CP) Let $(u_0, \{\Gamma(t; 0)\}_t)$ be a solution to (LOP) and let $l(t)$ be the length of $\Gamma(t; 0)$ and set $S_I = \{(t, s) : t \in I, s \in [0, l(t)]\}$. Then we need to find functions $u_1 : I \times D \rightarrow Y$ and $d_1 : S_I \rightarrow \mathbb{R}$ such that

$$\partial_t((\psi_l)_{,uu}(u_0)u_1) = L\Delta u_1, \quad \text{in } D^l(t; 0), t \in I, \quad (41)$$

$$\partial_t((\psi_s)_{,uu}(u_0)u_1) = L\Delta u_1, \quad \text{in } D^s(t; 0), t \in I \quad (42)$$

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

$$u_1 \text{ is continuous,} \quad (43)$$

$$[-L\nabla u_1]_s^l \cdot \nu = v[\psi,_{uu}(u_0)]_s^l u_1 + (\partial^\circ d_1)[\psi,_{,u}(u_0)]_s^l, \quad (44)$$

$$\omega_0(\partial^\circ d_1) = (\partial_{ss} + \kappa^2)d_1 - \frac{1}{2I}[\psi,_{,u}(u_0)]_s^l \cdot u_1. \quad (45)$$

Obviously, $(u_1, d_1) \equiv 0$ 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 (40) is crucial in order to guarantee that the undesired terms in (33) vanish.

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.

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

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

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:

$$\varepsilon(\omega_0 + \varepsilon\omega_1)\partial_t \varphi = \varepsilon\sigma\partial_{xx}\varphi - \frac{9\sigma}{\varepsilon}\varphi(1 - \varphi)(1 - 2\varphi) + \frac{1}{2}\lambda(u - u_m)h'(\varphi), \quad (46)$$

$$\partial_t \psi,_{,u} = \partial_t(c_v u - \lambda(1 - \tilde{h}(\varphi))) = K\partial_{xx}u. \quad (47)$$

This system differs from typical phase field systems (see e.g. [21]) by the term $\varepsilon\omega_1(u)$. 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 $u \rightarrow u_\infty$ as $x \rightarrow \infty$ there is the following travelling wave solution: Setting $u_i = c_v^{-1}\lambda + u_\infty$ we define

$$p(t) = v t = \omega_0^{-1} \lambda (u_m - u_i) t, \quad (48)$$

$$u = u_i, \quad x \leq v t, \quad (49)$$

$$u = u_\infty + (u_i - u_\infty) \exp(-K^{-1} c_v v (x - v t)), \quad x > v t. \quad (50)$$

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

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

we obtain the velocity $v = 1.0$, the value $u_i = -1.5$ at the interface and by (40) the correction term $\omega_1 \approx 0.013194444$.

We solved the differential equations on the time interval $I = [0, 0.1]$ for several values for ε . We chose Dirichlet boundary conditions for u given by the travelling wave solution (49),(50) to the sharp interface model and homogeneous Neumann boundary conditions for φ . To initialize φ we set

$$\varphi(0, x) := \frac{1}{2}(1 + \tanh(\frac{3}{2}z)) = \Phi_0(z), \quad z = \frac{x-x_0}{\varepsilon} \quad (51)$$

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 (23) with the boundary conditions $\Phi_0(z) \rightarrow 0, 1$ as $z \rightarrow \infty, -\infty$. Initial values for u were obtained by matching outer and inner solution to leading and first order obtained from the asymptotic expansions (see e.g. [18])

$$u(0, x) = u_0(0, x) + \varepsilon u_1(0, x) + U_0(0, z) + \varepsilon U_1(0, z) - \text{common part.}$$

The function $u_0(0, x)$ has the profile of the travelling wave solution:

$$u_0(0, x) = \begin{cases} u_\infty + (u_i - u_\infty) \exp(-\frac{cv}{K}v(x - x_0)), & x > x_0, \\ u_i, & x \leq x_0. \end{cases} \quad (52)$$

