

Comparison of a rapidly converging phase field model for interfaces in solids with the Allen-Cahn model

Hans-Dieter Alber[†]

Fachbereich Mathematik, Technische Universität Darmstadt
Schlossgartenstr. 7, 64289 Darmstadt, Germany

Peicheng Zhu^{1,2‡}

¹Basque Center for Applied Mathematics (BCAM)

Building 500, Bizkaia Technology Park, 48160 Derio, Spain

²IKERBASQUE, Basque Foundation for Science, 48011 Bilbao, Spain

Abstract

We compare two phase field models for interfaces in elastic solids carrying low surface energy. One model has hybrid properties of a Hamilton-Jacobi and a parabolic equation, the other is the Allen-Cahn model. For vanishing width of the interface we construct asymptotic solutions of second order for the hybrid model and of first order for the Allen-Cahn model. They show that to follow the interface precisely the width of the interface can be chosen much larger for the hybrid model than for the Allen-Cahn model and that the hybrid model can describe interfaces with nonlinear kinetic relation. This explains why numerical simulations based on the hybrid model are considerably more effective. These simulations are discussed in the last section.

1 Introduction and statement of results

In this article we consider two different phase field models for the evolution of a phase interface in an elastically deformable solid. We compare the properties of these models by constructing asymptotic solutions of these models with respect to a small parameter ν , which determines the width of the diffusive phase interface. We call the first model hybrid model; the explanation for this name is given later in this introduction. The second model is the Allen-Cahn model. In numerical experiments we observed that simulations of the movement of phase interfaces carrying low surface energy based on the hybrid model run faster than corresponding simulations based on the Allen-Cahn model by a large factor. At the end of this article we present the results of these experiments in two space dimensions, where this factor has the value of 50 or larger. Our theoretical investigations explain this observation.

It is a fundamental result of the theory of phase field models that the propagation speed of the diffusive interface is up to an error term equal to the propagation speed of an interface from a sharp interface model and that this sharp interface model can be determined by constructing an asymptotic solution to the phase field model. Since this

[†]alber@mathematik.tu-darmstadt.de

[‡]zhu@bcamath.org

error term tends to zero for $\nu \rightarrow 0$, the sharp interface model is the limit model for the phase field model. It turns out that the difference of the two phase field models can be understood if the two limit models are known and if in addition the error term for the hybrid model is known with second order accuracy. This term can be determined with high accuracy by constructing asymptotic solutions of higher order. For the hybrid model we therefore construct such an asymptotic solutions of second order; for the Allen-Cahn model, on the other hand, we only need to construct an asymptotic solution of first order.

To formulate both models let Ω be an open subset in \mathbb{R}^3 . It represents the material points of a solid body. The material structure of this body can be in two different phase states. The phase state of the material is characterized by the values of a smooth order parameter $S(t, x) \in \mathbb{R}$. The material is in phase 1 or 2 at the material point $x \in \Omega$ at time t if the value $S(t, x)$ is close to 0 or 1. The other unknowns are the displacement $u(t, x) \in \mathbb{R}^3$ of the point x at time t and the Cauchy stress tensor $T(t, x) \in \mathcal{S}^3$, where \mathcal{S}^3 denotes the set of symmetric 3×3 -matrices. In the domain $[0, \infty) \times \Omega$ these unknowns must satisfy the equations of the hybrid model

$$-\operatorname{div}_x T = \mathbf{b}, \quad (1.1)$$

$$T = D(\varepsilon(\nabla_x u) - \bar{\varepsilon}S), \quad (1.2)$$

$$\partial_t S = -f(\psi_S(\varepsilon(\nabla_x u), S) - \nu \Delta_x S) |\nabla_x S|, \quad (1.3)$$

or, alternatively, of the Allen-Cahn model

$$-\operatorname{div}_x T = \mathbf{b}, \quad (1.4)$$

$$T = D(\varepsilon(\nabla_x u) - \bar{\varepsilon}S), \quad (1.5)$$

$$\partial_t S = -f(\psi_S(\varepsilon(\nabla_x u), S) - \mu \Delta_x S). \quad (1.6)$$

(1.1), (1.2) or (1.4), (1.5), respectively, are the equations of linear elasticity, which are coupled to the evolution equations (1.3) or (1.6) for the order parameter. In these equations $\nabla_x u$ denotes the 3×3 -matrix of first order derivatives of u , the deformation gradient, and

$$\varepsilon(\nabla_x u) = \frac{1}{2}(\nabla_x u + (\nabla_x u)^T) \in \mathcal{S}^3$$

is the strain tensor, where $(\nabla_x u)^T$ denotes the transposed matrix. $\bar{\varepsilon} \in \mathcal{S}^3$ is a given matrix, the transformation strain. The elasticity tensor $D : \mathcal{S}^3 \rightarrow \mathcal{S}^3$ is a linear, symmetric, positive definite mapping, $\nu > 0$ and $\mu > 0$ are small parameters, and $\mathbf{b} : [0, \infty) \times \Omega \rightarrow \mathbb{R}^3$ is the given volume force. $\psi_S = \frac{\partial}{\partial S} \psi$ is the partial derivative of the function

$$\psi(\varepsilon, S) = \frac{1}{2}(D(\varepsilon - \bar{\varepsilon}S)) : (\varepsilon - \bar{\varepsilon}S) + \hat{\psi}(S), \quad (1.7)$$

with a double well potential $\hat{\psi} : \mathbb{R} \rightarrow \mathbb{R}$. Here the scalar product of two matrices is denoted by $A : B = \sum a_{ij} b_{ij}$. We thus have

$$\psi_S(\varepsilon, S) = -T : \bar{\varepsilon} + \hat{\psi}'(S). \quad (1.8)$$

ψ is a part of the free energy. The total free energies corresponding to the model (1.1) – (1.3) and to the model (1.4) – (1.6) are given by the sums

$$\psi(\varepsilon, S) + \frac{\nu}{2} |\nabla_x S|^2, \quad \psi(\varepsilon, S) + \frac{\mu}{2} |\nabla_x S|^2, \quad (1.9)$$

respectively. The function $f : \mathbb{R} \rightarrow \mathbb{R}$ in (1.3) and (1.6) is a linear or nonlinear constitutive function. We require that it satisfies

$$r \cdot f(r) \geq 0 \tag{1.10}$$

for all $r \in \mathbb{R}$. This condition guaranties that for the free energies (1.9) the Clausius-Duhem inequality is satisfied by the models, cf. [3].

The systems (1.1) – (1.3) and (1.4) – (1.6) of partial differential equations must be supplemented by initial and boundary conditions. To see what conditions are required note that if the function $x \mapsto S(t, x)$ is known for a fixed time t , then $x \mapsto (u(t, x), T(t, x))$ must be determined by solving the elliptic systems (1.1), (1.2) or (1.4), (1.5). To this end we need boundary conditions for (u, T) . For example, we can prescribe standard Dirichlet or Neumann boundary conditions for these elliptic systems. To solve the evolution equations (1.3) or (1.6) we need initial and boundary conditions for S . Since we only consider situations where the material is in phase 1 at the boundary, we always choose the homogeneous boundary condition $S(t, x) = 0$, $x \in \partial\Omega$.

The evolution equation (1.3) differs from the corresponding equation (1.6) only by the gradient term $|\nabla_x S|$. If one sets $\nu = 0$, then (1.3) becomes a Hamilton-Jacobi transport equation. The equations (1.1), (1.2) coupled to this Hamilton-Jacobi equation can in principle be used as a phase field model. Yet, if one starts with smooth initial data $S(0, x)$, then for growing t the transition of S from 0 to 1 becomes steeper until after a finite time the gradient becomes infinite. This behavior can be read off from the classical solution formulas for partial differential equations of first order. Since in a phase field model one wants that the transition of the order parameter is smooth for all times, the parameter ν must be chosen positive. In this case (1.3) becomes a degenerate parabolic evolution equation and the gradient $|\nabla_x S|$ stays bounded for all times. Still, also for positive ν the equation (1.3) has some properties which one would expect from a hyperbolic Hamilton-Jacobi equation. This is why we call (1.1) – (1.3) a hybrid model.

The Hamilton-Jacobi equation was obtained in [1] by a mathematical procedure starting from a sharp interface problem, which will be shown in Section 2 to be the limit problem of the model (1.1) – (1.3) for $\nu \rightarrow 0$. In this procedure the notion of a classical solution of the sharp interface problem was generalized by defining measure valued solutions. This wider class of solutions in turn allowed solutions, which are smooth in the whole domain, and for which it could be shown that they satisfy the system (1.1) – (1.3) with $\nu = 0$. In [2, 3] the hybrid model was obtained by adding the term $\nu \Delta_x S$ to the Hamilton-Jacobi equation to avoid that the gradient of S can become infinite.

The questions arise, in what way the solutions of the models (1.1) – (1.3) and (1.4) – (1.6) differ and which one of the two models should be preferred to simulate a given physical situation. As already mentioned, to answer these questions we construct in the theoretical part of this paper asymptotic solutions both of first and second order to the hybrid model for $\nu \rightarrow 0$ and an asymptotic solution of first order to the rescaled Allen-Cahn model for $\mu \rightarrow 0$. The construction of the asymptotic solutions for the hybrid model is contained in Section 2, the proofs of the theorems and lemmas stated there are given in Section 3. The asymptotic solution for the Allen-Cahn model is constructed in Section 4, the proofs are contained in Section 5. Numerical experiments are discussed in Section 6.

In the remainder of this introduction we explain the motivation of our investigations. In particular, we discuss why it is not sufficient to know the corresponding limit models

for the two phase field models and why we need an asymptotic solution of second order for the hybrid model to explain the higher numerical efficiency of this model when the interface carries low surface energy. To this end we need to state next the sharp interface limit models, which are determined in Sections 3 and 5.

Let $0 \leq t_1 < t_2 < \infty$ be given fixed times and let Γ be a sufficiently smooth three-dimensional manifold embedded in $Q = [t_1, t_2] \times \Omega \subseteq \mathbb{R}^4$ such that for all $t \in [t_1, t_2]$ the sharp interface between the two material phases of Ω is given by the two-dimensional manifold

$$\Gamma(t) = \{x \in \Omega \mid (t, x) \in \Gamma\} \quad (1.11)$$

embedded in Ω . The two different phases are characterized by the values of the order parameter \hat{S} , which in the sharp interface models is piecewise constant and only takes the values 0 or 1 with a jump along Γ . For $x \in \Gamma(t)$ let $n(t, x) \in \mathbb{R}^3$ be the unit normal vector pointing into the region where $\hat{S} = 1$. This defines a vector field

$$n : \Gamma \rightarrow \mathbb{R}^3. \quad (1.12)$$

If V is a neighborhood of $\Gamma(t)$ and if w is a function defined on $V \setminus \Gamma(t)$, which has limit values on both sides of $\Gamma(t)$, we set for $\eta \in \Gamma(t)$

$$w^{(\pm)}(\eta) = \lim_{\substack{\xi \rightarrow 0 \\ \xi > 0}} w(\eta \pm \xi n(t, \eta)), \quad [w](\eta) = w^{(+)}(\eta) - w^{(-)}(\eta). \quad (1.13)$$

In the sharp interface models we denote the unknown displacement by $\hat{u}(t, x) \in \mathbb{R}^3$ and the unknown Cauchy stress tensor by $\hat{T}(t, x) \in \mathcal{S}^3$. The limit model to the hybrid model (1.1) – (1.3) consists of the equations

$$-\operatorname{div}_x \hat{T} = \mathbf{b}, \quad (1.14)$$

$$\hat{T} = D(\varepsilon(\nabla_x \hat{u}) - \bar{\varepsilon} \hat{S}), \quad (1.15)$$

$$s = f(n \cdot [\hat{C}]n), \quad (1.16)$$

$$[\hat{u}] = 0, \quad (1.17)$$

$$[\hat{T}]n = 0. \quad (1.18)$$

(1.14) and (1.15) must hold on $Q \setminus \Gamma$ whereas (1.16) – (1.18) are posed on Γ . Here

$$\hat{C}(\nabla_x \hat{u}, \hat{S}) = \psi(\varepsilon(\nabla_x \hat{u}), \hat{S})I - (\nabla_x \hat{u})^T \hat{T} \quad (1.19)$$

denotes the Eshelby tensor, where I is the 3×3 -unit matrix and where $(\nabla_x \hat{u})^T \hat{T}$ denotes the matrix product. ψ is defined in (1.7), and D , $\bar{\varepsilon}$, \mathbf{b} are defined as in (1.1) – (1.3). The equation (1.16), the kinetic relation, determines the normal speed s of the interface $\Gamma(t)$. The normal speed is measured positive in direction of n . We note that the constitutive function f , which can be nonlinear, is the same in the kinetic relation (1.16) of the limit model and in the evolution equation (1.3) of the phase field model. Note also that the system (1.14) – (1.18) is the limit model of the phase field model (1.1) – (1.3) without rescaling.

It is well known on the other hand, that in limit model to the Allen-Cahn model (1.4) – (1.6) the sharp interface has positive propagation speed only when the model equations

are suitably rescaled. The rescaled model equations are

$$-\operatorname{div}_x T = \mathbf{b}, \quad (1.20)$$

$$T = D(\varepsilon(\nabla_x u) - \bar{\varepsilon}S), \quad (1.21)$$

$$\partial_t S = -\frac{1}{(\mu\lambda)^{1/2}}f(W_S(\varepsilon(\nabla_x u), S) + \frac{1}{\mu^{1/2}}\hat{\psi}'(S) - \mu^{1/2}\lambda \Delta_x S), \quad (1.22)$$

where

$$W(\varepsilon, S) = \frac{1}{2}(D(\varepsilon - \bar{\varepsilon}S)) : (\varepsilon - \bar{\varepsilon}S) \quad (1.23)$$

is the elastic energy, where

$$W_S(\varepsilon, S) = \partial_S W(\varepsilon, S) = -T : \bar{\varepsilon}, \quad (1.24)$$

and where $\lambda, \mu > 0$ are constants. We remark that differently from (1.9), the free energy corresponding to this rescaled model is equal to the sum

$$W(\varepsilon, S) + \frac{1}{\mu^{1/2}}\hat{\psi}(S) + \frac{\mu^{1/2}\lambda}{2}|\nabla_x S|^2.$$

In Section 4 we show that the constitutive function in the kinetic relation of the sharp interface limit model can be obtained by application of a relatively complicated integral operator to the function f in (1.22). This integral operator simplifies when f is linear. For our purposes here it suffices to consider this simpler case. We thus assume that the function f in (1.22) is of the form

$$f(r) = cr, \quad (1.25)$$

with a positive constant $c > 0$. It is shown in [29] that in this case the sharp interface limit model to (1.20) – (1.22) consists of the equations (1.14), (1.15), (1.17), (1.18) and of the kinetic relation

$$s = \frac{c}{c_1}(n \cdot [\hat{C}]n + \lambda^{1/2}c_1\kappa_\Gamma), \quad (1.26)$$

which replaces (1.16). Here the constant c_1 is given by

$$c_1 = \int_0^1 \sqrt{2\hat{\psi}(\zeta)} d\zeta > 0. \quad (1.27)$$

and $\kappa_\Gamma(t, x)$ denotes twice the mean curvature of the surface $\Gamma(t)$ at the point $x \in \Gamma(t)$ with the convention, that the sign of $\kappa_\Gamma(t, x)$ is positive if the center of curvature lies in the direction of $n(t, x)$.

Thus, if we choose f of the form (1.25) also in (1.3), then the limit models of the phase field models differ essentially only in the curvature term $c\lambda^{1/2}\kappa_\Gamma$, which appears in (1.26) but is not present in (1.16). Since λ in (1.22) must be chosen positive, it follows that the coefficient in front of the curvature is positive and that this curvature term is always part of the driving force in the kinetic relation (1.26).

Therefore in the limit model for the Allen-Cahn phase field model the contribution of the curvature to the driving force of the interface cannot be avoided, whereas the kinetic relation to the limit model for the hybrid phase field model does not contain a curvature term.

This suggests that it is advantageous to use the model (1.1) – (1.3) when the interface carries low or no surface energy, since in this case the curvature is not part of the driving force. This is the case for example in martensitic phase transitions. Yet, it is not immediately clear what the advantage actually is. Namely, the true propagation speed of the diffusive interface described by an exact solution of the phase field model (1.1) – (1.3) differs from the propagation speed of the sharp interface determined by the model (1.14) – (1.18) by an error $E^{(h)}(\nu)$, which is the sum of two terms $E_1^{(h)}(\nu)$ and $E_2^{(h)}(\nu)$. This can be seen from the asymptotic solution of second order constructed in Section 2. The term $E_1^{(h)}(\nu)$ is simply the difference of the propagation speeds of the diffusive interfaces modelled by the exact solution and the second order asymptotic solution of (1.1) – (1.3), the second term originates from an additional curvature term of the order $O(\nu^{1/2})$, by which the driving force of the diffusive interface modelled by the second order asymptotic solution differs from the driving force $n \cdot [\hat{C}]n$ in (1.16). This additional term generates the second error term $E_2^{(h)}(\nu) = O(\nu^{1/2})$, which is curvature dependent. Since the error, up to which the second order asymptotic solution satisfies (1.1) – (1.3), is of order $O(\nu)$, as will be seen, one expects that the error term $E_1^{(h)}(\nu)$ tends to zero for $\nu \rightarrow 0$.

Thus, fixing $\nu > 0$ in the evolution equation (1.3) determines the amount, by which the curvature contributes to the driving force of the diffusive interface modelled by (1.1) – (1.3) and determines at the same time the accuracy, with which the propagation speed of this diffusive interface approximates the propagation speed of the sharp interface modelled by (1.14) – (1.18).

On the other hand, we can make the coefficient multiplying the mean curvature in the kinetic relation (1.26) small by choosing the parameter λ in the rescaled Allen-Cahn equation (1.22) small. Thus, to given $\nu > 0$ in (1.3) choose $\lambda > 0$ in (1.22) small enough such that the term $c\lambda^{1/2}\kappa_\Gamma$ in the kinetic relation (1.26) has the same size as the curvature term of order $O(\nu^{1/2})$ contributing to the driving force of the diffusive interface modelled by (1.1) – (1.3). This amounts to choosing $\lambda \approx \nu$. Subsequently choose $\mu > 0$ in (1.22) small enough such that the difference $E^{(AC)}(\mu)$ of the propagation speeds of the diffusive interface modelled by (1.20) – (1.22) and the sharp interface modelled by (1.14), (1.15), (1.26), (1.17), (1.18) is of the same size as the error term $E^{(h)}(\nu)$. With this choice we have

$$E^{(AC)}(\mu) \approx E^{(h)}(\nu) = E_1^{(h)}(\nu) + E_2^{(h)}(\nu) \rightarrow 0, \quad \text{for } \nu \rightarrow 0,$$

so also μ must tend to zero, hence $\mu = o(1)$ for $\nu \rightarrow 0$.

With the parameters chosen in this way the diffusive interfaces of both models (1.1) – (1.3) and (1.20) – (1.22) approximate the evolution of the sharp interface determined by the model (1.14) – (1.18) with the same accuracy, whence we can model the evolution of a martensitic phase interface with both phase field models with the same precision. However, the asymptotic solutions show that the width of the diffusive interface in the hybrid model (1.1) – (1.3) is proportional to $\nu^{1/2}$, whereas the width of the interface in the Allen-Cahn model (1.20) – (1.22) is proportional to $(\mu\lambda)^{1/2}$. Thus, by our choice of the parameters λ, μ , for $\nu \rightarrow 0$ the diffusive interface has the width of the order $O(\nu^{1/2})$ in the hybrid model and of the order $O((o(1)\nu)^{1/2})$ in the Allen-Cahn model.