As we want $u_1 \equiv 0$ to be a solution to the correction problem we chose $u_1(0, x) = 0$. By equations (24) and (25), $U_0 \equiv u_i$ is the interface value which is constant in normal direction. Equation (18) implies $\partial_z U_1(z) \rightarrow \nabla \cdot u_0(x_0^-) = 0$ as $z \rightarrow -\infty$. As $u_1(0, x) = 0$ we have $\bar{u} = -\frac{v}{K}\lambda\tilde{H}$ by (30). With (29) we see that $A = v(\psi_s)_{,u}(U_0)$ which yields

$$U_1(0, z) = \frac{v}{K} \begin{cases} \lambda - z + \int_0^z (1 - \tilde{h} \circ \varphi_0)(z') dz' - \tilde{H}, & z > 0, \\ \lambda \int_z^0 (\tilde{h} \circ \varphi_0)(z') dz' - \tilde{H}, & z < 0. \end{cases}$$

The common part is $u_i - \frac{v\lambda}{K}z$ if $z > 0$ and u_i if $z < 0$.

The phase boundaries $\{\varphi = \frac{1}{2}\}$ were determined by linearly interpolating the values at the grid points. Subtracting from the computed transition point the exact position given by (48) we got up to the sign the values in Figure 1 on the 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

$$u(0, x) = u_0(0, x) \text{ or } \varphi = \chi_{[x_0, \infty]}$$

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 behaviour exactly. 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 $10/\sqrt{2}$. The deviations at $t = 8.0$ are

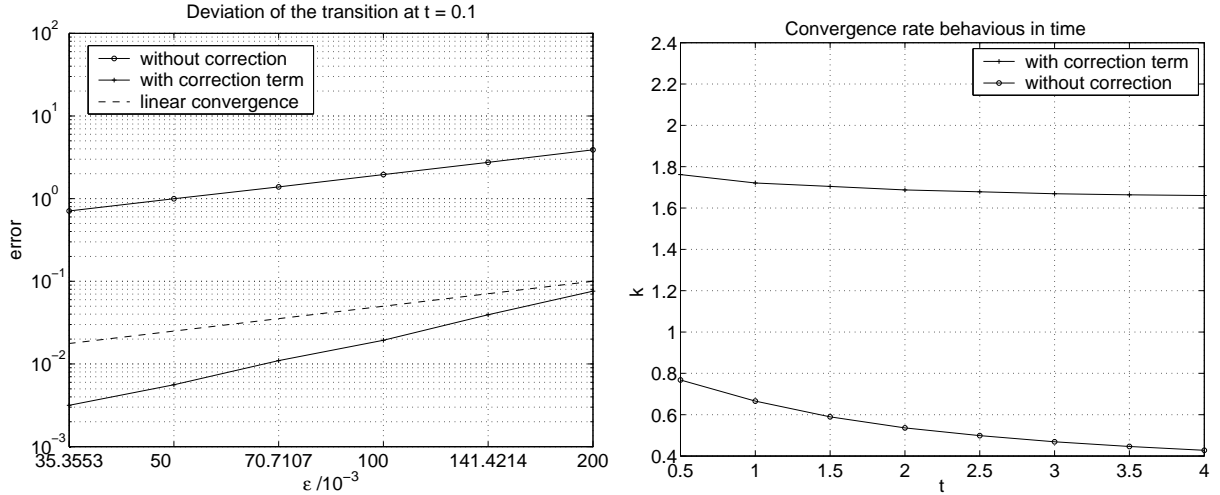


FIGURE 1. On the left: deviations of the phase boundaries measured from the exact interface position given by (48) over ε ; the resolution of the transition region is very fine such that the error caused by the discretization is negligible. On the right: behaviour of the numerically computed convergence rates (see Appendix E) in time for the angle $\beta = 15^\circ$ (see Sec. 4.2).

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 correction term. To get an error as obtained with 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 $dt \lesssim \Delta x^2$ 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

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

Then (46) has to be replaced by a variational inequality for φ but the asymptotic analysis can be done in a similar way (see [5]). 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 (47) for u remains the same except that ∂_{xx} is replaced by the Laplacian Δ .

We chose the following constants:

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

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

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

which is the solution to the variational inequality corresponding to (23) when restricted to a radial direction. Here, $r = \sqrt{x^2 + y^2}$ is the radius and we chose $r_0 = 0.8$. With $\tilde{h}(\varphi) = h(\varphi) = \varphi^2(3 - 2\varphi)$ we get the constants $I = \frac{1}{2}$, $H + \tilde{H} - 2J = \frac{23\pi^2}{1024}$ and hence $\omega_1 = \frac{\lambda^2}{K} \frac{H + \tilde{H} - 2J}{2I} \approx 0.554201419$. For u initially the 1D profile (52) of the travelling wave solution in Subsection 4.1 in radial direction was used. As in the 1D case $u_i = -1.5$, $v = \frac{\omega_0}{\lambda}(u_m - u_i) = 0.25$ 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 $\varphi = \frac{1}{2}$ 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		
	$\beta = 20^\circ$	$\beta = 15^\circ$	$\beta = 0^\circ$	$\beta = 20^\circ$	$\beta = 15^\circ$	$\beta = 0^\circ$
$\varepsilon = 0.2$	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 (see Appendix E 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. Besides we see that the change in the radius when changing ε is much smaller if a correction ω_1 is considered. In Figure 1 the time behaviour 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 u -dependent correction term. In this subsection we will demonstrate that our approach in fact makes it possible to obtain a superior approximation behaviour also in this case.

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

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

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

$$u^{(0)} = u_m - \frac{G}{\lambda}(u^{(1)})^2(3 - 2u^{(1)}) \quad (53)$$

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

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

For the isothermal case, i.e. $u^{(0)}$ is constant, we solved (3) 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 (52) for $u^{(0)}$,

$$u^{(1)}(0, x) = \begin{cases} u_{\infty}^{(1)} + (u_i - u_{\infty}^{(1)}) \exp(-\frac{1}{d}v(x - x_0)), & x > x_0, \\ u_i^{(1)}, & x \leq x_0. \end{cases} \quad (54)$$

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

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

Due to the fraction this is numerically instable as $h_s(\varphi) \rightarrow 0$. Defining $\beta = 6Gh_s(\varphi)$ we set $u^{(1)} = c$ if $\beta \leq 10^{-4}$, 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 decay $c^{(l)}$ and $u^{(1)}$ exponentially to this value by setting $u_{\infty}^{(1)} = 0.456$. For $u^{(1)} = u_i^{(1)} = 0.6$ we obtain in equilibrium $u_{eq}^{(0)} \approx -1.648$ and an equilibrium temperature of $T_{eq} \approx 0.6067$. To make the front move we initialized with an undercooling of $T = 0.55$, i.e. $u^{(0)} \equiv \frac{-1}{0.55}$. Formula (48) yields an estimation of the initial velocity of the front: with $\omega_0 = 0.08$ we have $v \approx \frac{\lambda}{\omega_0}(u_{eq}^{(0)} - u^{(0)}) \approx 0.2$. The initial position of the front $x_0 = 8.0$ was appropriately chosen such that there were not much interactions with the external boundary. Initial values for φ again were defined as in (51). By (40), 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 (54) does not describe the profile of a travelling wave solution, but a nearly travelling wave solution can be observed (see Figure 2). We computed the following transition points of φ at $t = 20.0$:

ε	without correction				with correction			
	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

There are nearly no ε -dependend differences in the interface position when the correction term is taken into account. Deviations of several grid points are possible without correction. Hence, a superior approximation is obtained when taking the correction term into account.

4.4. Binary non-isothermal case. Now we will demonstrate that a better convergence behaviour can also be observed if several conserved quantities are considered. We postulate the following reduced grand canonical potential:

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

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 $[c(u)]_s^l = G$ and $[e(u)]_s^l = \lambda$ are independent of u we obtain a constant correction term (h and \tilde{h} are chosen as above) $\omega_1 = \left(\frac{\lambda^2}{K} + \frac{G^2}{d}\right) \frac{H + \tilde{H} - 2J}{2I} \approx 0.86555555$. Usually temperature diffusivity is much faster than mass diffusivity so that the influence of the concentration part on the correction term is much larger.