The width of the interface in the Allen-Cahn model is therefore smaller by a factor of the order $o(1)^{1/2}$ than in the hybrid model. In a numerical simulation the discretization must be chosen fine enough such that the transition of the order parameter from 0 to 1

in the diffusive interface can be resolved. Consequently, if we base the simulation on the Allen-Cahn model we must choose the discretization finer by the factor $o(1)^{1/2}$ than if we base it on the hybrid model. Since in these nonlinear problems also the time steps must be chosen smaller if the space discretization is refined to get a convergent iteration scheme, a simulation based on the hybrid model will therefore be more effective and take only $o(1)^{k/2}$ -times the computing time of a simulation based on the Allen-Cahn model, where $k > 1$ depends on the space dimension and on the numerical scheme, but in three space dimensions will be larger than 4.

The actual gain in the efficiency depends on the form of the $o(1)$ term and on the value of ν . If the usual asymptotics is valid for the error, by which the asymptotic solutions approximate the exact solutions of the phase field models, we have that

$$E^{(AC)}(\mu) = O(\mu^{1/2}) \quad \text{and} \quad E^{(h)}(\nu) = E_1^{(h)}(\nu) + E_2^{(h)}(\nu) = O(\nu) + O(\nu^{1/2}) = O(\nu^{1/2}).$$

This implies that we must choose $\mu \approx \nu$, hence $o(1) = O(\nu)$, which means that the computing time for the hybrid model is $o(1)^{k/2} = O(\nu^{k/2})$ times the computing time for the Allen-Cahn model.

When we want to simulate an interface with a negligible surface energy, ν must be chosen small enough that the $O(\nu^{1/2})$ -curvature term contributing to the driving force of the diffusive interface is negligible. The numerical example presented in Section 6 shows that the value of $\nu = 0.00125$ is still considerably too large for this in the situation considered there. Of course, the actual value of ν depends on the parameters of the problem, but we believe that the picture emerging from this example is qualitatively correct. A reduction of the computing time by the factor $\frac{1}{O(\nu^{k/2})}$ is therefore a big gain.

For a phase field model consisting of the Allen-Cahn equation coupled to the heat equation it has been shown in [35, 5, 20, 31] that by choosing the parameters of the model suitably it can be achieved that the difference of the propagation speeds of the diffusive interface and the sharp interface is of the order $O(\mu)$. We do not know whether such a result can also be achieved for the model (1.20) – (1.22). If it is possible, we would have $E^{(AC)}(\mu) = O(\mu)$. By the reasoning above this would lead to the choice $\mu \approx \nu^{1/2}$, hence $o(1) = O(\nu^{1/2})$. In this case the computing time for the hybrid model would be $o(1)^{k/2} = O(\nu^{k/4})$ times the computing time for the Allen-Cahn model, still a big advantage.

For a rigorous proof of the above statements it would be necessary to derive estimates for the difference of the propagation speeds of the diffusive interfaces modelled by the exact solution and by the asymptotic solution. At present, such estimates are not available for the hybrid model. Proving such estimates would also mean to prove existence of solutions. For the hybrid model there is up to now only the existence proof in [2] available, which is valid in one space dimension. To prove existence of solutions in higher space dimensions and to derive such estimates is an open problem. Therefore it only remains to test the validity of the statements by numerical computations. The test computations in two space dimensions presented in Section 6 clearly confirm the statements about the numerical effectivity of the two phase field models.

Besides the higher numerical efficiency of the hybrid model in the simulation of interfaces carrying low surface energy, another advantage is that the constitutive function f in the kinetic relation (1.16) is the same as the function f in the evolution equation (1.3), even if f is nonlinear. As we already mentioned, this is different for the Allen-Cahn

model, where the constitutive function in the kinetic relation of the sharp interface model is obtained by application of a nonlinear integral operator to the function f in (1.22). This integral operator, which will be determined in Section 4, has smoothing properties and is therefore not surjective. Consequently, not every nonlinear kinetic relation in a sharp interface model can be approximated by the Allen-Cahn phase field model.

We end this introduction by a short discussion of the literature. Related to the hybrid model is [33], where a phase field model was introduced and studied numerically, which essentially consists of the equations (1.1), (1.2) and of the Hamilton-Jacobi equation obtained by setting $\nu = 0$ in (1.3), supplemented by a numerical reinitialisation procedure. This reinitialisation procedure is necessary to avoid the steepening or flattening of the slope of the order parameter and the possible blow up of the gradient during the time evolution.

Much more references exist, which are related to the Allen-Cahn model, and we can only mention some of them. In [34, 25, 32] and other articles the convergence of planar solutions of the Allen-Cahn equation to traveling wave solutions for $t \rightarrow \infty$ has been studied. In the non-planar case asymptotic solutions to this equation are constructed in [10, 42] and in other references. The asymptotic solutions indicate that the propagation speed of the diffusive interface from an exact solutions converges to the propagation speed of the sharp interface moving by mean curvature when the width of the diffusive interface tends to zero. That this is indeed the case when the limit problem has a solution with a smooth interface is shown in [40]; that this holds in general without assuming classical solvability of the limit problem is proved in [24] using the level set approach and viscosity solutions.

On another line of development, phase field models for solidification, which consist of the Allen-Cahn equation coupled to the heat equation, were introduced in [27, 9, 21, 11, 13]. Using asymptotic solutions it is shown there that the limit model is the Mullins-Sekerka problem with kinetic undercooling. Under the assumption that there exists a smooth sharp interface solving the Mullins-Sekerka problem it was proved in [12] that the propagation speed of the diffusive interface from an exact solution of this phase field model indeed converges to the propagation speed of the sharp interface; in [43] this result is shown to hold without the assumption on classical solvability of the limit problem.

For these phase field models it has been observed in [35] that if one introduces a μ -dependent kinetic coefficient and chooses the double well potential and coupling terms suitably, then one can achieve that the propagation speed of the diffusive interface converges to the propagation speed of the sharp interface of second order. By the notations used in (1.22) this is convergence of order μ . The proof is based on the construction of an asymptotic solution of second order and needs additional special assumptions. These special assumptions have been removed and the result has been generalized in [5, 31, 20]. A similar idea is also present in [26].

Related to these solidification models is the Cahn-Hilliard equation. By formal asymptotics it was shown in [41] that the propagation speed of the diffusive interface from a solution to this equation tends to the propagation speed of the sharp interface in the Stefan problem when the width of the diffusive interface tends to zero. This was proved rigorously in [6] under the assumption that there is a smooth sharp interface solving the Stefan problem. As in the convergence proofs given in [40, 12], the proof is based on the construction of an asymptotic solution and on a spectral estimate, which is needed to estimate the difference of the exact solution and the asymptotic solution. This spectral

estimate is derived in [17]. Using energy methods and without the assumption on the solvability of the Stefan problem, the convergence result was proved in [44] for the radial symmetric case and in [18] for the general case.

In [29] the model (1.4) – (1.6) is derived based on considerations from thermodynamics. This model describes the time evolution of phases in a solid, whose volume is not conserved. When the volume is conserved one uses instead the model, which consists of the elasticity equations coupled to the Cahn-Hilliard equation. This alternative model is used in [28] to study the evolution of the phases in Nickel-based superalloys. The sharp interface limit problem for this phase field model is determined in [37] by constructing asymptotic solutions, existence of solutions is obtained in [16, 8, 30].

From many other applications of phase field models we only mention here [38], where a model for a binary mixture of fluids is formulated, which consists of the coupled Euler and Cahn-Hilliard equations.

Existence, uniqueness and regularity of classical solutions of the Stefan problem was obtained in [22, 23], global existence of weak solutions of the Stefan problem with Gibbs-Thomson condition was obtained in [39]. Local existence of solutions of the Mullins-Sekerka problem with kinetic undercooling is proved in [19], global existence of solutions follows from the convergence result in [43].

2 Asymptotic solutions for the hybrid model

In this section we construct asymptotic solutions to the model (1.1) – (1.3) for $\nu \rightarrow 0$ of first and second order. That is, we construct two family of functions $\{(u^{(\nu)}, T^{(\nu)}, S^{(\nu)})\}_\nu$, which satisfy the equations (1.1) – (1.3) up to an error, which tends to zero for $\nu \rightarrow 0$. For the family of solutions of second order the L^1 -norm of the residue, with which these equations are satisfied, can be estimated by $C\nu$, for the family of solutions of first order by $C\nu^{1/2}$.

In Section 2.1 we construct the asymptotic family of second order. Our main result for it is the estimate of the residue, which is stated in Theorem 2.7 at the end of this section. The proofs of Theorem 2.7 and of some preparatory results are postponed to Section 3. In Section 2.2 we construct the asymptotic family of first order and state the residue estimate for it in Theorem 2.9. We believe that this first order asymptotic family is of interest, since it can be constructed under weaker assumptions than the second order family. The proof of Theorem 2.9 is however omitted, since it is obtained by a considerable simplification of the proof of Theorem 2.7.

To construct the family of asymptotic solutions we need an inner expansion, but no outer expansion. This is different from the Allen-Cahn model, for which also an outer expansion is needed. Though the proof of the residue estimate is technical and though in this paper we do not use this estimate of the residue to estimate the difference of the exact and asymptotic solutions of the model (1.1) – (1.3), we consider it important to give a complete proof and not only a formal asymptotic expansion, since besides the inner expansion other inequalities are necessary to prove the residue estimate. The proof of these inequalities is by no means obvious. Without such a complete proof one could therefore not be sure that our construction really yields a family of asymptotic solutions.

2.1 Asymptotic solution of second order

2.1.1 Preparatory results

To construct the asymptotic solution $(u^{(\nu)}, T^{(\nu)}, S^{(\nu)})$ we start with some assumptions, definitions and other preparations. In the following we always assume that the parameter ν varies in an interval $(0, \nu_0]$ with a fixed number $\nu_0 > 0$, which we choose sufficiently small, according to our needs. The unit sphere in \mathbb{R}^3 is denoted by

$$\mathbb{S}^2 = \{e \in \mathbb{R}^3 \mid |e| = 1\}.$$

With the notations introduced previously let $(\hat{u}, \hat{T}, \hat{S}, \Gamma)$ be a solution of the sharp interface model

$$-\operatorname{div}_x \hat{T} = \mathbf{b}, \quad (2.1)$$

$$\hat{T} = D(\varepsilon(\nabla_x \hat{u}) - \bar{\varepsilon} \hat{S}), \quad (2.2)$$

$$s = f\left(n \cdot [\hat{C}]n + \nu^{1/2}(\omega_1(n)\kappa_\Gamma + B(n)\nabla_\Gamma n)\right), \quad (2.3)$$

$$[\hat{u}] = 0, \quad (2.4)$$

$$[\hat{T}]n = 0. \quad (2.5)$$

The equations (2.1), (2.2) must hold on the set $Q \setminus \Gamma$ and (2.3) – (2.5) are posed on the three-dimensional manifold Γ . For $(t, x) \in \Gamma$ we denote by $\nabla_\Gamma n(t, x) \in \mathbb{R}^{3 \times 3}$ the surface gradient of the normal vector field n at $x \in \Gamma(t)$. The surface gradient is defined below. $\omega_1(n(t, x)) > 0$ is a positive scalar and $B(n(t, x)) : \mathbb{R}^{3 \times 3} \rightarrow \mathbb{R}$ is a linear mapping. The functions

$$\omega_1 : \mathbb{S}^2 \rightarrow (0, \infty), \quad e \mapsto B(e) : \mathbb{S}^2 \rightarrow L(\mathbb{R}^{3 \times 3}, \mathbb{R})$$

appearing here are defined in Lemma 2.6 after the construction of the asymptotic solution. The differentiability properties of these functions depend on the differentiability of the potential $\hat{\psi}$ in (1.7), and we can achieve that both ω_1 and B are m -times continuously differentiable for any integer m by choosing $\hat{\psi}$ with order of differentiability high enough.

The equations (2.1) – (2.5) differ from (1.14) – (1.18) only by the term $\nu^{1/2}(\omega_1(n)\kappa_\Gamma + B(n)\nabla_\Gamma n)$ in the kinetic relation (2.3). Clearly, because of this term the manifold Γ and the function $(\hat{u}, \hat{T}, \hat{S})$ depend on ν , hence

$$(\hat{u}, \hat{T}, \hat{S}, \Gamma) = (\hat{u}^{(\nu)}, \hat{T}^{(\nu)}, \hat{S}^{(\nu)}, \Gamma^{(\nu)}).$$

We denote by $\gamma^{(\nu)}$ the set of all $(t, x) \in Q \setminus \Gamma^{(\nu)}$ with $\hat{S}^{(\nu)}(t, x) = 0$ and by $\gamma^{(\nu)'}$ the set of all $(t, x) \in Q \setminus \Gamma^{(\nu)}$ with $\hat{S}^{(\nu)}(t, x) = 1$, hence $\gamma^{(\nu)} \cup \gamma^{(\nu)'} = Q \setminus \Gamma^{(\nu)}$.

The family $\{(\hat{u}^{(\nu)}, \hat{T}^{(\nu)}, \hat{S}^{(\nu)}, \Gamma^{(\nu)})\}_{0 < \nu \leq \nu_0}$ is the basis for our construction of the asymptotic solution. We require that this family satisfies the following

Assumption A. For every ν let $\Gamma^{(\nu)}$ be a three-dimensional C^4 -manifold embedded in Q , such that the set $\Gamma^{(\nu)}$ is a compact subset of Q , such that the two-dimensional manifold $\Gamma^{(\nu)}(t)$ does not have a boundary for all $t \in [t_1, t_2]$, and such that all derivatives of a parametrization of $\Gamma^{(\nu)}$ up to order four are bounded uniformly with respect to $\nu \in (0, \nu_0]$. We assume that the family $\{(\hat{u}^{(\nu)}, \hat{T}^{(\nu)})\}_{0 < \nu \leq \nu_0}$ belongs to the space $C^5(\gamma^{(\nu)} \cup \gamma^{(\nu)'}) \times C^4(\gamma^{(\nu)} \cup \gamma^{(\nu)'})$ and that this family is bounded in the norm of this space. Moreover, we assume that all derivatives of $\hat{u}^{(\nu)}$ up to order five and all derivatives

of $\hat{T}^{(\nu)}$ up to order four have continuous extensions from $\gamma^{(\nu)}$ to $\gamma^{(\nu)} \cup \Gamma^{(\nu)}$ and from $\gamma^{(\nu)'}$ to $\gamma^{(\nu)'} \cup \Gamma^{(\nu)}$. Furthermore, we assume that the right hand side $\mathbf{b} : Q \rightarrow \mathbb{R}^3$ of (2.1) is continuous.

From now on we always drop the index ν in $(\hat{u}^{(\nu)}, \hat{T}^{(\nu)}, \hat{S}^{(\nu)}, \Gamma^{(\nu)})$ and in $\gamma^{(\nu)}, \gamma^{(\nu)'}$ to simplify the notation. Thus, in this section $(\hat{u}, \hat{T}, \hat{S}, \Gamma)$ always denotes the solution of (2.1) – (2.5) to the value of the parameter ν just considered and we write $\gamma = \{(t, x) \in Q \mid \hat{S}(t, x) = 0\}$, $\gamma' = \{(t, x) \in Q \mid \hat{S}(t, x) = 1\}$.

By these assumptions we can choose $\delta > 0$ sufficiently small such that the set

$$\mathcal{U} = \{(t, \eta + n(t, \eta)\xi) \mid (t, \eta) \in \Gamma, |\xi| < \delta\} \subset [t_1, t_2] \times \mathbb{R}^3$$

is contained in Q . The set $\mathcal{U}(t) = \{x \in \Omega \mid (t, x) \in \mathcal{U}\} \subset \Omega$ is a neighborhood of $\Gamma(t)$ for every $t \in [t_1, t_2]$, with $\Gamma(t)$ defined in (1.11). By choosing δ smaller if necessary, we can guarantee that

$$(t, \eta, \xi) \mapsto (t, x(t, \eta, \xi)) = (t, \eta + n(t, \eta)\xi) : \Gamma \times (-\delta, \delta) \rightarrow \mathcal{U} \quad (2.6)$$

is an invertible C^3 -mapping, where n denotes the normal vector field defined in (1.12). This implies that for ξ satisfying $-\delta < \xi < \delta$

$$\Gamma_\xi = \{(t, \eta + n(t, \eta)\xi) \mid (t, \eta) \in \Gamma\}$$

is a C^3 -parallel manifold of Γ embedded in \mathcal{U} , and

$$\Gamma_\xi(t) = \{x \in \Omega \mid (t, x) \in \Gamma_\xi\}$$

is a C^3 -parallel manifold of $\Gamma(t)$ embedded in $\mathcal{U}(t)$. Though (t, η) is a point on the manifold Γ , we say that the mapping (2.6) defines new coordinates (t, η, ξ) in \mathcal{U} .