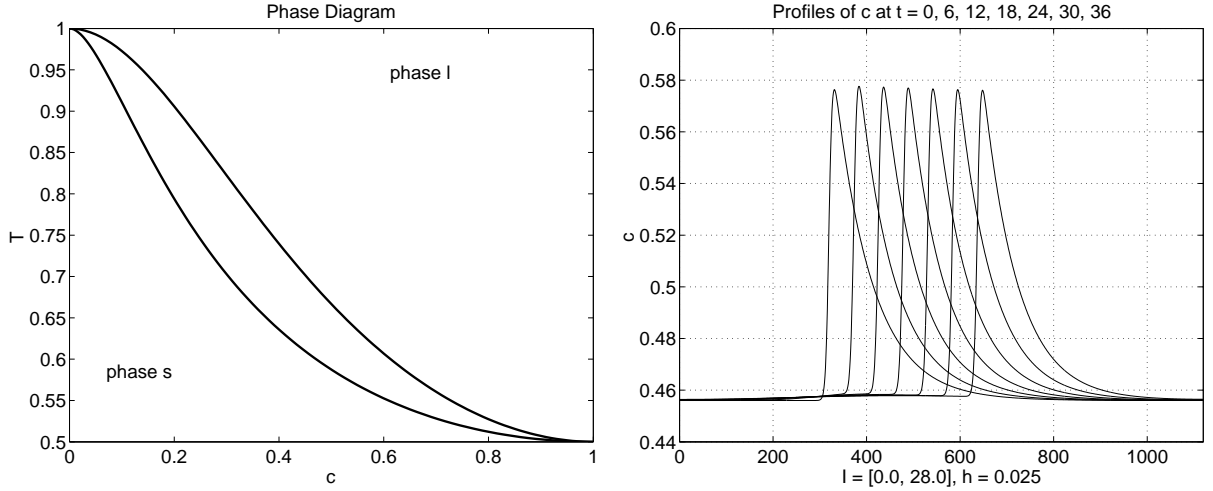


FIGURE 2. On the left: phase diagram for a binary mixture computed from (53). On the right: profiles of the solution c for the binary system in Sec. 4.3 during the evolution, $\varepsilon = 0.4$; the figure indicates already that there is only a negligible influence of the boundary conditions on the evolution as gradients of c don't vanish only in the transition region. But simulations on domains with different lengths were performed to verify this conjecture.

In equilibrium (see Appendix A for the conditions) we have the linear relation $u_{eq}^{(1)} - u_e = u_{eq}^{(0)} - u_m$. For $u^{(1)} = u_e = 0.6$ and $u^{(0)} = u_m = -1.0$ ($\leadsto T^{(0)} = T_m = 1.0$) 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 again were defined as in (51) 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 $u^{(0)}$ in $x = 1.4$, but on the other boundary point we imposed the Dirichlet boundary condition $u^{(0)}(x = 0.0) = -1.25$ which corresponds to an undercooling of $\frac{1}{5}$ 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:

	$\Delta x \backslash \varepsilon$	$0.4/\sqrt{2}$	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 $\varepsilon = \frac{0.2}{\sqrt{2}}$ 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 Appendix E) we obtained values of $k \approx 1.78$ with correction term and $k \approx 0.57$ without correction term when the runs for $\varepsilon \in \{\frac{0.4}{\sqrt{2}}, \frac{0.2}{\sqrt{2}}, \frac{0.1}{\sqrt{2}}\}$ are compared. Similar results were obtained at the 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 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 behaviour 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.

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APPENDIX A. REMARKS ON THERMODYNAMICS

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

$$f : \mathbb{R} \times \Sigma^N \rightarrow \mathbb{R}, \quad (T, c) \mapsto f(T, c).$$

Here, T is the temperature and $c = (c^{(1)}, \dots, c^{(N)})$ 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 c . Its derivative operates on the tangential space of the domain, i.e. on $\mathbb{R} \times T\Sigma^N \subset \mathbb{R}^{N+1}$, and its gradient can naturally be interpreted as a vector in $\mathbb{R} \times T\Sigma^N$, hence

$$Df : \mathbb{R} \times \Sigma^N \rightarrow \mathbb{R} \times T\Sigma^N, \quad (T, c) \mapsto Df(T, c) = (\partial_T f, \partial_c f) =: (-s, \mu).$$

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

$$df = -sdT + \mu \cdot dc.$$

The internal energy e is the Legendre transformed 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 . It holds

$$de = df + sdT + Tds = Tds + \mu \cdot dc$$

leading to

$$ds = \frac{1}{T}de - \frac{\mu}{T}dc =: -u^{(0)}de - \tilde{u}dc.$$

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

$$-s : \mathbb{R} \times \Sigma^N \rightarrow \mathbb{R}, \quad \bar{c} \mapsto -s(\bar{c})$$

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

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

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

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

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

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

This motivates to identify $d\psi(u)$ with $\bar{c}(u)$ and to write

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

In particular, we see

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

One can think of f , s and ψ to be 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 will enter the equations in Sections 2, 3 and 4.