Let $\tau_1, \tau_2 \in \mathbb{R}^3$ be two orthogonal unit vectors tangent to $\Gamma_\xi(t)$ at $x \in \Gamma_\xi(t)$. For functions $w : \Gamma_\xi(t) \rightarrow \mathbb{R}$, $W : \Gamma_\xi(t) \rightarrow \mathbb{R}^3$ and $\hat{W} : \Gamma_\xi(t) \rightarrow \mathbb{R}^{3 \times 3}$ we define the surface gradients and the surface divergences

$$\nabla_{\Gamma_\xi} w = (\partial_{\tau_1} w)\tau_1 + (\partial_{\tau_2} w)\tau_2, \quad (2.7)$$

$$\nabla_{\Gamma_\xi} W = (\partial_{\tau_1} W) \otimes \tau_1 + (\partial_{\tau_2} W) \otimes \tau_2, \quad (2.8)$$

$$\operatorname{div}_{\Gamma_\xi} W = \tau_1 \cdot \partial_{\tau_1} W + \tau_2 \cdot \partial_{\tau_2} W = \sum_{i=1}^2 \tau_i \cdot (\nabla_{\Gamma_\xi} W)\tau_i, \quad (2.9)$$

$$\operatorname{div}_{\Gamma_\xi} \hat{W} = (\partial_{\tau_1} \hat{W})\tau_1 + (\partial_{\tau_2} \hat{W})\tau_2, \quad (2.10)$$

where for vectors $c, d \in \mathbb{R}^3$ we define a 3×3 -matrix by

$$c \otimes d = (c_i d_j)_{i,j=1,2,3}.$$

For brevity we write $\nabla_\Gamma = \nabla_{\Gamma_0}$ and $\operatorname{div}_\Gamma = \operatorname{div}_{\Gamma_0}$. Clearly, we have $\nabla_{\Gamma_\xi} w : \Gamma_\xi \mapsto \mathbb{R}^3$, $\nabla_{\Gamma_\xi} W : \Gamma_\xi \mapsto \mathbb{R}^{3 \times 3}$, $\operatorname{div}_{\Gamma_\xi} W : \Gamma_\xi \mapsto \mathbb{R}$, $\operatorname{div}_{\Gamma_\xi} \hat{W} : \Gamma_\xi \mapsto \mathbb{R}^3$. With these definitions we have the splittings

$$\nabla_x W(t, x) = \partial_\xi W(t, \eta, \xi) \otimes n(t, \eta) + \nabla_{\Gamma_\xi} W(t, \eta, \xi), \quad (2.11)$$

$$\operatorname{div}_x \hat{W}(t, x) = (\partial_\xi \hat{W}(t, \eta, \xi))n(t, \eta) + \operatorname{div}_{\Gamma_\xi} \hat{W}(t, \eta, \xi), \quad (2.12)$$

where, as usual, $W(t, \eta, \xi) = W(t, \eta + n(t, \eta)\xi)$. Let $J \subseteq \mathbb{R}$ be an interval. To define $\nabla_\eta W$ for a mapping $W : \Gamma \times J \rightarrow \mathbb{R}^3$, consider the function $\eta \mapsto W_{t, \xi}(\eta) = W(t, \eta, \xi)$, which is defined on $\Gamma(t)$. To this function (2.8) can be applied. We set

$$\nabla_\eta W(t, \eta, \xi) = \nabla_\eta W_{t, \xi}(\eta) = \nabla_\Gamma W_{t, \xi}(\eta) \in \mathbb{R}^{3 \times 3}. \quad (2.13)$$

With (2.7), (2.9), (2.10) we define in the same way

$$\nabla_\eta w(t, \eta, \xi) = \nabla_\Gamma w_{t, \xi}(\eta) \in \mathbb{R}^3, \quad (2.14)$$

$$\operatorname{div}_\eta W(t, \eta, \xi) = \operatorname{div}_\Gamma W_{t, \xi}(\eta) = \sum_{i=1}^2 \tau_i \cdot (\nabla_\eta W(t, \eta, \xi)) \tau_i \in \mathbb{R}, \quad (2.15)$$

$$\operatorname{div}_\eta \hat{W}(t, \eta, \xi) = \operatorname{div}_\Gamma \hat{W}_{t, \xi}(\eta) \in \mathbb{R}^3. \quad (2.16)$$

The connection between the gradients $\nabla_\eta W$ and $\nabla_{\Gamma_\xi} W$ is given by the chain rule, which yields

$$\nabla_\eta W(t, \eta, \xi) = (\nabla_{\Gamma_\xi} W(t, \eta + n(t, \eta)\xi)) (I + \xi \nabla_\eta n(t, \eta)). \quad (2.17)$$

In particular, we have $\nabla_\eta W(t, \eta, 0) = \nabla_\Gamma W(t, \eta)$. Similar formulas and relations hold for $\nabla_\eta w$, $\operatorname{div}_\eta W$, $\operatorname{div}_\eta \hat{W}$. If $W : \mathcal{U} \rightarrow \mathbb{R}^3$ is constant on all the lines normal to $\Gamma(t)$, for all t , we have $W(t, \eta, \xi) = W(t, \eta)$. For such functions we sometimes interchangeably use the notations $\nabla_\eta W$ and $\nabla_\Gamma W$. Similarly, we interchangeably use the notations $\nabla_\eta w$ and $\nabla_\Gamma w$, $\operatorname{div}_\eta W$ and $\operatorname{div}_\Gamma W$, $\operatorname{div}_\eta \hat{W}$ and $\operatorname{div}_\Gamma \hat{W}$ if w and \hat{W} are independent of ξ .

To construct the asymptotic solution we need information about the jump behavior of \hat{u} and \hat{T} at Γ . This information, which is used throughout our investigations, is collected in the next two lemmas.

Lemma 2.1 *Let $n \in \mathbb{R}^3$ be a unit vector. Then the linear mapping $L_n : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ defined by*

$$L_n z \rightarrow (D\varepsilon(z \otimes n))n : \mathbb{R}^3 \rightarrow \mathbb{R}^3$$

is invertible.

Proof: For $\hat{z} \in \mathbb{R}^3$ and $\alpha \in \mathcal{S}^3$ we have $\hat{z} \cdot (\alpha n) = (\hat{z} \otimes n) : \alpha$. This yields for $z \in \mathbb{R}^3$ with $z \neq 0$ that $z \cdot (D\varepsilon(z \otimes n))n = (z \otimes n) : D\varepsilon(z \otimes n) = \varepsilon(z \otimes n) : D\varepsilon(z \otimes n) > 0$, since by assumption the mapping $D : \mathcal{S}^3 \rightarrow \mathcal{S}^3$ is positive definite. We also used that $\varepsilon(z \otimes n) \neq 0$. For, otherwise we would have $z \otimes n + n \otimes z = 0$. This would imply $|z|^2 = (z \otimes n) : (z \otimes n) = -(n \otimes z) : (z \otimes n) = -(n \cdot z)^2$, which can not hold for $z \neq 0$. Therefore the linear mapping $z \mapsto (D\varepsilon(z \otimes n))n$ is injective, hence it is invertible. \blacksquare

Choose $\phi \in C^\infty(Q)$ such that $\phi = 0$ outside the set \mathcal{U} and $\phi = 1$ in a neighborhood of Γ . We set

$$\xi^+ = \begin{cases} \xi, & \xi \geq 0, \\ 0, & \xi < 0. \end{cases} \quad 1^+(\xi) = \begin{cases} 1, & \xi \geq 0, \\ 0, & \xi < 0. \end{cases} \quad (2.18)$$

Lemma 2.2 (i) *For $(t, \eta) \in \Gamma$ set*

$$u^*(t, \eta) = [\partial_\xi \hat{u}](t, \eta, 0), \quad (2.19)$$

$$a^*(t, \eta) = [\partial_\xi^2 \hat{u}](t, \eta, 0), \quad (2.20)$$

and define $v : Q \rightarrow \mathbb{R}^3$ by the equation

$$\hat{u}(t, x) = \left(u^*(t, \eta) \xi^+ + \frac{1}{2} a^*(t, \eta) (\xi^+)^2 \right) \phi(t, x) + v(t, x), \quad (2.21)$$

where (t, η, ξ) are the new coordinates of $(t, x) \in \mathcal{U}$. Then for $i + j \leq 3$ and $i + j + l \leq 5$ the derivatives $\partial_t^i \nabla_{\Gamma_\xi}^j \partial_\xi^l v$ exist in $\gamma \cup \gamma'$ and are continuous. For $i + j \leq 3$ and $l \leq 2$ these derivatives exist in \hat{Q} and are continuous.

(ii) The jumps of $\nabla_x \hat{u}$ and \hat{T} across the interface Γ satisfy

$$[\varepsilon(\nabla_x \hat{u})] = \varepsilon(u^* \otimes n), \quad [\hat{T}] = D(\varepsilon(u^* \otimes n) - \bar{\varepsilon}). \quad (2.22)$$

(iii) Let $n : \Gamma \rightarrow \mathbb{R}^3$ be the unit normal vector field from (1.12). Then the functions $u^* : \Gamma \rightarrow \mathbb{R}^3$ and $a^* : \Gamma \rightarrow \mathbb{R}^3$ are the unique solutions of the equations

$$(D\varepsilon(u^* \otimes n))n = (D\bar{\varepsilon})n, \quad (2.23)$$

$$(D\varepsilon(a^* \otimes n))n = -(D\varepsilon(\nabla_\Gamma u^*))n - \operatorname{div}_\Gamma D\varepsilon(u^* \otimes n). \quad (2.24)$$

(iv) Define a scalar product $\alpha :_D \beta$ on \mathcal{S}^3 by $\alpha :_D \beta = \alpha \cdot (D\beta)$, for $\alpha, \beta \in \mathcal{S}^3$. For a unit vector $n \in \mathbb{R}^3$ let a linear subspace of \mathcal{S}^3 be given by

$$\mathcal{S}_n^3 = \left\{ \frac{1}{2}(\omega \otimes n + n \otimes \omega) \mid \omega \in \mathbb{R}^3 \right\}, \quad (2.25)$$

let $P_n : \mathcal{S}^3 \rightarrow \mathcal{S}^3$ be the projection onto \mathcal{S}_n^3 , which is orthogonal with respect to the scalar product $\alpha :_D \beta$ and let $Q_n = I - P_n$. Then, with the unit normal vector field $n : \Gamma \rightarrow \mathbb{R}^3$,

$$[\varepsilon(\nabla_x \hat{u})] = P_n \bar{\varepsilon}, \quad [\hat{T}] = -D(I - P_n) \bar{\varepsilon}. \quad (2.26)$$

(v) Let the infinitely differentiable function $p : \mathbb{S}^2 \rightarrow \mathbb{R}$ be defined by

$$p(n) = -\bar{\varepsilon} : D(I - P_n) \bar{\varepsilon}. \quad (2.27)$$

Then we have for all $(t, \eta) \in \Gamma$ that

$$\bar{\varepsilon} : [\hat{T}](t, \eta) = p(n(t, \eta)), \quad (2.28)$$

where $n = n(t, \eta)$ is the unit normal vector to Γ at (t, η) . This implies

$$0 \geq \bar{\varepsilon} : [\hat{T}](t, \eta) \geq -\bar{\varepsilon} : D\bar{\varepsilon}, \quad \text{for all } (t, \eta) \in \Gamma. \quad (2.29)$$

(iv) Let $\langle \hat{T} \rangle = \frac{1}{2}(\hat{T}^{(+)} + \hat{T}^{(-)})$. The jump of the Eshelby tensor \hat{C} defined in (1.19) satisfies

$$n \cdot [\hat{C}]n = [\hat{\psi}] - \bar{\varepsilon} : \langle \hat{T} \rangle. \quad (2.30)$$

Proof: By Assumption A the function \hat{u} is five times continuously differentiable in $\gamma \cup \Gamma$ and in $\gamma' \cup \Gamma$. Therefore (2.19) and (2.20) imply that u^* is four times continuously differentiable and a^* is three-times continuously differentiable. From the right hand side of the equation

$$v(t, x) = \hat{u}(t, x) - \left(u^*(t, \eta) \xi^+ + \frac{1}{2} a^*(t, \eta) (\xi^+)^2 \right) \phi(t, x)$$

we consequently see that for $i + j \leq 3$ and $i + j + l \leq 5$ the derivatives $\partial_t^i \nabla_{\Gamma_\xi}^j \partial_\xi^l v$ exist in the domain $\gamma \cup \gamma'$ and are continuous. By construction, for $i + j \leq 3$ and $l \leq 2$ these derivatives can be joined continuously across Γ . From this we see by well known considerations from calculus that these derivatives exist in all points of Γ and that they are continuous in $\gamma \cup \gamma' \cup \Gamma = Q$. This proves (i).

We use (2.11) to compute from (2.21) that in a neighborhood of Γ where $\phi = 1$

$$\begin{aligned} \nabla_x \hat{u} &= \partial_\xi \hat{u} \otimes n + \nabla_{\Gamma_\xi} \hat{u} \\ &= (u^* \otimes n)1^+ + (a^* \otimes n + \nabla_{\Gamma_\xi} u^*)\xi^+ + \frac{1}{2}(\nabla_{\Gamma_\xi} a^*)(\xi^+)^2 + \nabla_x v, \end{aligned} \quad (2.31)$$

with 1^+ defined in (2.18). Since $\nabla_x v$ is continuous, we have $[\nabla_x v] = 0$, which together with (2.31) yields $[\varepsilon(\nabla_x \hat{u})] = \varepsilon(u^* \otimes n)$. This is the first equality in (2.22). Insertion of (2.31) into (2.2) yields

$$\hat{T} = D(\varepsilon(u^* \otimes n) - \bar{\varepsilon})1^+ + D\varepsilon\left((a^* \otimes n + \nabla_{\Gamma_\xi} u^*)\xi^+ + \frac{1}{2}(\nabla_{\Gamma_\xi} a^*)(\xi^+)^2 + \nabla_x v\right). \quad (2.32)$$

Using again that $[\nabla_x v] = 0$, we conclude from this equation that the second equality in (2.22) holds. To prove (iii), we multiply (2.32) from the right with n and infer from the resulting equation and from (2.5) that

$$(D(\varepsilon(u^* \otimes n) - \bar{\varepsilon}))n = 0. \quad (2.33)$$

This shows that u^* solves (2.23). To verify (2.24), we insert (2.32) into (2.1). Noting the splitting (2.12) of the divergence operator, we calculate that

$$\begin{aligned} 0 &= \operatorname{div}_x \hat{T} + \mathbf{b} \\ &= \partial_\xi (D(\varepsilon(u^* \otimes n) - \bar{\varepsilon})1^+)n + \partial_\xi (D\varepsilon(a^* \otimes n + \nabla_{\Gamma_\xi} u^*)\xi^+)n \\ &\quad + \partial_\xi \left(\frac{1}{2}D\varepsilon(\nabla_{\Gamma_\xi} a^*)(\xi^+)^2\right)n \\ &\quad + \operatorname{div}_{\Gamma_\xi} D(\varepsilon(u^* \otimes n) - \bar{\varepsilon})1^+ + \operatorname{div}_{\Gamma_\xi} D\left(\varepsilon(a^* \otimes n + \nabla_{\Gamma_\xi} u^*)\xi^+ + \frac{1}{2}(\nabla_{\Gamma_\xi} a^*)(\xi^+)^2\right) \\ &\quad + \operatorname{div}_x D\varepsilon(\nabla_x v) + \mathbf{b}. \end{aligned} \quad (2.34)$$

By (2.21) and (2.1), (2.2) we have in the domain γ that

$$\operatorname{div}_x D\varepsilon(\nabla_x v) + \mathbf{b} = \operatorname{div}_x \hat{T} + \mathbf{b} = 0.$$

Γ is a part of the boundary of γ . Consequently, since by Assumption A the function \mathbf{b} and by (i) the function $\nabla_x v$ are both continuous at Γ , we obtain from this equation with the notation introduced in (1.13) that

$$(\operatorname{div}_x D\varepsilon(\nabla_x v) + \mathbf{b})^{(+)} = (\operatorname{div}_x D\varepsilon(\nabla_x v) + \mathbf{b})^{(-)} = 0, \quad \text{on } \Gamma. \quad (2.35)$$

This relation and (2.34), (2.33) imply

$$0 = \lim_{\xi \rightarrow 0^+} (\operatorname{div}_x \hat{T} + \mathbf{b}) = (D\varepsilon(a^* \otimes n + \nabla_{\Gamma} u^*))n + \operatorname{div}_{\Gamma} D\varepsilon(u^* \otimes n).$$

Therefore a^* solves (2.24). It follows from Lemma 2.1 that the solutions u^* and a^* are unique. This proves (ii).

Statement (iv) is proved in [4, Lemma]. Clearly, the second equation in (2.26) follows from the first equation and from (2.22). To prove statement (v), note that (2.26) and (2.27) yield

$$\bar{\varepsilon} : [\hat{T}](t, \eta) = -\bar{\varepsilon} : D(I - P_{n(t, \eta)})\bar{\varepsilon} = p(n(t, \eta)).$$

Since $I - P_n$ is a projector orthogonal with respect to the scalar product $\alpha :_D \beta$, this implies

$$\bar{\varepsilon} : [\hat{T}] = -\bar{\varepsilon} : D(I - P_n)\bar{\varepsilon} = -\bar{\varepsilon} :_D (I - P_n)\bar{\varepsilon} = -(I - P_n)\bar{\varepsilon} :_D (I - P_n)\bar{\varepsilon},$$

The inequalities in (2.29) are obvious consequences of this equation.

The equation (2.30) is verified in [3, equation (2.4)] and in [4, Section 3]. We omit the proof here. \blacksquare

2.1.2 Construction of the asymptotic solution

Now we can state the ansatz for the asymptotic solution $(u^{(\nu)}, T^{(\nu)}, S^{(\nu)})$. To this end we note that (2.21) can be written in the form

$$\hat{u}(t, x) = \phi(t, x) \left(\nu^{\frac{1}{2}} u^*(t, \eta) \left(\frac{\xi}{\nu^{1/2}} \right)^+ + \nu a^*(t, \eta) \frac{1}{2} \left(\left(\frac{\xi}{\nu^{1/2}} \right)^+ \right)^2 \right) + v(t, x). \quad (2.36)$$

This suggests to choose an ansatz of the form

$$u^{(\nu)}(t, x) = \phi(t, x) \sum_{i=0}^1 \nu^{\frac{1+i}{2}} u_i(t, \eta, \frac{\xi}{\nu^{1/2}}) + v(t, x), \quad (2.37)$$

where the functions $u^* \zeta^+$ and $a^* \frac{1}{2} (\zeta^+)^2$ in (2.36) are replaced by suitable functions $u_0(t, \eta, \zeta)$ and $u_1(t, \eta, \zeta)$, which both take values in \mathbb{R}^3 . For the other two components in the asymptotic solution we make the ansatz

$$S^{(\nu)}(t, x) = \phi(t, x) \sum_{i=0}^1 \nu^{\frac{i}{2}} S_i(t, \eta, \frac{\xi}{\nu^{1/2}}) + (1 - \phi(t, x)) \hat{S}(t, x), \quad (2.38)$$

$$T^{(\nu)}(t, x) = D \left(\varepsilon (\nabla_x u^{(\nu)}(t, x)) - \bar{\varepsilon} S^{(\nu)}(t, x) \right), \quad (2.39)$$

where the functions S_0 and S_1 are real valued. We want that $S^{(\nu)}$ is a transition profile connecting the state $S^{(\nu)} = 0$ to the state $S^{(\nu)} = 1$. Therefore we require that there exist functions $a : \Gamma \rightarrow (-\infty, 0)$ and $b : \Gamma \rightarrow (0, \infty)$ such that

$$S_0(t, \eta, \frac{\xi}{\nu^{1/2}}) + \nu^{\frac{1}{2}} S_1(t, \eta, \frac{\xi}{\nu^{1/2}}) = \begin{cases} 0, & (t, x(t, \eta, \xi)) \in \mathcal{U}, \xi \leq \nu^{1/2} a(t, \eta), \\ 1, & (t, x(t, \eta, \xi)) \in \mathcal{U}, \xi \geq \nu^{1/2} b(t, \eta). \end{cases} \quad (2.40)$$

Here and everywhere in the paper we only consider values of the parameter $\nu > 0$, which are sufficiently small such that $-\delta < \nu^{1/2} a(t, \eta) < \nu^{1/2} b(t, \eta) < \delta$. If such functions a and b exist, then

$$\Gamma[\nu] = \{(t, x(t, \eta, \xi)) \mid (t, \eta) \in \Gamma, \nu^{1/2} a(t, \eta) \leq \xi \leq \nu^{1/2} b(t, \eta)\} \subseteq \mathcal{U} \quad (2.41)$$

is the transitional region, where the order parameter $S^{(\nu)}$ changes from 0 to 1. The thickness of the transitional region decreases like $\nu^{1/2}$ for $\nu \rightarrow 0$. For fixed ν the thickness is not constant but depends on the point $(t, \eta) \in \Gamma$. Because of the coordinate transformation (2.6) we always identify $\Gamma[\nu]$ with the set

$$\{(t, \eta, \xi) \mid (t, \eta) \in \Gamma, \nu^{1/2}a(t, \eta) \leq \xi \leq \nu^{1/2}b(t, \eta)\} \subseteq \Gamma \times (-\delta, \delta).$$

The equations (2.38) and (2.40) imply that

$$S^{(\nu)}(t, x) = \hat{S}(t, x), \quad \text{for } (t, x) \in Q \setminus \Gamma[\nu]. \quad (2.42)$$

To determine the functions u_0 , u_1 , S_0 and S_1 we insert the asymptotic solution $(u^{(\nu)}, T^{(\nu)}, S^{(\nu)})$ into the equations (1.1) – (1.3) and collect terms with the same power of ν . This yields a recursively solvable system of four ordinary differential equations of second order, which must be satisfied by the function $\zeta \mapsto (u_0, u_1, S_0, S_1)(t, \eta, \zeta)$ for every value of the parameter $(t, \eta) \in \Gamma$. Since in the asymptotic solution the value $\xi/\nu^{1/2}$ is inserted for ζ in the third argument of in the functions u_0 , u_1 , S_0 , S_1 , and since ξ varies in the interval $[\nu^{1/2}a(t, \eta), \nu^{1/2}b(t, \eta)]$, it follows that the differential equations must be satisfied for every value of ζ from the interval $[a(t, \eta), b(t, \eta)]$. The solution (u_0, u_1, S_0, S_1) depends on the parameter $(t, \eta) \in \Gamma$, since the coefficients in the system of differential equations depend on this parameter. To state the system of differential equations we sometimes drop the arguments t and η for simplicity in notation, but all functions depend on these arguments. For functions w depending on (t, η, ζ) we write $w' = \partial_\zeta w$, $w'' = \partial_\zeta^2 w$. Here and later we also use the notations

$$T_0(t, \eta, \zeta) = D\left(\varepsilon(u_0'(t, \eta, \zeta) \otimes n(t, \eta)) - \bar{\varepsilon}S_0(t, \eta, \zeta)\right), \quad (2.43)$$

$$T_1(t, \eta, \zeta) = D\left(\varepsilon(u_1'(t, \eta, \zeta) \otimes n(t, \eta) + \nabla_\eta u_0(t, \eta, \zeta)) - \bar{\varepsilon}S_1(t, \eta, \zeta)\right), \quad (2.44)$$

$$S_i^{(-1)}(t, \eta, \zeta) = \int_{-\infty}^{\zeta} S_i(t, \eta, \vartheta) d\vartheta, \quad i = 0, 1, \quad (2.45)$$

$$S_0^{(-2)}(t, \eta, \zeta) = \int_{-\infty}^{\zeta} S_0^{(-1)}(t, \eta, \vartheta) d\vartheta, \quad (2.46)$$

$$\begin{aligned} \tilde{\psi}(t, \eta, S) &= \hat{\psi}(S) - \hat{\psi}(0)(1 - S) - \hat{\psi}(1)S + \frac{1}{2}\bar{\varepsilon} : [\hat{T}](t, \eta)S(1 - S) \\ &= \hat{\psi}(S) - \hat{\psi}(0)(1 - S) - \hat{\psi}(1)S + \frac{1}{2}p(n(t, \eta))S(1 - S), \end{aligned} \quad (2.47)$$

with the infinitely differentiable function p defined in (2.27) and with $\tilde{\psi}_S = \partial_S \tilde{\psi}$, as usual. We call $\tilde{\psi}$ the effective double well potential. With these notations the differential equations are

$$T_0'(\zeta)n = 0, \quad (2.48)$$

$$T_1'(\zeta)n = -\text{div}_\eta T_0(\zeta), \quad (2.49)$$

$$\tilde{\psi}_S(S_0(\zeta)) - S_0''(\zeta) = 0, \quad (2.50)$$

$$\tilde{\psi}_{SS}(S_0(\zeta))S_1(\zeta) - S_1''(\zeta) = g_1(t, \eta, \zeta) + \omega(t, \eta), \quad (2.51)$$

where

$$g_1(t, \eta, \zeta) = -\kappa_\Gamma S_0'(\zeta) + \partial_\xi \sigma_1(0)\zeta + \sigma_2(\zeta) - \frac{\partial_t S_0(\zeta)}{f'(n \cdot [\hat{C}]n)S_0'(\zeta)} \varphi_\nu(t, \eta, \zeta), \quad (2.52)$$

with the constitutive function f from (1.3), where

$$\sigma_1(\xi) = \sigma_1(t, \eta, \xi) = \bar{\varepsilon} : D\varepsilon(\nabla_x v(t, x)), \quad x = \eta + n(t, \eta)\xi, \quad (2.53)$$

$$\sigma_2(t, \eta, \zeta) = \bar{\varepsilon} : D\varepsilon(((a^* \otimes n)S_0^{(-1)} + \nabla_\eta u_0 + \partial_\zeta u_{11} \otimes n)), \quad (2.54)$$

$$\partial_\zeta u_{11}(t, \eta, \zeta) = -L_n^{-1} \left((D\varepsilon(u^* \otimes \nabla_\eta S_0^{(-1)}))n + (D(\varepsilon(u^* \otimes n) - \bar{\varepsilon}))\nabla_\eta S_0^{(-1)} \right), \quad (2.55)$$

and where

$$\omega(t, \eta) = - \int_{a(t, \eta)}^{b(t, \eta)} g_1(t, \eta, \vartheta) S_0'(t, \eta, \vartheta) d\vartheta. \quad (2.56)$$

In (2.52) $[\hat{C}]$ is the jump of the Eshelby tensor defined in (1.19), hence $n \cdot [\hat{C}]n$ is a function of (t, η) alone. Finally, to define the function φ_ν we need to introduce the core region $\Gamma_{k, \nu}[a, b]$ and the boundary region $\tilde{\Gamma}_{k, \nu}[a, b]$ of $\Gamma[a, b]$ to a given constant $k > 0$: We set

$$\Gamma_{k, \nu}[a, b] = \{(t, \eta, \zeta) \mid (t, \eta) \in \Gamma, a(t, \eta) + \nu^{1/2}k \leq \zeta \leq b(t, \eta) - \nu^{1/2}k\}, \quad (2.57)$$

and $\tilde{\Gamma}_{k, \nu}[a, b] = \Gamma[a, b] \setminus \Gamma_{k, \nu}[a, b]$. Now let $\varphi_\nu \in C_0^\infty(\Gamma[a, b])$ be a function satisfying

$$0 \leq \varphi_\nu \leq 1, \quad \varphi_\nu = 1 \text{ on } \Gamma_{k, \nu}[a, b], \quad |D_{t, \eta, \zeta}^\alpha \varphi_\nu| \leq \nu^{-|\alpha|/2} K, \text{ for all } \alpha \in \mathbb{N}_0^4, |\alpha| \leq 2. \quad (2.58)$$

For the functions S_0 and S_1 conditions at the boundary of the interval $[a(t, \eta), b(t, \eta)]$ are obtained from the condition (2.40). Since this condition must be satisfied for all sufficiently small $\nu > 0$, it follows that

$$S_0(t, \eta, a(t, \eta)) = 0, \quad S_0(t, \eta, b(t, \eta)) = 1, \quad (2.59)$$

$$S_1(t, \eta, a(t, \eta)) = S_1(t, \eta, b(t, \eta)) = 0. \quad (2.60)$$

The differential equations (2.50), (2.51) together with these boundary conditions determine S_0 and S_1 on the set

$$\Gamma[a, b] = \{(t, \eta, \zeta) \mid (t, \eta) \in \Gamma, a(t, \eta) \leq \zeta \leq b(t, \eta)\}, \quad (2.61)$$

which we do not identify with a subset of $(t_1, t_2) \times \Omega$, differently from $\Gamma[\nu]$. In accordance with (2.40) we extend S_0, S_1 from $\Gamma[a, b]$ to the set $\Gamma \times \mathbb{R}$ by

$$S_0(t, \eta, \zeta) = \begin{cases} 0, & \zeta < a(t, \eta), \\ 1, & \zeta > b(t, \eta), \end{cases} \quad S_1(t, \eta, \zeta) = 0, \quad \zeta \in \mathbb{R} \setminus [a(t, \eta), b(t, \eta)]. \quad (2.62)$$

We also need to define the functions u_0 and u_1 outside of the set $\Gamma[a, b]$. As will be seen, we need that there is a function $c_+ : \Gamma \rightarrow \mathbb{R}^3$ such that for all $(t, \eta, \xi) \in \mathcal{U} \setminus \Gamma[\nu]$

$$\begin{aligned} & \sum_{i=0}^1 \nu^{\frac{1+i}{2}} u_i(t, \eta, \frac{\xi}{\nu^{1/2}}) \\ &= \left(\nu^{\frac{1}{2}} u^*(t, \eta) \left(\frac{\xi}{\nu^{1/2}} \right)^+ + \nu a^*(t, \eta) \frac{1}{2} \left(\left(\frac{\xi}{\nu^{1/2}} \right)^+ \right)^2 \right) + \begin{cases} 0, & \xi \leq a(t, \eta), \\ \nu c_+(t, \eta), & \xi \geq b(t, \eta). \end{cases} \end{aligned} \quad (2.63)$$

This equation holds for all sufficiently small $\nu > 0$ if and only if for all $(t, \eta) \in \Gamma$ and all $\zeta \in \mathbb{R} \setminus [a(t, \eta), b(t, \eta)]$

$$u_0(t, \eta, \zeta) = u^*(t, \eta)\zeta^+, \quad (2.64)$$

$$u_1(t, \eta, \zeta) = \frac{1}{2}a^*(t, \eta)(\zeta^+)^2 + c_+(t, \eta)1^+(\zeta), \quad (2.65)$$

where $1^+(\zeta) = 1$ for $\zeta \geq 0$ and $1^+(\zeta) = 0$ for $\zeta < 0$. Since we require that u_0 and u_1 are at least continuously differentiable, (2.64) prescribes the values of $u_0(\zeta)$ and of $u_0'(\zeta)$ for $\zeta = a(t, \eta)$ and $\zeta = b(t, \eta)$. Since (2.48) is a second order equation for u_0 on the interval $[a(t, \eta), b(t, \eta)]$, we can in general only satisfy two boundary conditions. To satisfy all four boundary conditions, we need a symmetry condition for the potential $\hat{\psi}$, which we state below in the existence theorem for this differential equation. The equation (2.65) prescribes $u_1'(\zeta)$ at the boundary of the interval $[a(t, \eta), b(t, \eta)]$ and the value $u_1(a(t, \eta)) = 0$. Though the differential equation (2.49) for u_1 is also of second order, we show in the existence theorem following below that these three boundary conditions can be satisfied because of the symmetry condition for $\hat{\psi}$.

2.1.3 Main theorems

To complete the construction of the asymptotic solution $(u^{(\nu)}, T^{(\nu)}, S^{(\nu)})$ we must show that the boundary value problem for (u_0, u_1, S_0, S_1) , which consists of the differential equations (2.48) – (2.51) and the boundary conditions (2.59), (2.60), (2.64), (2.65) can be solved. The next three theorems show that the solution can indeed be determined recursively.

From (2.47) we see that $\tilde{\psi}$ depends on (t, η) only via the dependence of the unit normal vector field $(t, \eta) \mapsto n(t, \eta) : \Gamma \rightarrow \mathbb{S}^2$ on these variables, hence $\tilde{\psi}(t, \eta, S) = \tilde{\psi}(n(t, \eta), S)$, where the function

$$(n, S) \mapsto \tilde{\psi}(n, S) : \mathbb{S}^2 \times \mathbb{R} \rightarrow \mathbb{R}$$

is infinitely differentiable with respect to n and has the same order of differentiability with respect to $S \in \mathbb{R}$ as the function $\hat{\psi}$. Now consider the initial value problem

$$\partial_\zeta S_0(n, \zeta) = \sqrt{2\tilde{\psi}(n, S_0(n, \zeta))}, \quad S_0(n, 0) = \frac{1}{2}. \quad (2.66)$$

with $n \in \mathbb{S}^2$. Differentiation of this first order differential equation with respect to ζ shows that if the solution $S_0(n, \zeta)$ is two times differentiable with respect to ζ , then $S_0(t, \eta, \zeta) = S_0(n(t, \eta), \zeta)$ solves the second order differential equation (2.50). To solve the boundary value problem (2.50), (2.59) it therefore suffices to study the initial value problem (2.66). The differentiability properties of $S_0(t, \eta, \zeta)$ with respect to (t, η) then follow from the differentiability properties of the solution $S_0(n, \zeta)$ of (2.66) with respect to n and from the differentiability properties of the normal vector field $(t, \eta) \mapsto n(t, \eta)$ via the chain rule.

To state the properties of $S_0(n, \zeta)$ in the next theorem we need the function $q : \mathbb{S}^2 \times \mathbb{R} \rightarrow \mathbb{R}$ defined by

$$q(n, S) = \hat{\psi}(0)(1 - S) + \hat{\psi}(1)S - \frac{1}{2}p(n)S(1 - S),$$

with p given in (2.27). The function q is infinitely differentiable with respect to n . Since (2.27) – (2.29) imply

$$0 \leq -p(n) = -\bar{\varepsilon} : [\hat{T}] \leq \bar{\varepsilon} : D\bar{\varepsilon}, \quad (2.67)$$

we see that $S \mapsto q(n, S)$ is a concave polynomial of second order whose graph passes through the points $(0, \hat{\psi}(0))$ and $(1, \hat{\psi}(1))$. Note that $\tilde{\psi}(n, S) = \hat{\psi}(S) - q(n, S)$.

Theorem 2.3 *Suppose that the function $\hat{\psi} : \mathbb{R} \rightarrow \mathbb{R}$ has the following properties:*

1. *there is $m \geq 4$ such that $\hat{\psi} \in C^m(\mathbb{R}, \mathbb{R})$,*
2. *$\hat{\psi}(S) - q(n, S) = \tilde{\psi}(n, S) > 0$ for all $0 < S < 1$ and all $n \in \mathbb{S}^2$,*
3. *there is $c_0 > 0$ such that for all $n \in \mathbb{S}^2$*

$$\hat{\psi}'(0) - \partial_S q(n, 0) = \partial_S \tilde{\psi}(n, 0) \geq c_0, \quad \hat{\psi}'(1) - \partial_S q(n, 1) = \partial_S \tilde{\psi}'(n, 1) \leq -c_0. \quad (2.68)$$

Then the following assertions hold:

- (i) *For all $n \in \mathbb{S}^2$ there exist numbers $-\infty < \tilde{a}(n) < 0 < \tilde{b}(n) < \infty$ and a unique solution $\zeta \mapsto S_0(n, \zeta) : [\tilde{a}, \tilde{b}] \rightarrow [0, 1]$ of (2.66), which is strictly increasing and satisfies*

$$S_0(n, \tilde{a}(n)) = 0, \quad S_0(n, \tilde{b}(n)) = 1, \quad \partial_\zeta S_0(n, \tilde{a}(n)) = \partial_\zeta S_0(n, \tilde{b}(n)) = 0.$$

$\partial_\zeta^i S_0$ belongs to the space $C^{m-1}(\mathbb{S}^2[\tilde{a}, \tilde{b}])$ for $i = 0, \dots, 2$, where

$$\mathbb{S}^2[\tilde{a}, \tilde{b}] = \{(n, \zeta) \mid n \in \mathbb{S}^2, \tilde{a}(n) \leq \zeta \leq \tilde{b}(n)\}.$$

For $n \in \mathbb{S}^2$ we have

$$\nabla_n S_0(n, \tilde{a}(n)) = \nabla_n S_0(n, \tilde{b}(n)) = 0.$$

The functions $n \mapsto \tilde{a}(n)$ and $n \mapsto \tilde{b}(n)$ belong to the space $C^{m-1}(\mathbb{S}^2)$.

- (ii) *The functions $a : \Gamma \rightarrow (-\infty, 0)$ and $b : \Gamma \rightarrow (0, \infty)$ defined by $a(t, \eta) = \tilde{a}(n(t, \eta))$, $b(t, \eta) = \tilde{b}(n(t, \eta))$ belong to $C^3(\Gamma)$. Moreover, the function*

$$(t, \eta, \zeta) \mapsto S_0(t, \eta, \zeta) = S_0(n(t, \eta), \zeta) : \Gamma[a, b] \rightarrow \mathbb{R}$$

satisfies the differential equation (2.50) on $\Gamma[a, b]$ and we have $\partial_\zeta^i S_0 \in C^3(\Gamma[a, b])$ for $i = 0, \dots, m-1$. Also,

$$S_0(t, \eta, a) = 0, \quad S_0(t, \eta, b) = 1, \quad \partial_\zeta S_0(t, \eta, a) = \partial_\zeta S_0(t, \eta, b) = 0, \quad (2.69)$$

where $a = a(t, \eta)$ and $b = b(t, \eta)$, and

$$\partial_t S_0(t, \eta, \zeta) = 0, \quad \nabla_\eta S_0(t, \eta, \zeta) = 0, \quad \text{for } \zeta = a(t, \eta), b(t, \eta). \quad (2.70)$$

- (iii) *Assume that $\hat{\psi}$ has the properties 1. – 3. and the following additional property:*

4. *for all $S \in [-\frac{1}{2}, \frac{1}{2}]$*

$$\hat{\psi}(\frac{1}{2} + S) = \hat{\psi}(\frac{1}{2} - S). \quad (2.71)$$

Then S_0 is of the form

$$S_0(t, \eta, \zeta) = S_*(t, \eta, \zeta) + \frac{1}{2}, \quad (2.72)$$

with $S_*(t, \eta, \zeta) = -S_*(t, \eta, -\zeta)$ and the interval $[a(t, \eta), b(t, \eta)]$ is symmetric with respect to 0, hence $a(t, \eta) = -b(t, \eta)$.

Remarks. The symmetry condition (2.71) implies $\hat{\psi}(0) = \hat{\psi}(1)$.