APPENDIX B. TRANSFORMATION OF DERIVATIVES NEAR THE INTERFACE

Let $\varepsilon_0 > 0$. Near the interface $\Gamma(t; 0)$ we consider the diffeomorphisms

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

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 such that 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

$$\begin{aligned}
D(F_\varepsilon^{-1})(t, x) &= (DF_\varepsilon)^{-1}(t, x) = \begin{pmatrix} \partial_t t(t, x) & \nabla_x t(t, x) \\ \partial_t s(t, x) & \nabla_x s(t, x) \\ \partial_t z(t, x) & \nabla_x z(t, x) \end{pmatrix} \\
&= \begin{pmatrix} 1 & (0, 0) \\ -\frac{1}{1-\kappa(\varepsilon z+d_\varepsilon)}(v_\tau + (\varepsilon z + d_\varepsilon)\tau \cdot \partial_t \nu) & \frac{1}{1-\kappa(\varepsilon z+d_\varepsilon)}\tau^\perp \\ \frac{1}{\varepsilon} \left(-\partial_t d_\varepsilon + \frac{\partial_s d_\varepsilon(\varepsilon z+d_\varepsilon)}{1-\kappa(\varepsilon z+d_\varepsilon)}\tau \cdot \partial_t \nu + \frac{\partial_s d_\varepsilon}{1-\kappa(\varepsilon z+d_\varepsilon)}v_\tau - v \right) & \frac{1}{\varepsilon}\nu^T - \frac{\partial_s d_\varepsilon}{\varepsilon(1-\kappa(\varepsilon z+d_\varepsilon))}\tau^\perp \end{pmatrix}
\end{aligned}$$

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

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

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

where $\partial^\circ = \partial_t - v_\tau \partial_s$ is the (intrinsic) normal-time-derivative (see e.g. [14]).

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.

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

By (9) 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 $d_\varepsilon = d(t, s; \varepsilon) = \varepsilon d_1(t, s) + \varepsilon^2 d_2(t, s) + \dots$. We want to identify the functions v_i , κ_i in terms of the functions $d_i(t, s)$, $i = 1, 2, \dots$, $v := v(t, s; 0)$ and $\kappa := \kappa(t, s; 0)$.

The unit tangential 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

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

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

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

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

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

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

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

APPENDIX D. DERIVATION OF MATCHING CONDITIONS

In this appendix we will derive the conditions (16)-(19) for u . Analogous results can be obtained for φ .

By (12) and (13) the functions $\hat{u}_k(t, s, r) = u_k(t, x)$ 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 smoothly and uniformly be extended onto $\Gamma(t; 0)$ from both sides as $r \searrow 0$ and $r \nearrow 0$ respectively. An expansion in Taylor series in $r = 0$ yields

$$\hat{u}_k(t, s, r) = \hat{u}_k(t, s, 0^+) + \partial_r \hat{u}_k(t, s, 0^+) r + \frac{1}{2} \partial_{rr} \hat{u}_k(t, s, 0^+) r^2 + O(r^3), \quad r \in (0, \delta_0], \quad (55)$$

$$\hat{u}_k(t, s, r) = \hat{u}_k(t, s, 0^-) + \partial_r \hat{u}_k(t, s, 0^-) r + \frac{1}{2} \partial_{rr} \hat{u}_k(t, s, 0^-) r^2 + O(r^3), \quad r \in [-\delta_0, 0). \quad (56)$$

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

$$\hat{u}(t, s, r; \varepsilon) = \sum_{k=0}^N \varepsilon^k \hat{u}_k(t, s, r) + O(\varepsilon^{N+1}) \quad (57)$$

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

We assume that the functions $U_k(t, s, z)$ in (14) 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.