It is not immediately clear how to verify that $\hat{\psi}$ has the properties 2 and 3 stated in this theorem. Yet, a condition, which guarantees that $\hat{\psi}$ has these properties and which can be checked easily, is obtained from the estimate (2.67). Namely, from this estimate we immediately see that $\hat{\psi}$ has these properties if

$$\begin{aligned}\hat{\psi}(S) &> \hat{\psi}(0)(1-S) + \hat{\psi}(1)S + \frac{1}{2}\bar{\varepsilon} : D\bar{\varepsilon} S(1-S), \quad \text{for all } 0 < S < 1, \\ \hat{\psi}'(0) &> \hat{\psi}(1) - \hat{\psi}(0) + \frac{1}{2}\bar{\varepsilon} : D\bar{\varepsilon}, \quad \hat{\psi}'(1) < \hat{\psi}(1) - \hat{\psi}(0) - \frac{1}{2}\bar{\varepsilon} : D\bar{\varepsilon}.\end{aligned}$$

Proof of the theorem: The statement (i) of this theorem is obtained by a slight and obvious modification of the proof of Theorem 1.1 in [4]. Since $S_0(t, \eta, \zeta) = S_0(n(t, \eta), \zeta)$ with the unit normal vector field n to the manifold Γ , statement (ii) is an immediate consequence of (i) and of the chain rule, noting that by Assumption A we have $n \in C^3(\Gamma)$. Finally, to prove (iii) note that (2.47) and (2.71) imply

$$\tilde{\psi}(t, \eta, \frac{1}{2} + S) = \tilde{\psi}(t, \eta, \frac{1}{2} - S). \quad (2.73)$$

Let $S_0(t, \eta, \zeta) = S_0(n(t, \eta), \zeta)$ be the solution of (2.66). To simplify the notation we drop the variables (t, η) . Define

$$S_*(\zeta) = \begin{cases} S_0(\zeta) - \frac{1}{2}, & 0 \leq \zeta \leq b(t, \eta), \\ -S_*(-\zeta), & -b(t, \eta) \leq \zeta \leq 0. \end{cases}$$

Then $S_*(\zeta) + \frac{1}{2}$ satisfies the differential equation from the initial value problem (2.66) for $0 \leq \zeta \leq b$. For $-b \leq \zeta \leq 0$ we thus obtain together with (2.73) that

$$\begin{aligned}\partial_\zeta(S_*(\zeta) + 1/2) &= \partial_\zeta(S_*(-\zeta) + 1/2) \\ &= \sqrt{2\tilde{\psi}(S_*(-\zeta) + 1/2)} = \sqrt{2\tilde{\psi}(-S_*(-\zeta) + 1/2)} = \sqrt{2\tilde{\psi}(S_*(\zeta) + 1/2)}.\end{aligned}$$

Consequently, $S_* + \frac{1}{2}$ satisfies this differential equation in the whole interval $[-b, b]$. Since also $S_*(0) + \frac{1}{2} = \frac{1}{2}$, it follows that $S_* + \frac{1}{2}$ is equal to the unique solution S_0 of this problem. \blacksquare

Theorem 2.4 (i) Let $S_0 = S_0(t, \eta, \zeta)$ be the function constructed in Theorem 2.3. Then $S'_0 = \partial_\zeta S_0$ is an eigenfunction to the eigenvalue zero of the linear boundary value problem

$$\tilde{\psi}_{SS}(S_0(\zeta))S_1(\zeta) - S''_1(\zeta) = f_1(t, \eta, \zeta), \quad S_1(t, \eta, a(t, \eta)) = S_1(t, \eta, b(t, \eta)) = 0. \quad (2.74)$$

(ii) Assume that $f_1 \in C(\Gamma[a, b])$ satisfies

$$\int_{a(t, \eta)}^{b(t, \eta)} f_1(t, \eta, \zeta) S'_0(t, \eta, \zeta) d\zeta = 0. \quad (2.75)$$

Then there are solutions $S_1 : \Gamma[a, b] \rightarrow \mathbb{R}$ of the boundary value problem (2.74).

(iii) Assume that $\hat{\psi}$ has the properties 1. – 4. stated in Theorem 2.3, let $f \in C^3(\mathbb{R}, \mathbb{R})$ satisfy $f'(r) \geq c_1 > 0$ for all $r \in \mathbb{R}$ and let φ_ν in (2.52) be chosen such that

$$\varphi_\nu(t, \eta, \zeta) = \varphi_\nu(t, \eta, -\zeta). \quad (2.76)$$

Then the function g_1 defined in (2.52) belongs to the space $C^2(\Gamma[a, b])$, the function ω defined in (2.56) belongs to $C^2(\Gamma)$ and the function $f_1 = g_1 + \omega$ satisfies (2.75). Moreover, there is a solution S_1 of the boundary value problem (2.51), (2.60), which belongs to $C^2(\Gamma[a, b])$ and satisfies

$$|\partial_\zeta^i S_1|, |\partial_t S_1|, |\nabla_\eta S_1| \leq K_1, \text{ for } i = 0, \dots, 2, \quad |\nabla_\eta^2 S_1| \leq (|\ln \nu| + 1)K_2. \quad (2.77)$$

Proof: Since $S'_0(\zeta)$ vanishes for $\zeta = a$ and $\zeta = b$, by (2.69), statement (i) of this theorem follows by differentiation of (2.50) with respect to ζ . Statement (ii) is a well known result from the spectral theory of selfadjoint differential operators. It remains to verify (iii). To see that $f_1 = g_1 + \omega$ satisfies (2.75), note that

$$\int_a^b \omega S'_0(\zeta) d\zeta = \omega(S_0(b) - S_0(a)) = \omega,$$

by (2.69). The statement follows by combination of this equation with (2.56). From (ii) we obtain now that the boundary value problem (2.51), (2.60) has a solution S_1 . To show that there is a solution with the regularity and boundedness properties stated in (iii) is more involved because of the term $\frac{\partial_t S_0(\zeta)}{f'(n \cdot [\bar{C}]_n) S'_0(\zeta)}$ appearing in g_1 . Therefore we postpone this part of the proof to Section 3. \blacksquare

Theorem 2.5 *Let $S_0, S_1 : \Gamma \times \mathbb{R} \rightarrow \mathbb{R}$ be given differentiable functions satisfying the condition (2.62). Suppose that S_0 satisfies the symmetry condition (2.72). Then there are continuously differentiable functions $u_0, u_1 : \Gamma \times \mathbb{R} \rightarrow \mathbb{R}^3$, which fulfill the differential equations (2.48), (2.49) on $\Gamma \times \mathbb{R}$ and the conditions (2.64) and (2.65). These functions have the form*

$$u_0(t, \eta, \zeta) = u^*(t, \eta) S_0^{(-1)}(t, \eta, \zeta), \quad (2.78)$$

$$u_1(t, \eta, \zeta) = u^*(t, \eta) S_1^{(-1)}(t, \eta, \zeta) + a^*(t, \eta) S_0^{(-2)}(t, \eta, \zeta) + u_{11}(t, \eta, \zeta), \quad (2.79)$$

$$u_{11}(t, \eta, \zeta) = -L_n^{-1} \left((D\varepsilon(u^* \otimes \nabla_\eta S_0^{(-2)}))n + (D(\varepsilon(u^* \otimes n) - \bar{\varepsilon}))\nabla_\eta S_0^{(-2)} \right), \quad (2.80)$$

where L_n is the linear mapping from Lemma 2.1. The functions u_0 and u_1 are uniquely determined.

The **proof** of this theorem is given in Section 3.

These three theorems show that we can first solve (2.50) for S_0 , then determine u_0 from (2.48), next solve (2.51) for S_1 , and finally determine u_1 from (2.49).

Now we are in a position to define the functions ω_1 and B appearing in the kinetic relation (2.3).

Lemma 2.6 *Assume that S_0 and φ_ν satisfy the symmetry conditions (2.72) and (2.76), respectively. Then the function ω defined in (2.56) satisfies*

$$\omega(n(t, \eta)) = \omega_1(n(t, \eta)) \kappa_\Gamma(t, \eta) + B(n(t, \eta)) \nabla_\Gamma n(t, \eta), \quad (2.81)$$

where the function $\omega_1 : \mathbb{S}^2 \rightarrow (0, \infty)$ is given by

$$\omega_1(n) = \int_0^1 \sqrt{2\tilde{\psi}(n, \vartheta)} d\vartheta, \quad (2.82)$$

and where for every unit vector $n \in \mathbb{R}^3$ the linear mapping $B(n) : \mathbb{R}^{3 \times 3} \rightarrow \mathbb{R}$ is defined by

$$B(n(t, \eta)) \nabla_{\Gamma} n(t, \eta) = - \int_{a(t, \eta)}^{b(t, \eta)} \sigma_2(t, \eta, \vartheta) S'_0(t, \eta, \vartheta) d\vartheta. \quad (2.83)$$

with σ_2 given in (2.54).

Proof: The function $\zeta \mapsto S_*(\zeta)$ in the symmetry condition (2.72) is odd, whence $\zeta \mapsto \partial_t S_0(\zeta) = \partial_t S_*(\zeta)$ is odd and $\zeta \mapsto S'_0(\zeta) = S'_*(\zeta)$ is even. Since $\zeta \mapsto \partial_{\xi} \sigma_1(0) \zeta$ is odd, since by (2.76) the function $\zeta \mapsto \varphi_{\nu}(\zeta)$ is even, since $f'(n \cdot [\hat{C}]n)$ is independent of ζ and since $a(t, \eta) = -b(t, \eta)$, it follows that

$$\int_a^b \partial_{\xi} \sigma_1(0) \zeta S'_0(\zeta) d\zeta = 0, \quad \int_a^b \frac{\partial_t S_0(\zeta) \varphi_{\nu}(\zeta)}{f'(n \cdot [\hat{C}]n)} S'_0(\zeta) d\zeta = 0,$$

because the integrands are odd. These equations and (2.56), (2.52) together yield

$$\omega(t, \eta) = \omega_1(n(t, \eta)) \kappa_{\Gamma}(t, \eta) - \int_{a(t, \eta)}^{b(t, \eta)} \sigma_2(t, \eta, \vartheta) S'_0(t, \eta, \vartheta) d\vartheta. \quad (2.84)$$

with

$$\omega_1(n) = \int_a^b S'_0(\vartheta)^2 d\vartheta = \int_a^b \sqrt{2\tilde{\psi}(S_0(\zeta))} S'_0(\zeta) d\zeta = \int_0^1 \sqrt{2\tilde{\psi}(n, \vartheta)} d\vartheta. \quad (2.85)$$

In this computation we used (2.66).

Next we show that the second term on the right hand side of (2.84) is of the form of a linear mapping applied to the surface gradient $\nabla_{\Gamma} n(t, \eta)$. Examination of the definition of σ_2 in (2.54), (2.55) and in (2.78) shows that $\int_a^b \sigma_2 S'_0 d\vartheta$ is a sum, every summand of which contains one of the terms

$$\int_a^b S_0^{(-1)}(\vartheta) S'_0(\vartheta) d\vartheta = \tilde{b}(n) - \int_{\tilde{a}(n)}^{\tilde{b}(n)} S_0^2(n, \vartheta) d\theta, \quad (2.86)$$

$$\begin{aligned} \int_a^b \nabla_{\eta} S_0^{(-1)}(\vartheta) S'_0(\vartheta) d\vartheta &= - \int_a^b \nabla_{\eta} S_0(\vartheta) S_0(\vartheta) d\theta \\ &= - \left(\int_{\tilde{a}(n)}^{\tilde{b}(n)} (\nabla_n S_0(n, \vartheta))^T S_0(n, \vartheta) d\theta \right) \nabla_{\Gamma} n. \end{aligned} \quad (2.87)$$

In (2.86) we integrated by parts using that $S_0^{(-1)}(b) = b$, which is implied by (2.64) and by (2.78). In the integration by parts in (2.87) we employed (2.70). To get the last equality sign in (2.87) we also used that $\nabla_{\eta} S_0(n(t, \eta), \vartheta) = (\nabla_n S_0(n(t, \eta), \vartheta))^T \nabla_{\eta} n(t, \eta)$ and wrote $\nabla_{\Gamma} n = \nabla_{\eta} n$, by our convention. The functions \tilde{a} and \tilde{b} are defined in Theorem 2.3.

The right hand side of (2.86) is a real valued function, which only depends on the normal vector n , and the right hand side in (2.87) is of the form of a linear mapping applied to the surface gradient $\nabla_{\Gamma} n$ of the normal vector; the coefficients in the linear mapping depend only on n , in a nonlinear way.

If we insert these terms into the sum composing $\int_a^b \sigma_2 S'_0 d\vartheta$ and observe that u^* and the linear mapping L_n both are functions depending on n only, which follows from (2.23)

and from Lemma 2.1, and that a^* is obtained by application of a linear mapping to $\nabla_\Gamma n$, with coefficients of the linear mapping depending on n only, which is implied by (2.24), we see by examining (2.54), (2.55) and (2.78) again, that in fact every summand is of the form of such a linear mapping applied to $\nabla_\Gamma n$. Consequently, $\int_a^b \sigma_2 S'_0 d\vartheta$ itself is of this form, hence for every unit vector $n \in \mathbb{R}^3$ there is a linear mapping $B(n) : \mathbb{R}^{3 \times 3} \rightarrow \mathbb{R}$ satisfying (2.83). We can thus replace the second term on the right hand side of (2.84) by the left hand side of (2.83). Combination of the resulting equation with (2.85) yields (2.81). \blacksquare

The next theorem shows that $(u^{(\nu)}, T^{(\nu)}, S^{(\nu)})$ satisfies the model equations (1.1) – (1.3) up to an error decreasing to zero with vanishing parameter ν , and is therefore indeed an asymptotic solution. This is the main result of this section. To state the theorem we need the core region $\Gamma_k[\nu]$ and the boundary region $\tilde{\Gamma}_k[\nu]$ of $\Gamma[\nu]$ to a given constant $k > 0$, which are defined by

$$\Gamma_k[\nu] = \{(t, x(t, \eta, \xi)) \mid (t, \eta) \in \Gamma, \nu^{1/2}a(t, \eta) + \nu k \leq \xi \leq \nu^{1/2}b(t, \eta) - \nu k\} \quad (2.88)$$

and by $\tilde{\Gamma}_k[\nu] = \Gamma[\nu] \setminus \Gamma_k[\nu]$. If we identify (t, x) with (t, η, ξ) and set $\zeta = \frac{\xi}{\nu^{1/2}}$, as usual, then (t, η, ξ) belongs $\Gamma_k[\nu]$ or to $\tilde{\Gamma}_k[\nu]$, if and only if (t, η, ζ) belongs to $\Gamma_{k, \nu}[a, b]$ or to $\tilde{\Gamma}_{k, \nu}[a, b]$, respectively. The sets $\Gamma_{k, \nu}[a, b]$ and $\tilde{\Gamma}_{k, \nu}[a, b]$ are defined in (2.57).

Theorem 2.7 *Assume that $\hat{\psi}$ has the properties 1. – 4. stated in Theorem 2.3, that the symmetry condition (2.76) for φ_ν is fulfilled and that $f \in C^3(\mathbb{R}, \mathbb{R})$ satisfies $f'(r) \geq c_1 > 0$ for all $r \in \mathbb{R}$. Let the functions ω_1 in and B in the kinetic relation (2.3) of the sharp interface model (2.1) – (2.5) be defined by (2.82) and (2.83).*

Assume that $(\hat{u}, \hat{T}, \hat{S}, \Gamma)$ is a solution of this sharp interface model in the domain Q , which satisfies Assumption A. For $\nu > 0$ let the function $(u^{(\nu)}, T^{(\nu)}, S^{(\nu)})$ be defined by (2.37) – (2.39) with u_0, u_1, S_0, S_1 given in Theorem 2.3 – Theorem 2.5.

Then $(u^{(\nu)}, T^{(\nu)}, S^{(\nu)})$ belongs to the space $C^2(Q) \times C^1(Q) \times (C^1(Q) \cap C^2(\Gamma[\nu]))$ and satisfies (1.2) identically and (1.1) and (1.3) asymptotically. More precisely, there are constants $k > 0, K_1, \dots, K_4 > 0$ such that

$$|\operatorname{div}_x T^{(\nu)}(t, x) + \mathbf{b}(t, x)| \leq \begin{cases} K_1 \nu^{1/2}, & (t, x) \in \Gamma[\nu], \\ K_2 \nu, & (t, x) \in Q \setminus \Gamma[\nu], \end{cases} \quad (2.89)$$

and

$$\begin{aligned} & \left\| \partial_t S^{(\nu)} + f\left(\psi_S(\varepsilon(\nabla_x u^{(\nu)}), S^{(\nu)}) - \nu \Delta_x S^{(\nu)}\right) \Big| \nabla_x S^{(\nu)} \right\|_{L^\infty(V)} \\ & \leq \begin{cases} K_3 \nu^{1/2}, & \text{for } V = \Gamma_k[\nu], \\ K_4, & \text{for } V = \tilde{\Gamma}_k[\nu], \\ 0, & \text{for } V = Q \setminus \Gamma[\nu]. \end{cases} \end{aligned} \quad (2.90)$$

From the definitions (2.41) and (2.88) we see that there are constants $K_5, K_6 > 0$ such that $\operatorname{meas}(\Gamma_k[\nu]) < \operatorname{meas}(\Gamma[\nu]) \leq K_5 \nu^{1/2}$ and $\operatorname{meas}(\tilde{\Gamma}_k[\nu]) \leq K_6 \nu$. Therefore the following result is an immediate consequence of this theorem.

Corollary 2.8 *There are constants K_7, K_8 such that*

$$\|\operatorname{div}_x T^{(\nu)} + \mathbf{b}\|_{L^1(Q)} \leq K_7 \nu, \quad (2.91)$$

$$\left\| \partial_t S^{(\nu)} + f\left(\psi_S(\varepsilon(\nabla_x u^{(\nu)}), S^{(\nu)}) - \nu \Delta_x S^{(\nu)}\right) |\nabla_x S^{(\nu)}| \right\|_{L^1(Q)} \leq K_8 \nu. \quad (2.92)$$

2.2 Asymptotic solution of first order

In this section we construct the family $(u^{(\nu)}, T^{(\nu)}, S^{(\nu)})$ of asymptotic solution of first order to the model (1.1) – (1.3). This first order family can be constructed under weaker assumptions for the potential $\hat{\psi}$ and the nonlinearity f than the second order family. In particular, the nonlinearity f needs not to be one-to-one or differentiable.

We use the notations introduced previously, but redefine some of these notations in this section.

The construction of the asymptotic solution of first order is based on the sharp interface model (1.14) – (1.18). Thus, let $(\hat{u}, \hat{T}, \hat{S}, \Gamma)$ be a given solution of this model. We denote by γ the set of all $(t, x) \in Q \setminus \Gamma$ with $\hat{S}(t, x) = 0$ and by γ' the set of all $(t, x) \in Q \setminus \Gamma$ with $\hat{S}(t, x) = 1$, hence $\gamma \cup \gamma' = Q \setminus \Gamma$. For this solution we make the following

Assumption B. Let Γ be a three dimensional C^3 -manifold embedded in Q , such that the set Γ is a compact subset of Q and the two dimensional manifold $\Gamma(t)$ does not have a boundary for all $t \in [t_1, t_2]$. Let the function (\hat{u}, \hat{T}) belong to the space $C^3(\gamma \cup \gamma') \times C^2(\gamma \cup \gamma')$. We assume that the derivatives of \hat{u} up to order three and the derivatives of \hat{T} up to order two have continuous extensions from γ to $\gamma \cup \Gamma$ and from γ' to $\gamma' \cup \Gamma$.

Let $\phi \in C^\infty(Q)$ be a function, which vanishes outside of the set \mathcal{U} and is equal to one in a neighborhood of Γ . With u^* defined in (2.19) we decompose the function \hat{u} in the form

$$\hat{u}(t, x) = u^*(t, \eta) \xi^+ \phi(t, x) + v(t, x), \quad (t, x) \in \mathcal{U}. \quad (2.93)$$

This defines the function $v : Q \rightarrow \mathbb{R}^3$. As in Lemma 2.2 it follows from Assumption B that for $i+j \leq 2$ and $i+j+l \leq 3$ the derivatives $\partial_t^i \nabla_{\Gamma}^j \partial_\xi^l v$ exist in $\gamma \cup \gamma'$ and are bounded and continuous. For $i+j \leq 2$ and $l \leq 1$ these derivatives can be joined continuously across Γ , whence these derivatives exist in Q and are continuous. With the functions ϕ and v defined in this way we make for the asymptotic solution the ansatz

$$u^{(\nu)}(t, x) = \nu^{1/2} u_0(t, \eta, \frac{\xi}{\nu^{1/2}}) \phi(t, x) + v(t, x), \quad (2.94)$$

$$S^{(\nu)}(t, x) = S_0(t, \eta, \frac{\xi}{\nu^{1/2}}) \phi(t, x) + \hat{S}(t, x) (1 - \phi(t, x)), \quad (2.95)$$

$$T^{(\nu)}(t, x) = D(\varepsilon(\nabla_x u^{(\nu)}(t, x)) - \bar{\varepsilon} S^{(\nu)}(t, x)), \quad (2.96)$$

where the functions u_0 and S_0 are defined as in the previous section. That is, for S_0 we require that there exist functions $a : \Gamma \rightarrow (-\infty, 0)$ and $b : \Gamma \rightarrow (0, \infty)$ such that

$$\tilde{\psi}_S(S_0(t, \eta, \zeta)) - S_0''(t, \eta, \zeta) = 0, \quad \zeta \in [a(t, \eta), b(t, \eta)], \quad (2.97)$$

$$S_0(t, \eta, \zeta) = \begin{cases} 0, & (t, \eta) \in \Gamma, \zeta \leq a(t, \eta), \\ 1, & (t, \eta) \in \Gamma, \zeta \geq b(t, \eta). \end{cases} \quad (2.98)$$

For u_0 we set

$$u_0(t, \eta, \zeta) = u^*(t, \eta) S_0^{(-1)}(t, \eta, \zeta), \quad (2.99)$$

with $S_0^{(-1)}$ defined in (2.45). We assume that the potential $\hat{\psi}$ has the properties 1. – 3. stated in Theorem 2.3. However, in the present case it suffices to require in property 1 that $m \geq 3$. The proof of Theorem 2.3 in [4] shows that also under this weaker assumption there exist functions $a : \Gamma \rightarrow (-\infty, 0)$, $b : \Gamma \rightarrow (0, \infty)$ and S_0 , which satisfy (2.66) and (2.97), (2.98) and for which statement (i) of Theorem 2.3 remains true without modification, statement (ii) remains true with the sole modifications that a and b belong to $C^2(\Gamma)$ and $\partial_\zeta^i S_0 \in C^2(\Gamma[a, b])$ for $i = 0, \dots, 2$. We do not need to require that $\hat{\psi}$ has property 4 of Theorem 2.3. Therefore potentials with $\hat{\psi}(0) \neq \hat{\psi}(1)$ are allowed.

The asymptotic solution thus constructed has the following convergence properties:

Theorem 2.9 *Let the hypotheses 1. – 3. in Theorem 2.3 be satisfied and let $f : \mathbb{R} \rightarrow \mathbb{R}$ be an increasing, Lipschitz continuous function. Assume that $(\hat{u}, \hat{T}, \hat{S}, \Gamma)$ is a solution of the sharp interface model (1.14) – (1.18) in the domain Q , which satisfies Assumption B. For $\nu > 0$ let the function $(u^{(\nu)}, T^{(\nu)}, S^{(\nu)})$ be defined by (2.94) – (2.96) with S_0 and u_0 satisfying (2.97) – (2.99).*

Then $(u^{(\nu)}, T^{(\nu)}, S^{(\nu)})$ belongs to the space $C^2(Q) \times C^1(Q) \times (C^1(Q) \cap C^2(\Gamma[\nu]))$, the divergence $\operatorname{div}_x T^{(\nu)}$ exists in Q and is continuous, and $(u^{(\nu)}, T^{(\nu)}, S^{(\nu)})$ satisfies (1.2) exactly and (1.1) and (1.3) asymptotically. Precisely, there are constants $K_1, \dots, K_3 > 0$ such that

$$\begin{aligned} |\operatorname{div}_x T^{(\nu)}(t, x) + \mathbf{b}(t, x)| &\leq \begin{cases} K_1, & (t, x) \in \Gamma[\nu], \\ K_2 \nu^{1/2}, & (t, x) \in Q \setminus \Gamma[\nu], \end{cases} \\ \left\| \partial_t S^{(\nu)} + f\left(\psi_S(\varepsilon(\nabla_x u^{(\nu)}), S^{(\nu)}) - \nu \Delta_x S^{(\nu)}\right) |\nabla_x S^{(\nu)}| \right\|_{L^\infty(V)} \\ &\leq \begin{cases} K_3, & \text{for } V = \Gamma[\nu], \\ 0, & \text{for } V = Q \setminus \Gamma[\nu]. \end{cases} \end{aligned}$$

Since $\operatorname{meas}(\Gamma[\nu]) \leq K_4 \nu^{1/2}$, this theorem has the following corollary:

Corollary 2.10 *There are constants K_5, K_6 such that*

$$\begin{aligned} \|\operatorname{div}_x T^{(\nu)} + \mathbf{b}\|_{L^1(Q)} &\leq K_5 \nu^{1/2}, \\ \left\| \partial_t S^{(\nu)} + f\left(\psi_S(\varepsilon(\nabla_x u^{(\nu)}), S^{(\nu)}) - \nu \Delta_x S^{(\nu)}\right) |\nabla_x S^{(\nu)}| \right\|_{L^1(Q)} &\leq K_6 \nu^{1/2}. \end{aligned}$$

The proof of Theorem 2.9 runs along the same lines as the proof of Theorem 2.7, but is much less technical and is obtained by modifications and simplifications of the latter proof. Therefore we do not give the proof, but leave the necessary modifications of the investigations in Section 3 to the reader.

3 Proof of the main theorems from Section 2.1

In Sections 3.1 – 3.3 we prove Theorems 2.4, 2.5 and 2.7. The proof of some technical estimates, which are needed in Sections 3.1 and 3.3.3, is postponed to Section 3.4. This latter proof uses solely properties of the function S_0 from Theorem 2.3.

3.1 Proof of Theorem 2.4

Only statement (iii) must be verified. For the proof we use a result from [4]. In the proof of lemma 4.1 of that article it has been shown that a solution of the boundary value problem (2.51), (2.60) is given by

$$w(t, \eta, \zeta) = \int_{a(t, \eta)}^{b(t, \eta)} G(t, \eta; \zeta, \vartheta) (g_1(t, \eta, \vartheta) + \omega(t, \eta)) d\vartheta, \quad (3.1)$$

with the Green's function G defined as follows: For fixed ϑ with $a < \vartheta < b$ the function G is a solution of the differential equation

$$(\tilde{\psi}_{SS}(S_0) - \partial_\zeta^2)G(\zeta, \vartheta) = C_\vartheta, \quad a < \zeta < d, \quad \zeta \neq \vartheta, \quad (3.2)$$

with the constant $C_\vartheta = -S'_0(\vartheta)$, and of the initial and jump conditions

$$G(a, \vartheta) = \partial_\zeta G(a, \vartheta) = 0, \quad (3.3)$$

$$G(\vartheta+, \vartheta) = G(\vartheta-, \vartheta), \quad (3.4)$$

$$\partial_\zeta G(\vartheta+, \vartheta) = \partial_\zeta G(\vartheta-, \vartheta) - 1. \quad (3.5)$$

It is also shown in [4] that

$$G(b, \vartheta) = 0. \quad (3.6)$$

From Theorem 2.3 we have $S_0 \in C^3(\Gamma[a, b])$. Since by assumption $\hat{\psi}_{SS} \in C^2(\mathbb{R})$, we conclude that $\hat{\psi}_{SS}(S_0) \in C^2(\Gamma[a, b])$. From this result, from the definition of $\tilde{\psi}$ in (2.47) and from Assumption A we obtain that the coefficient function $(t, \eta, \zeta) \mapsto \tilde{\psi}_{SS}(t, \eta, S_0(t, \eta, \zeta))$ in (3.2) belongs to $C^2(\Gamma[a, b])$. Since also $a, b \in C^3(\Gamma)$, by Theorem 2.3, we conclude from the standard theory of the linear initial- and transmission problem (3.2) – (3.5) that $(t, \eta, \zeta, \vartheta) \mapsto G(t, \eta; \zeta, \vartheta)$ is two times continuously differentiable with bounded derivatives at all points $(t, \eta, \zeta, \vartheta)$ with $\zeta \neq \vartheta$. However, G need not be symmetric with respect to the ζ and ϑ variables. Therefore we replace the Green's function G in (3.1) by the modified Green's function

$$G_1(t, \eta; \zeta, \vartheta) = G(t, \eta; \zeta, \vartheta) - d_1(t, \eta, \vartheta)S'_0(\zeta) - d_2(t, \eta, \zeta)S'_0(\vartheta) - S'_0(\zeta)d_3(t, \eta)S'_0(\vartheta), \quad (3.7)$$

where

$$\begin{aligned} d_1(t, \eta, \vartheta) &= \frac{1}{\|S'_0\|_{L^2([a, b])}^2} \int_a^b G(t, \eta; \zeta, \vartheta) S'_0(\zeta) d\zeta, \\ d_2(t, \eta, \zeta) &= \frac{1}{\|S'_0\|_{L^2([a, b])}^2} \int_a^b G(t, \eta; \zeta, \vartheta) S'_0(\vartheta) d\vartheta, \\ d_3(t, \eta, \zeta) &= \frac{1}{\|S'_0\|_{L^2([a, b])}^4} \int_a^b \int_a^b S'_0(\zeta) G(t, \eta; \zeta, \vartheta) S'_0(\vartheta) d\vartheta d\zeta. \end{aligned}$$

For $(t, \eta) \in \Gamma$ we define the integral operator $\mathcal{K}_{t, \eta}$ on $L^2([a(t, \eta), b(t, \eta)])$ by

$$\mathcal{K}_{t, \eta}(w) = \int_{a(t, \eta)}^{b(t, \eta)} G_1(t, \eta; \zeta, \vartheta) w(\vartheta) d\vartheta.$$

Using that the function $S'_0(t, \eta, \cdot)$ belongs to the one dimensional kernel of the differential operator $\tilde{\psi}_{SS}(S'_0) - \partial_\zeta^2$, that $g_1(t, \eta, \cdot) + \omega(t, \eta)$ is orthogonal to S'_0 , by definition of ω in (2.56), and that (3.1) yields a solution of the boundary value problem (2.51), (2.60), we see immediately from the definition of G_1 in (3.7) that

$$S_1(t, \eta, \zeta) = \mathcal{K}_{t, \eta}(g_1(t, \eta, \cdot) + \omega(t, \eta)) \quad (3.8)$$

is another solution of this boundary value problem. To see that the Green's function G_1 is symmetric with respect to ζ and ϑ , note that S'_0 belongs to the kernel of $\mathcal{K}_{t, \eta}$ and that the orthogonal space of S'_0 is mapped to itself by $\mathcal{K}_{t, \eta}$. Both properties follow from (3.7). Therefore, since S'_0 spans the kernel of the operator $\tilde{\psi}_{SS}(S_0) - \partial_\zeta^2$, it follows that $\mathcal{K}_{t, \eta}$ maps this kernel to $\{0\}$ and the orthogonal space of this kernel to itself. Using these properties and the fact that $\tilde{\psi}_{SS}(S_0) - \partial_\zeta^2$ is a symmetric differential operator, we can show by the usual method that

$$G_1(t, \eta; \zeta, \vartheta) = G_1(t, \eta; \vartheta, \zeta),$$

hence, from (3.3) and (3.6),

$$G_1(t, \eta; \zeta, a(t, \eta)) = G_1(t, \eta; a(t, \eta), \zeta) = 0, \quad (3.9)$$

$$G_1(t, \eta; \zeta, b(t, \eta)) = G_1(t, \eta; b(t, \eta), \zeta) = 0. \quad (3.10)$$

From the differentiability properties of G stated above, from $S_0 \in C^3(\Gamma[a, b])$ and from the definition of G_1 in (3.7) we see that $(t, \eta, \zeta, \vartheta) \mapsto G_1(t, \eta; \zeta, \vartheta)$ is two times continuously differentiable with bounded derivatives at all points $(t, \eta, \zeta, \vartheta)$ with $\zeta \neq \vartheta$.

Now let

$$\begin{aligned} g_2(t, \eta, \zeta) &= -\kappa_\Gamma S'_0(\zeta) + \partial_\xi \sigma_1(0)\zeta + \sigma_2(\zeta), \\ g_3(t, \eta, \zeta) &= -\frac{\partial_t S_0(\zeta) \varphi_\nu(t, \eta, \zeta)}{f'(n \cdot [\hat{C}]n) S'_0(\zeta)}, \end{aligned} \quad (3.11)$$

$$F_i(t, \eta, \zeta) = \int_a^b G_1(t, \eta; \zeta, \vartheta) g_i(t, \eta, \vartheta) d\vartheta, \quad i = 2, 3, \quad (3.12)$$

$$F_4(t, \eta, \zeta) = \int_a^b G_1(t, \eta; \zeta, \vartheta) d\vartheta \omega(t, \eta).$$

(2.52) and (3.8) imply that

$$g_1 = g_2 + g_3, \quad S_1 = \sum_{i=2}^4 F_i. \quad (3.13)$$

By inspection of the definition of σ_1 and σ_2 in (2.53) – (2.55), using the differentiability properties of v stated in Lemma 2.2, we see that the derivatives of g_2 with respect to (t, η) up to order 2 are continuous in $\Gamma[a, b]$. This implies that $F_2 \in C^2(\Gamma[a, b])$.

Noting the regularity of Γ stated in Assumption A, the definition of σ_2 in (2.54), (2.55) and the differentiability properties of S_0 and a, b stated in Theorem 2.3, we conclude from (2.84), (2.85) that ω belongs to $C^2(\Gamma)$. This yields that $F_4 \in C^2(\Gamma[a, b])$.

From (2.30) and from the regularity properties of \hat{T} required in Assumption A we see that $n \cdot [\hat{C}]n \in C^2(\Gamma)$. Since $\varphi_\nu \in C_0^\infty(\Gamma[a, b])$ and since by assumption f is three times

continuously differentiable, we conclude from the properties of S_0 stated in Theorem 2.3 that $g_3 \in C^2(\Gamma[a, b])$. This implies that $F_3 \in C^2(\Gamma[a, b])$.

From these results and from (3.13) we infer that $g_1, S_1 \in C^2(\Gamma[a, b])$. To finish the proof it remains to show that S_1 satisfies the estimates (2.77). Since F_2 and F_4 are bounded in the norm of $C^2(\Gamma[a, b])$, uniformly with respect to ν , it is seen from (3.13) that the inequalities (2.77) are implied by the estimates

$$|\partial_\zeta^i F_3| \leq C_1 \quad i = 0, \dots, 2, \quad (3.14)$$

$$|\partial_t F_3|, |\nabla_\eta F_3| \leq C_2, \quad (3.15)$$

$$|\nabla_\eta^2 F_3| \leq (|\ln \nu| + 1)C_3. \quad (3.16)$$

To prove these estimates we use Lemma 3.8 and the estimate

$$|G_1(t, \eta; \zeta, \vartheta)| \leq Cd, \quad (3.17)$$

where d denotes the distance of ϑ to the boundary of the interval $[a(t, \eta), b(t, \eta)]$, with the constant C independent of $(t, \eta, \zeta, \vartheta)$. This estimate follows from (3.9), (3.10) and the uniform boundedness of the derivatives $\partial_\vartheta G_1(t, \eta; \zeta, \vartheta)$ by application of the mean value theorem.

To verify (3.16) note that (3.12) yields

$$\begin{aligned} \nabla_\eta^2 F_3(t, \eta, \zeta) &= \int_a^b \nabla_\eta^2 G_1(t, \eta; \zeta, \vartheta) g_3(t, \eta, \vartheta) d\vartheta \\ &\quad + 2 \int_a^b \nabla_\eta G_1(t, \eta; \zeta, \vartheta) \otimes \nabla_\eta g_3(t, \eta, \vartheta) d\vartheta \\ &\quad + \int_a^b G_1(t, \eta; \zeta, \vartheta) \nabla_\eta^2 g_3(t, \eta, \vartheta) d\vartheta. \end{aligned} \quad (3.18)$$

Though the limits of integration a and b depend on (t, η) , no boundary terms appear in this formula, because by (3.11) the function g_3 vanishes in a neighborhood of the boundary of $\Gamma[a, b]$, since $\varphi_\nu \in C_0^\infty(\Gamma[a, b])$. We have that $|\nabla_\eta G_1|, |\nabla_\eta^2 G_1| \leq C_1$ and $|g_3| \leq K_0$. The latter estimate follows from (3.75) and from the assumption that $f'(r) \geq c_1 > 0$. From (3.17), (3.18), (3.90) and from the definition of $\Gamma_{k, \nu}[a, b]$ in (2.57) we thus obtain

$$\begin{aligned} |\nabla_\eta^2 F_3(t, \eta, \zeta)| &\leq \int_a^b C_1 K_1 d\vartheta \\ &\quad + 2 \int_{a+k\nu^{1/2}}^{b-k\nu^{1/2}} C_1 K_1 d^{-1} d\vartheta + 2 \left(\int_a^{a+k\nu^{1/2}} + \int_{b-k\nu^{1/2}}^b \right) C_1 K_1 \nu^{-1/2} d\vartheta \\ &\quad + \int_{a+k\nu^{1/2}}^{b-k\nu^{1/2}} CdK_1 d^{-2} d\vartheta + \left(\int_a^{a+k\nu^{1/2}} + \int_{b-k\nu^{1/2}}^b \right) CdK_1 d^{-1} \nu^{-1/2} d\vartheta \\ &\leq \hat{K}_1 + \hat{K}_2 |\ln(k\nu^{1/2})| + \hat{K}_3 + \hat{K}_4 |\ln(k\nu^{1/2})| + \hat{K}_5. \end{aligned}$$

(3.16) follows from this estimate. The proofs of (3.14) and (3.15) run along the same lines, but are simpler. We leave these proofs to the reader. \blacksquare

3.2 Proof of Theorem 2.5

With the definition of T_0 in (2.43) the differential equation (2.48) can be written in the form

$$\partial_\zeta (D(\varepsilon(\partial_\zeta u_0 \otimes n) - \bar{\varepsilon} S_0)) n = 0, \quad (3.19)$$

hence

$$(D(\varepsilon(\partial_\zeta u_0 \otimes n) - \bar{\varepsilon} S_0)) n = c_1,$$

where $c_1(t, \eta)$ is a constant of integration. By Lemma 2.1, the linear mapping $z \mapsto L_n(z) = (D\varepsilon(z \otimes n))n$ is invertible, whence

$$\partial_\zeta u_0 = L_n^{-1}((D\bar{\varepsilon})n S_0 + c_1),$$

and so

$$\partial_\zeta u_0 = u^* S_0 + c_2,$$

with $u^*(t, \eta)$ defined in (2.23) and with $c_2(t, \eta) = L_n^{-1}c_1(t, \eta)$. Consequently u_0 satisfies (3.19) and the equivalent equation (2.48) if and only if

$$u_0 = u^* S_0^{-1} + c_2 \zeta + c_3,$$

with arbitrary constants $c_2(t, \eta)$, $c_3(t, \eta)$ of integration. Since by condition (2.64) the function u_0 must vanish for $\zeta \leq a(t, \eta)$ and since $S_0^{(-1)}(\zeta) = 0$ for such ζ , we conclude that (2.64) holds for $\zeta \in (-\infty, a(t, \eta))$ if and only if $c_2 = c_3 = 0$, that is, if and only if u_0 is of the form given in (2.78). It remains to show that this u_0 satisfies the condition (2.64) for $\zeta \geq b(t, \eta)$. We use (2.62) and (2.72) to compute for $\zeta \geq b(t, \eta) = -a(t, \eta)$ that

$$\begin{aligned} S_0^{(-1)}(t, \eta, \zeta) &= \int_{-\infty}^{\zeta} S_0(t, \eta, \vartheta) d\vartheta = \int_{a(t, \eta)}^{b(t, \eta)} S_0(t, \eta, \vartheta) d\vartheta + \int_{b(t, \eta)}^{\zeta} d\vartheta \\ &= \int_{-b(t, \eta)}^{b(t, \eta)} \left(S_*(t, \eta, \vartheta) + \frac{1}{2} \right) d\vartheta + \zeta - b(t, \eta) = \zeta, \end{aligned} \quad (3.20)$$

since $S_*(t, \eta, \vartheta)$ is an odd function with respect to ϑ . This equation implies that u_0 from (2.78) satisfies (2.64) for $\zeta \in (b(t, \eta), \infty)$.