$$U_k(t, s, z) \approx U_{k,0}^\pm(t, s) + U_{k,1}^\pm(t, s) z + U_{k,2}^\pm(t, s) z^2 + \cdots + U_{k,n_k}^\pm(t, s) z^{n_k}, \quad z \rightarrow \pm\infty \quad (58)$$

with $n_k \in \mathbb{N}$ for all k . Besides we assume that the expansion (14) 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 $\zeta \in (\frac{\delta_0}{2}, \delta_0)$ and $\varepsilon \in (0, \varepsilon_0]$ and consider the intermediate variable $\zeta\varepsilon^\alpha$. The expansion (57) is valid with $r = \zeta\varepsilon^\alpha$ for ε small enough. We can use (55) and get (dropping the uniform dependence on (t, s))

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

Using (56) the same can be written for $-\zeta \in (\frac{\delta_0}{2}, \delta_0)$ with 0^+ replaced by 0^- .

Now, for ζ positive again (14) is valid for the choice $z = \zeta\varepsilon^{\alpha-1}$. Using (58) and again dropping the dependence on (t, s) we obtain

$$\begin{aligned}U(\zeta\varepsilon^{\alpha-1}; \varepsilon) &= \varepsilon^0 U_{0,0}^+ + \varepsilon^{\alpha-1} U_{0,1}^+ \zeta + \dots + \varepsilon^{n_0(\alpha-1)} U_{0,n_0}^+ \zeta^{n_0} \\ &\quad + \varepsilon^1 U_{1,0}^+ + \varepsilon^{1+\alpha-1} U_{1,1}^+ \zeta + \dots + \varepsilon^{1+n_1(\alpha-1)} U_{1,n_1}^+ \zeta^{n_1} \\ &\quad + \varepsilon^2 U_{2,0}^+ + \varepsilon^{2+\alpha-1} U_{2,1}^+ \zeta + \dots + \varepsilon^{2+n_2(\alpha-1)} U_{2,n_2}^+ \zeta^{n_2} + \dots\end{aligned}$$

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

The expansions of U and \hat{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 U and \hat{u} yields the following relations between the coefficients $U_{k,n}^+$ on the one hand and the derivatives $\partial_r^j u(0^+)$ on the other hand for $k \leq 2$:

$$\begin{aligned}U_{0,0}^+ &= \hat{u}_0(0^+), & U_{0,i}^+ &= 0, \quad 1 \leq i \leq n_0, \\ U_{1,0}^+ &= \hat{u}_1(0^+), \quad U_{1,1}^+ = \partial_r \hat{u}_0(0^+), & U_{1,i}^+ &= 0, \quad 2 \leq i \leq n_1, \\ U_{2,0}^+ &= \hat{u}_2(0^+), \quad U_{2,1}^+ = \partial_r \hat{u}_1(0^+), \quad U_{2,2}^+ = \frac{1}{2} \partial_{rr} \hat{u}_0(0^+), & U_{2,i}^+ &= 0, \quad 3 \leq i \leq n_2.\end{aligned}$$

Obviously from the definition of r , a derivative of some function with respect to r corresponds to the derivative with respect to x into the direction $\nu = \nu(t, s(t, x); 0)$. Hence, we can replace $\partial_r \hat{u}_k$ by $\nabla u_k \cdot \nu$. As ν is independent of r we can also replace $\partial_{rr} \hat{u}_k$ by $\nu \cdot D^2 u_k \nu$. We use (58) again and obtain the following matching conditions (compare (16)-(19)): As $z \rightarrow \pm\infty$

$$\begin{aligned}U_0(z) &\approx u_0(0^\pm), \\ U_1(z) &\approx u_1(0^\pm) + (\nabla u_0(0^\pm) \cdot \nu)z, \\ \partial_z U_1(z) &\approx \nabla u_0(0^\pm) \cdot \nu, \\ \partial_z U_2(z) &\approx \nabla u_1(0^\pm) \cdot \nu + (\nu \cdot D^2 u_0(0^\pm) \nu)z.\end{aligned}$$

APPENDIX E. ORDER OF CONVERGENCE

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

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

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 terms

$$\frac{Err(\varepsilon) - Err(\frac{\varepsilon}{m})}{Err(\frac{\varepsilon}{m}) - Err(\frac{\varepsilon}{m^2})} = (\frac{1}{m})^{-k} = m^k$$

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

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