Next, with (2.44) we write (2.49) in the form

$$\partial_\zeta (D(\varepsilon(\partial_\zeta u_1 \otimes n + \nabla_\eta u_0) - \bar{\varepsilon} S_1)) n + \operatorname{div}_\eta T_0 = 0. \quad (3.21)$$

For the solution u_1 of this equation we make the ansatz (2.79). Using the equations

$$\begin{aligned} \partial_\zeta \nabla_\eta u_0 &= (\nabla_\eta u^*) S_0 + u^* \otimes \nabla_\eta S_0, \\ \operatorname{div}_\eta T_0 &= \operatorname{div}_\eta \left(D(\varepsilon(u^* \otimes n) - \bar{\varepsilon}) S_0 \right) \\ &= \operatorname{div}_\eta (D\varepsilon(u^* \otimes n)) S_0 + (D(\varepsilon(u^* \otimes n) - \bar{\varepsilon})) \nabla_\eta S_0, \end{aligned}$$

which follow from (2.78) and (2.43), we obtain by insertion of (2.78) and (2.79) into (3.21) that

$$\begin{aligned} \partial_\zeta \left(D(\varepsilon(u^* \otimes n) - \bar{\varepsilon}) n S_1 \right) + \left((D\varepsilon(u^* \otimes n + \nabla_\eta u^*)) n + \operatorname{div}_\eta (D\varepsilon(u^* \otimes n)) \right) S_0 \\ + (D\varepsilon(\partial_\zeta^2 u_{11} \otimes n + u^* \otimes \nabla_\eta S_0)) n + (D(\varepsilon(u^* \otimes n) - \bar{\varepsilon})) \nabla_\eta S_0 = 0. \end{aligned}$$

(2.23) and (2.24) show that the first and second term on the left hand side vanish. This implies that u_1 satisfies (2.49) if and only if u_{11} satisfies the differential equation

$$D\varepsilon(\partial_\zeta^2 u_{11} \otimes n)n = -(D\varepsilon(u^* \otimes \nabla_\eta S_0))n - \left(D(\varepsilon(u^* \otimes n) - \bar{\varepsilon})\right)\nabla_\eta S_0. \quad (3.22)$$

We apply the inverse L_n^{-1} to this equation and integrate twice to find

$$u_{11} = -L_n^{-1}\left((D\varepsilon(u^* \otimes \nabla_\eta S_0^{(-2)}))n + (D(\varepsilon(u^* \otimes n) - \bar{\varepsilon}))\nabla_\eta S_0^{(-2)}\right) + c_1\zeta + c_2, \quad (3.23)$$

where $c_1(t, \eta)$, $c_2(t, \eta)$ are constants of integration. u_1 must vanish in the region $\{(t, \eta, \zeta) \mid (t, \eta) \in \Gamma, \zeta \leq a(t, \eta)\}$, by condition (2.65). By (2.62), the functions S_0 and S_1 vanish in this region, whence also $S_i^{(-1)}$, $S_0^{(-2)}$ and $\nabla_\eta S_0^{(-2)}$ vanish there. Consequently, u_1 defined by (2.79) vanishes in this region if and only if u_{11} vanishes there, and this in turn holds if and only if we choose $c_1(t, \eta) = c_2(t, \eta) = 0$ in (3.23). This yields the form of u_{11} given in (2.80). It remains to show that the function u_1 defined by (2.79), (2.80) fulfills (2.65) for $\zeta \geq b(t, \eta)$. Using (3.20), we compute for these ζ that

$$S_0^{(-2)}(t, \eta, \zeta) = \int_{-\infty}^{b(t, \eta)} S_0^{(-1)}(t, \eta, \vartheta) d\vartheta + \int_{b(t, \eta)}^{\zeta} \vartheta d\vartheta = \frac{1}{2}\zeta^2 + c_3(t, \eta), \quad (3.24)$$

with

$$c_3(t, \eta) = \int_{a(t, \eta)}^{b(t, \eta)} S_0^{(-1)}(t, \eta, \vartheta) d\vartheta - \frac{1}{2}b(t, \eta)^2.$$

(3.24) implies

$$\nabla_\eta S_0^{(-2)}(t, \eta, \zeta) = \nabla_\eta c_3(t, \eta) = c_4(t, \eta),$$

for $\zeta \geq b(t, \eta)$. Insertion of this equation into (2.80) yields

$$u_{11}(t, \eta, \zeta) = c_5(t, \eta), \quad \text{for } \zeta \geq b(t, \eta), \quad (3.25)$$

with a suitable function c_5 . By definition $S_1(t, \eta, \zeta)$ vanishes for $|\zeta| \geq b(t, \eta)$, which yields

$$S_1^{(-1)}(t, \eta, \zeta) = \int_{-\infty}^{\zeta} S_1(t, \eta, \vartheta) d\vartheta = \int_{a(t, \eta)}^{b(t, \eta)} S_1(t, \eta, \vartheta) d\vartheta = c_6(t, \eta),$$

for $\zeta \geq b(t, \eta)$. Combination of this result with (2.79), (3.24) and (3.25) yields

$$u_1(t, \eta, \zeta) = \frac{1}{2}a^*\zeta^2 + c_+(t, \eta), \quad \text{for } \zeta \geq b(t, \eta),$$

with $c_+ = u^*c_6 + a^*c_3 + c_5$, which proves that (2.65) is satisfied for $\zeta \geq b(t, \eta)$. The proof of Theorem 2.5 is complete. \blacksquare

3.3 Proof of Theorem 2.7

To prove this theorem we compute asymptotic expansions for the terms $\text{div}_x T^\nu + \mathbf{b}$ and $\partial_t S^{(\nu)} + f(\psi_S - \nu \Delta_x S^{(\nu)})|\nabla_x S^{(\nu)}|$ in powers of $\nu^{1/2}$. The former expansion is computed in Section 3.3.1, the latter in Section 3.3.2. It will be seen that the leading terms in these expansions of first and second order vanish if T_0 , T_1 , S_0 and S_1 satisfy the differential equations (2.48) – (2.51). To complete the proof we show in Section 3.3.3 how the

inequalities (2.89) and (2.90) can be obtained by combining these expansions with some other estimates.

The results in the next two sections are derived in a sequence of lemmas. In the derivations we need some technical details, which we collect here. As always, we identify $(t, x) \in \mathcal{U}$ with $(t, \eta, \xi) \in \Gamma \times (-\delta, \delta)$ via the coordinate transformation (2.6). The parameter ν varies in the interval $(0, \nu_0]$ with $\nu_0 > 0$ chosen small enough small such that the set $\Gamma[\nu_0]$ is contained in the neighborhood of Γ where ϕ has the constant value 1. We set $\zeta = \xi/\nu^{1/2}$. Though we have $|\xi| < \delta$, the value $|\zeta|$ can be large for sufficiently small values of ν . However, if $(t, x) = (t, \eta, \xi) \in \Gamma[\nu]$, then we have $(t, \eta, \zeta) \in \Gamma[a, b]$ with $\Gamma[a, b]$ defined in (2.61). Such (t, η, ξ) and (t, η, ζ) satisfy the estimates

$$|\xi| \leq \nu^{1/2}b(t, \eta) \leq \nu^{1/2}C, \quad |\zeta| \leq b(t, \eta) \leq C, \quad (3.26)$$

with a suitable constant C independent of t, η, ν . Here we used that by the assumptions of Theorem 2.7 the potential ψ satisfies (2.71), whence $a(t, \eta) = -b(t, \eta)$.

Note that by (2.17) we have for $x \in \Gamma_\xi(t)$ that

$$\nabla_{\Gamma_\xi} W(t, x) = (\nabla_\eta W(t, \eta, \xi))A(t, \eta, \xi), \quad (3.27)$$

where $A(t, \eta, \xi) \in \mathbb{R}^{3 \times 3}$ is the inverse of the linear mapping $(I + \xi \nabla_\eta n(t, \eta)) : \mathbb{R}^3 \rightarrow \mathbb{R}^3$. From the mean value theorem we obtain the expansion

$$A(t, \eta, \xi) = I + \xi \hat{R}_A(t, \eta, \xi) = I + \nu^{1/2}R_A(t, \eta, \xi, \xi/\nu^{1/2}), \quad (3.28)$$

with the remainder term

$$R_A(t, \eta, \xi, \zeta) = \zeta \hat{R}_A(t, \eta, \xi),$$

which is bounded when (t, η, ξ) varies in $\Gamma[\nu]$, with a bound independent of ν . Insertion into (3.27) yields

$$\nabla_{\Gamma_\xi} W(t, x) = \nabla_\eta W(t, \eta, \xi) \left(I + \nu^{1/2}R_A(t, \eta, \xi, \frac{\xi}{\nu^{1/2}}) \right). \quad (3.29)$$

For $w : \mathcal{U} \rightarrow \mathbb{R}$ we consider $\nabla_{\Gamma_\xi} w$ and $\nabla_\eta w$ to be column vectors. For such w the equation corresponding to (3.29) is therefore

$$\nabla_{\Gamma_\xi} w(t, x) = A^T(t, \eta, \xi) \nabla_\eta w(t, \eta, \xi) = \left(I + \nu^{1/2}R_A^T(t, \eta, \xi, \frac{\xi}{\nu^{1/2}}) \right) \nabla_\eta w(t, \eta, \xi). \quad (3.30)$$

Furthermore, (2.9), (3.29) and (2.15) together yield for $W : \mathcal{U} \rightarrow \mathbb{R}^3$ that

$$\operatorname{div}_{\Gamma_\xi} W = \sum_{i=1}^2 \tau_i \cdot (\nabla_\eta W) (I + \nu^{1/2}R_A) \tau_i = \operatorname{div}_\eta W + \nu^{1/2} \operatorname{div}_{\Gamma, \xi} W, \quad (3.31)$$

with the remainder term

$$\operatorname{div}_{\Gamma, \xi} W(t, \eta, \xi) = \sum_{i, j=1}^2 \tau_i \cdot (\nabla_\eta W_{t, \xi}) R_A \tau_i, \quad (3.32)$$

and this equation implies for $\hat{W} : \mathcal{U} \rightarrow \mathbb{R}^{3 \times 3}$ with $\operatorname{div}_{\Gamma, \xi} \hat{W} = \sum_{i, j=1}^2 (\partial_{\tau_j} \hat{W}_{t, \xi}) \tau_i (\tau_j \cdot R_A \tau_i)$ that

$$\operatorname{div}_{\Gamma_\xi} \hat{W}(t, \eta, \xi) = \operatorname{div}_\eta \hat{W} + \nu^{1/2} \operatorname{div}_{\Gamma, \xi} \hat{W}. \quad (3.33)$$

The terms $\operatorname{div}_{\Gamma, \xi} W$ and $\operatorname{div}_{\Gamma, \xi} \hat{W}$ are bounded when (t, η, ξ) varies in $\Gamma[\nu]$ with a bound independent of ν .

3.3.1 Asymptotic expansion of $\operatorname{div}_x T^{(\nu)} + \mathbf{b}$

Lemma 3.1 *Assume that $(u^{(\nu)}, T^{(\nu)}, S^{(\nu)})$ is given by (2.37) – (2.39) and that T_0, T_1 are defined by (2.43), (2.44). Then in the neighborhood of Γ where $\phi = 1$ we have*

$$T^{(\nu)}(t, x) = T_0 + \nu^{1/2}T_1 + \nu D\varepsilon((\nabla_\eta u_0)R_A + \nabla_{\Gamma_\xi} u_1) + D\varepsilon(\nabla_x v), \quad (3.34)$$

$$\begin{aligned} \operatorname{div}_x T^{(\nu)}(t, x) &= \nu^{-1/2}(\partial_\zeta T_0)n + ((\partial_\zeta T_1)n + \operatorname{div}_\eta T_0) \\ &\quad + \nu^{1/2}(\operatorname{div}_{\Gamma_\xi} T_0 + \operatorname{div}_{\Gamma_\xi} T_1) + \nu \operatorname{div}_x D\varepsilon((\nabla_\eta u_0)R_A + \nabla_{\Gamma_\xi} u_1) \\ &\quad + \operatorname{div}_x D\varepsilon(\nabla_x v), \end{aligned} \quad (3.35)$$

where $n(t, x) = n(t, \eta)$ is the unit normal vector to $\Gamma(t)$, where R_A is the matrix function from (3.28), and where $\operatorname{div}_{\Gamma_\xi}$ is the differential operator from (3.32). The argument of the functions u_0, u_1, T_0 and T_1 is $(t, \eta, \frac{\xi}{\nu^{1/2}})$.

Proof: We insert (2.37) and (2.38) into (2.39) and obtain with the decomposition (2.11) of the gradient that

$$\begin{aligned} T^{(\nu)} &= D\left(\varepsilon(\nu^{1/2}\nabla_x u_0 + \nu\nabla_x u_1 + \nabla_x v) - \bar{\varepsilon}(S_0 + \nu^{1/2}S_1)\right) \\ &= D\left(\varepsilon(\partial_\zeta u_0 \otimes n + \nu^{1/2}\nabla_{\Gamma_\xi} u_0 + \nu^{1/2}\partial_\zeta u_1 \otimes n + \nu\nabla_{\Gamma_\xi} u_1) - \bar{\varepsilon}S_0 - \nu^{1/2}\bar{\varepsilon}S_1\right) \\ &\quad + D\varepsilon(\nabla_x v) \\ &= D\left(\varepsilon(\partial_\zeta u_0 \otimes n) - \bar{\varepsilon}S_0\right) + \nu^{1/2}D\left(\varepsilon(\partial_\zeta u_1 \otimes n + \nabla_\eta u_0(I + \nu^{1/2}R_A)) - \bar{\varepsilon}S_1\right) \\ &\quad + \nu D\varepsilon(\nabla_{\Gamma_\xi} u_1) + D\varepsilon(\nabla_x v). \end{aligned}$$

To get the last equality sign we used (3.29). Combination of this equation with (2.43), (2.44) yields (3.34).

From (3.34) and (2.12) we obtain

$$\begin{aligned} \operatorname{div}_x T^{(\nu)} &= \nu^{-1/2}(\partial_\zeta T_0)n + (\partial_\zeta T_1)n + \operatorname{div}_{\Gamma_\xi} T_0 + \nu^{1/2}\operatorname{div}_{\Gamma_\xi} T_1 \\ &\quad + \nu \operatorname{div}_x D\varepsilon((\nabla_\eta u_0)R_A + \nabla_{\Gamma_\xi} u_1) + \operatorname{div}_x D\varepsilon(\nabla_x v). \end{aligned}$$

This equation and (3.33) together imply (3.35). ■

From the regularity requirements for \hat{T} in Assumption A and from (2.1) we conclude that \mathbf{b} is continuously differentiable on γ' with bounded derivatives. Since by Lemma 2.2 the function v is continuously differentiable on Q , we thus obtain from (2.35) by the mean value theorem that

$$\operatorname{div}_x D\varepsilon(\nabla_x v) + \mathbf{b} = \xi \hat{R}_v(t, \eta, \xi), = \nu^{1/2}R_v(t, \eta, \xi, \xi/\nu^{1/2}), \quad (3.36)$$

where

$$R_v(t, \eta, \xi, \zeta) = \zeta \hat{R}_v(t, \eta, \xi). \quad (3.37)$$

The remainder term \hat{R}_v is bounded on the neighborhood \mathcal{U} of Γ and vanishes for $\xi < 0$.

Corollary 3.2 *If u_0, u_1, S_0, S_1 are such that the functions T_0 and T_1 defined by (2.43), (2.44) satisfy the differential equations (2.48), (2.49), then we have for $(t, \eta, \xi) \in \Gamma[\nu]$*

$$(\operatorname{div}_x T^{(\nu)} + \mathbf{b})(t, \eta, \xi) = \nu^{1/2}R_{\operatorname{div}+\mathbf{b}}(\nu, u_0, u_1, T_0, T_1, t, \eta, \xi), \quad (3.38)$$

where

$$R_{\text{div}+\mathbf{b}} = \text{div}_{\Gamma,\xi} T_0 + \text{div}_{\Gamma,\xi} T_1 + \nu^{1/2} \text{div}_x D\varepsilon((\nabla_\eta u_0)R_A + \nabla_{\Gamma_\xi} u_1) + R_v, \quad (3.39)$$

with the function R_v from (3.37).

Proof: Since $\Gamma[\nu]$ is contained in the neighborhood of Γ where ϕ has the constant value 1, we obtain from (3.35) and (2.48), (2.49) for $(t, \eta, \xi) \in \Gamma[\nu]$ that

$$\begin{aligned} \text{div}_x T^{(\nu)} + \mathbf{b} &= \nu^{1/2} \left(\text{div}_{\Gamma,\xi} T_0 + \text{div}_{\Gamma,\xi} T_1 + \nu^{1/2} \text{div}_x D\varepsilon((\nabla_\eta u_0)R_A + \nabla_{\Gamma_\xi} u_1) \right) \\ &\quad + \text{div}_x D\varepsilon(\nabla_x v) + \mathbf{b}. \end{aligned}$$

Insertion of (3.36) into this equation yields (3.38). ■

3.3.2 Asymptotic expansion of $\partial_t S^{(\nu)} + f(\psi_S - \nu \Delta_x S^{(\nu)}) |\nabla_x S^{(\nu)}|$

Our next goal is to compute an asymptotic expansion in terms of $\nu^{1/2}$ for the term

$$\partial_t S^{(\nu)} + f(\psi_S(\varepsilon(\nabla_x u^{(\nu)}), S^{(\nu)}) - \nu \Delta_x S^{(\nu)}) |\nabla_x S^{(\nu)}| \quad (3.40)$$

on the left hand side of (2.90). The expansion is valid in the region $\Gamma[\nu]$. As will be seen, the leading terms in this expansion of first and second order vanish if S_0 and S_1 satisfy the differential equations (2.50) and (2.51), provided that the normal speed s of the sharp interface Γ satisfies the kinetic relation (2.3).

In the first lemma we compute the expression obtained by insertion of (2.37) – (2.39) into the partial derivative $\psi_S = \partial_S \psi$ of the free energy. This expression shows how this partial derivative is connected to the jump of the Eshelby tensor across the sharp interface Γ .

Lemma 3.3 (i) Let T_0, T_1 be defined by (2.43), (2.44). Then the differential equations (2.48), (2.49) and the conditions (2.64), (2.65) imply

$$T_0 = D(\varepsilon(u^* \otimes n) - \bar{\varepsilon}) S_0, \quad (3.41)$$

$$\begin{aligned} T_1 &= D(\varepsilon(u^* \otimes n) - \bar{\varepsilon}) S_1 + D\varepsilon(a^* \otimes n + \nabla_\eta u^*) S_0^{(-1)} \\ &\quad + D\varepsilon(\partial_\zeta u_{11} \otimes n + u^* \otimes \nabla_\eta S_0^{(-1)}). \end{aligned} \quad (3.42)$$

(ii) Let $S^{(\nu)}$ and $T^{(\nu)}$ be defined by (2.38), (2.39). Then we have for all $(t, x) = (t, \eta, \xi)$ from the neighborhood of Γ where $\phi = 1$ that

$$\bar{\varepsilon} : T^{(\nu)}(t, x) = \bar{\varepsilon} : [\hat{T}] S^{(\nu)} + \sigma_1 + \nu^{1/2} \sigma_2 + \nu \sigma_3, \quad (3.43)$$

where $\sigma_1(t, \eta, \xi)$ and $\sigma_2(t, \eta, \frac{\xi}{\nu^{1/2}})$ are defined in (2.53), (2.54) and where

$$\sigma_3(t, \eta, \xi, \xi/\nu^{1/2}) = \bar{\varepsilon} : D\varepsilon((\nabla_\eta u_0)R_A + \nabla_{\Gamma_\xi} u_1). \quad (3.44)$$

Here R_A is the remainder term from (3.28).

(iii) With the notation introduced in (1.13) we have

$$\sigma_1(t, \eta, 0) = \bar{\varepsilon} : \hat{T}^{(-)}(t, \eta). \quad (3.45)$$

(iv) For the effective potential $\tilde{\psi}$ defined in (2.47) we have in the neighborhood of Γ where $\phi = 1$ that

$$\psi_S(\varepsilon(\nabla_x u^{(\nu)}), S^{(\nu)}) = \tilde{\psi}_S(t, \eta, S^{(\nu)}) + n \cdot [\hat{C}]n - \bar{\sigma}_1 - \nu^{1/2}\sigma_2 - \nu\sigma_3, \quad (3.46)$$

with $\bar{\sigma}_1(t, \eta, \xi) = \sigma_1(t, \eta, \xi) - \sigma_1(t, \eta, 0)$.

Proof: (3.41) and (3.42) are obtained by insertion of (2.78), (2.79) into (2.43), (2.44). To obtain (3.43) we multiply (3.34) by $\bar{\varepsilon}$, insert (3.41), (3.42) into the resulting equation and note the second equation in (2.22). To verify (3.45) note that by the definition of v in (2.21) we have $\hat{T} = D\varepsilon(\nabla_x v)$ on γ . This equation and the definition of σ_1 in (2.53) together imply (3.45), since v is continuously differentiable on Q , by Lemma 2.2.

To prove (3.46) we insert (3.43) into (1.8) to obtain

$$\begin{aligned} \psi_S(\varepsilon(\nabla_x u^{(\nu)}), S^{(\nu)}) &= \hat{\psi}'(S^{(\nu)}) - \bar{\varepsilon} : T^{(\nu)} \\ &= \hat{\psi}'(S^{(\nu)}) - \bar{\varepsilon} : [\hat{T}]S^{(\nu)} - \sigma_1 - \nu^{1/2}\sigma_2 - \nu\sigma_3 \\ &= \tilde{\psi}_S(t, \eta, S^{(\nu)}) - \frac{1}{2}\bar{\varepsilon} : [\hat{T}] + [\hat{\psi}] - \sigma_1 - \nu^{1/2}\sigma_2 - \nu\sigma_3. \end{aligned} \quad (3.47)$$

In the last equality we used (2.47). Now, (3.45) and (2.30) imply

$$\begin{aligned} -\frac{1}{2}\bar{\varepsilon} : [\hat{T}] + [\hat{\psi}] - \sigma_1 &= -\frac{1}{2}\bar{\varepsilon} : (\hat{T}^{(+)} - \hat{T}^{(-)}) + [\hat{\psi}] - \bar{\sigma}_1 - \bar{\varepsilon} : \hat{T}^{(-)} \\ &= [\hat{\psi}] - \bar{\varepsilon} : \langle \hat{T} \rangle - \bar{\sigma}_1 = n \cdot [\hat{C}]n - \bar{\sigma}_1, \end{aligned}$$

Insertion of this equation into (3.47) yields (3.46). \blacksquare

We next compute an asymptotic expansion for $\psi_S - \nu\Delta_x S^{(\nu)}$ in terms of $\nu^{1/2}$, which is valid on the domain $\Gamma[\nu]$. To simplify the notation we drop the arguments t and η in most of the following equations. As usual, we set $\zeta = \frac{\xi}{\nu^{1/2}}$.

To expand ψ_S we use (3.46). Since we have $\phi = 1$ in the domain $\Gamma[\nu]$, Taylor's formula and the definition of $S^{(\nu)}$ in (2.38) yield for the first term on the right hand side of (3.46) that

$$\tilde{\psi}_S(S^{(\nu)}) = \tilde{\psi}_S(S_0) + \tilde{\psi}_{SS}(S_0)\nu^{1/2}S_1 + \nu R_{\tilde{\psi}}(\nu, S_0, S_1). \quad (3.48)$$

To treat the third term in (3.46) note that $\xi \mapsto \sigma_1(\xi) \in C^1([-\delta, \delta]) \cap C^2([-\delta, 0]) \cap C^2((0, \delta])$, by definition of the function σ_1 in (2.53) and by the regularity properties of v given in Lemma 2.2. Since $\bar{\sigma}_1(0) = 0$, we thus obtain from Taylor's formula that

$$\bar{\sigma}_1(\xi) = (\partial_\xi \sigma_1(0))\xi + \sigma_1^*(\xi)\xi^2 = \nu^{1/2}(\partial_\xi \sigma_1(0))\frac{\xi}{\nu^{1/2}} + \nu R_{\sigma_1}(\xi) \left(\frac{\xi}{\nu^{1/2}} \right)^2. \quad (3.49)$$

To compute the expansion of $\nu\Delta_x S^{(\nu)}$ note that we have

$$\Delta_x S^{(\nu)}(x, t) = \partial_\xi^2 S^{(\nu)}(t, \eta, \xi) - \kappa(t, \eta, \xi) \partial_\xi S^{(\nu)}(t, \eta, \xi) + \Delta_{\Gamma_\xi} S^{(\nu)}(t, \eta, \xi), \quad (3.50)$$

with twice the mean curvature $\kappa(t, \eta, \xi)$ of the surface $\Gamma_\xi(t)$ and with the surface Laplacian $\Delta_{\Gamma_\xi} = \text{div}_{\Gamma_\xi} \nabla_{\Gamma_\xi}$. The mean value theorem yields

$$\kappa(t, \eta, \xi) = \kappa_\Gamma + \kappa^*(\xi)\xi = \kappa_\Gamma + \nu^{1/2}\kappa^*(\xi)\frac{\xi}{\nu^{1/2}}. \quad (3.51)$$

With the notations $S'_0 = \partial_\zeta S_0$ and $S''_0 = \partial_\zeta^2 S_0$ we thus obtain from (3.50), (3.51) and (2.38) that

$$\nu \Delta_x S^{(\nu)} = S''_0 \left(\frac{\xi}{\nu^{1/2}} \right) + \nu^{1/2} \left(S''_1 \left(\frac{\xi}{\nu^{1/2}} \right) - \kappa_\Gamma S'_0 \left(\frac{\xi}{\nu^{1/2}} \right) \right) + \nu R_\Delta \left(\nu, \xi, \frac{\xi}{\nu^{1/2}} \right), \quad (3.52)$$

where

$$|R_\Delta| = \left| -\kappa_\Gamma S'_1 - \left(\frac{\xi}{\nu^{1/2}} \right) \kappa^* S'_0 + \Delta_{\Gamma_\xi} S_0 + \nu^{1/2} \left(\Delta_{\Gamma_\xi} S_1 - \left(\frac{\xi}{\nu^{1/2}} \right) \kappa^* S'_1 \right) \right| \leq K. \quad (3.53)$$

K is independent of $\nu \in (0, \nu_0]$ and of $(t, \eta, \xi) \in \Gamma[\nu]$. This follows from (3.26), which implies $|\frac{\xi}{\nu^{1/2}}| \leq C$, from $S_0 \in C^3(\Gamma[a, b])$ and from the estimates (2.77). In particular, (2.77) yields

$$|\nu^{1/2} \Delta_{\Gamma_\xi} S_1| \leq \nu^{1/2} (|\ln \nu| + 1) C_1 \leq C_2.$$

We insert (3.48) and (3.49) into (3.46) and combine the result with (3.52). This yields the asymptotic expansion

$$\begin{aligned} & \psi_S(\varepsilon(\nabla_x u^{(\nu)}), S^{(\nu)}) - \nu \Delta_x S^{(\nu)} \\ &= \left(\tilde{\psi}_S(S_0) - S''_0 + n \cdot [\hat{C}]n \right) \\ & \quad + \nu^{1/2} \left(\tilde{\psi}_{SS}(S_0) S_1 - S''_1 + \kappa_\Gamma S'_0 - (\partial_\xi \sigma_1(0)) \zeta - \sigma_2 \right) \\ & \quad + \nu R_{\psi_S - \nu \Delta}(\nu, t, \eta, \nu^{1/2} \zeta, \zeta), \end{aligned} \quad (3.54)$$

with the remainder

$$R_{\psi_S - \nu \Delta}(\nu, t, \eta, \nu^{1/2} \zeta, \zeta) = R_{\tilde{\psi}} - R_{\sigma_1} \zeta^2 - \sigma_3 - R_\Delta. \quad (3.55)$$

Here the argument of the functions $(n \cdot [\hat{C}]n)$, κ_Γ and $\partial_\xi \sigma_1(0)$ is (t, η) , the argument of S_0, S_1, σ_2 is (t, η, ζ) and the argument of $\tilde{\psi}$ is (t, η, S_0) .

Corollary 3.4 *If S_0 satisfies the differential equation (2.50) and if f belongs to $C^2(\mathbb{R})$, then the asymptotic expansion*

$$\begin{aligned} & f\left(\psi_S(\varepsilon(\nabla_x u^{(\nu)}), S^{(\nu)}) - \nu \Delta_x S^{(\nu)}\right) \\ &= f(n \cdot [\hat{C}]n) \\ & \quad + \nu^{1/2} f'(n \cdot [\hat{C}]n) \left(\tilde{\psi}_{SS}(S_0) S_1 - S''_1 + \kappa_\Gamma S'_0 - (\partial_\xi \sigma_1(0)) \zeta - \sigma_2 \right) \\ & \quad + \nu R_f(\nu, t, \eta, \nu^{1/2} \zeta, \zeta), \end{aligned} \quad (3.56)$$

is valid in the set $\Gamma[\nu]$. The remainder term satisfies the inequality

$$|R_f(\nu, t, \eta, \nu^{1/2} \zeta, \zeta)| \leq K, \quad (3.57)$$

with a constant K , which is independent of $(\nu, t, \eta, \zeta) \in (0, \nu_0] \times \Gamma[a, b]$.

Proof: For brevity we use the notation

$$(\dots) = \left(\tilde{\psi}_{SS}(S_0) S_1 - S''_1 + \kappa_\Gamma S'_0 - (\partial_\xi \sigma_1(0)) \zeta - \sigma_2 \right). \quad (3.58)$$

If S_0 satisfies (2.50), then the right hand side of (3.54) reduces to $n \cdot [\hat{C}]n + \nu^{1/2}(\dots) + \nu R_{\psi_S - \nu\Delta}$. Whence, Taylor's theorem applied to the function f yields

$$\begin{aligned} f\left(\psi_S(\varepsilon(\nabla_x u^{(\nu)}), S^{(\nu)}) - \nu\Delta_x S^{(\nu)}\right) &= f(n \cdot [\hat{C}]n) \\ &+ f'(n \cdot [\hat{C}]n)(\nu^{1/2}(\dots) + \nu R_{\psi_S - \nu\Delta}) + \frac{1}{2}f''(\vartheta)(\nu^{1/2}(\dots) + \nu R_{\psi_S - \nu\Delta})^2, \end{aligned}$$

where $\vartheta(t, \eta, \zeta)$ is a suitable number between $n \cdot [\hat{C}]n$ and $n \cdot [\hat{C}]n + \nu^{1/2}(\dots) + \nu R_{\psi_S - \nu\Delta}$. This yields (3.56) with the remainder term

$$R_f = f'(n \cdot [\hat{C}]n) R_{\psi_S - \nu\Delta} + \frac{1}{2}f''(\vartheta)((\dots) + \nu^{1/2}R_{\psi_S - \nu\Delta})^2.$$

This equation shows that (3.57) holds if $R_{\psi_S - \nu\Delta}$ is bounded on the set $(0, \nu_0] \times \Gamma[a, b]$. By inspection we see that the terms $R_{\tilde{\psi}}$, $R_{\sigma_1}\zeta^2$ and σ_3 on the right hand side of (3.55) are bounded on $(0, \nu_0] \times \Gamma[a, b]$. Consequently, also $R_{\psi_S - \nu\Delta}$ is bounded on this set, by (3.55) and (3.53). \blacksquare

The leading term $f(n \cdot [\hat{C}]n$ in the asymptotic expansion (3.56) is independent of ξ and is therefore constant in the region $\Gamma[\nu]$ on all lines normal to the interface Γ . It will be seen in the following that this property makes it possible that the leading terms of asymptotic expansions of the two terms $\partial_t S^{(\nu)}$ and $f(\psi_S - \nu\Delta_x S^{(\nu)})|\nabla_x S^{(\nu)}|$ in the expression (3.40) add up to zero if the normal speed of the interface Γ is chosen suitably.

Lemma 3.5 *With the normal velocity $s(t, \eta)$ of the phase interface $\Gamma(t)$ at $\eta \in \Gamma(t)$ we have for $x = \eta + n(t, \eta)\xi$ that*

$$\partial_t S^{(\nu)}(t, x) = S_t^{(\nu)}(t, \eta, \xi) - \xi \partial_t n(t, \eta) \cdot \nabla_\eta S^{(\nu)}(t, \eta, \xi) - s(t, \eta) \partial_\xi S^{(\nu)}(t, \eta, \xi). \quad (3.59)$$

Proof: The chain rule yields

$$\partial_t S^{(\nu)}(t, x) = S_t^{(\nu)}(t, \eta, \xi) + \partial_t \eta(t, x) \cdot \nabla_\eta S^{(\nu)}(t, \eta, \xi) + \partial_t \xi(t, x) \partial_\xi S^{(\nu)}(t, \eta, \xi). \quad (3.60)$$

To determine the coefficients $\partial_t \eta$ and $\partial_t \xi$ note that

$$0 = \partial_t x = n \partial_t \xi + \xi \partial_t n + \partial_t \eta. \quad (3.61)$$

From $0 = \partial_t 1 = \partial_t |n|^2 = 2n \cdot \partial_t n$ we see that $\partial_t n$ is tangential to $\Gamma(t)$, whence (3.61) shows that $-n \partial_t \xi$ is the component of $\partial_t \eta$ normal to the surface $\Gamma(t)$ and $-\xi \partial_t n$ is the component tangential to this surface. Since by (2.14) and (2.7) the gradient $\nabla_\eta S^{(\nu)}$ is a tangential vector to $\Gamma(t)$, we infer from (3.61) that

$$\partial_t \eta \cdot \nabla_\eta S^{(\nu)} = -\xi \partial_t n \cdot \nabla_\eta S^{(\nu)} \quad (3.62)$$

and that

$$\partial_t \xi = -n \cdot \partial_t \eta.$$

From this equation, from $|x - \eta| = \text{dist}(x, \Gamma(t))$ and from the definition of the normal speed we obtain

$$\begin{aligned} s &= -\text{sign}(\xi) \frac{d}{dt} \text{dist}(x, \Gamma(t)) = -\text{sign}(\xi) \frac{\partial}{\partial t} |x - \eta| \\ &= \text{sign}(\xi) \frac{(x - \eta) \cdot \partial_t \eta}{|x - \eta|} = \text{sign}(\xi) \frac{\xi n \cdot \partial_t \eta}{|\xi|} = n \cdot \partial_t \eta = -\partial_t \xi. \end{aligned} \quad (3.63)$$

The statement of the lemma follows by insertion of this equation and of the equation (3.62) into (3.60). \blacksquare

We can now derive the asymptotic expansion for the expression in (3.40), which we write in a short form dropping the argument $(\varepsilon(\nabla_x u^{(\nu)}), S^{(\nu)})$ of ψ_S . Using again the notation (3.58), we obtain from Corollary 3.4, Lemma 3.5 and from the definition of $S^{(\nu)}$ in (2.38), after insertion of $\xi \partial_t n \cdot \nabla_\eta S^{(\nu)} = \nu^{1/2} \zeta \partial_t n \cdot \nabla_\eta S^{(\nu)}$ into (3.59), that

$$\begin{aligned}
& \partial_t S^{(\nu)} + f(\psi_S - \nu \Delta_x S^{(\nu)}) |\nabla_x S^{(\nu)}| \\
&= \partial_t S^{(\nu)} + f(\psi_S - \nu \Delta_x S^{(\nu)}) \left(\partial_\xi S^{(\nu)} + (|\nabla_x S^{(\nu)}| - \partial_\xi S^{(\nu)}) \right) \\
&= -s \partial_\xi S^{(\nu)} - \nu^{1/2} \zeta \partial_t n \cdot \nabla_\eta S^{(\nu)} + S_t^{(\nu)} \\
&\quad + \left(f(n \cdot [\hat{C}]n) + \nu^{1/2} f'(n \cdot [\hat{C}]n) (\dots) + \nu R_f \right) \partial_\xi S^{(\nu)} \\
&\quad + f(\psi_S - \nu \Delta_x S^{(\nu)}) (|\nabla_x S^{(\nu)}| - \partial_\xi S^{(\nu)}) \\
&= \left(-s + f(n \cdot [\hat{C}]n) \right) \partial_\xi S^{(\nu)} \\
&\quad + S_{0,t} + \nu^{1/2} f'(n \cdot [\hat{C}]n) (\dots) \partial_\xi S^{(\nu)} \\
&\quad + \nu^{1/2} (S_{1,t} - \zeta \partial_t n \cdot \nabla_\eta S^{(\nu)}) \\
&\quad + \nu R_f \partial_\xi S^{(\nu)} + f(\psi_S - \nu \Delta_x S^{(\nu)}) (|\nabla_x S^{(\nu)}| - \partial_\xi S^{(\nu)}) \\
&= \left(-s + f(n \cdot [\hat{C}]n) + \nu^{1/2} f'(n \cdot [\hat{C}]n) \left(\frac{S_{0,t}}{f'(n \cdot [\hat{C}]n) S'_0} + (\dots) \right) \right) \partial_\xi S^{(\nu)} \\
&\quad + \nu^{1/2} \left(S_{1,t} - \zeta \partial_t n \cdot \nabla_\eta S^{(\nu)} - \frac{S_{0,t}}{S'_0} S'_1 \right) \\
&\quad + \nu R_f \partial_\xi S^{(\nu)} + f(\psi_S - \nu \Delta_x S^{(\nu)}) (|\nabla_x S^{(\nu)}| - \partial_\xi S^{(\nu)}), \tag{3.64}
\end{aligned}$$

where we write $S_{i,t} = \partial_t S_i(t, \eta, \zeta)|_{\zeta=\xi/\nu^{1/2}}$ and employ the notation $S'_i = \partial_\zeta S_i$, as usual. To get the last equality we used that by (2.38)

$$\partial_\xi S^{(\nu)} = \nu^{-1/2} S'_0 + S'_1. \tag{3.65}$$

Corollary 3.6 *Assume that f satisfies the conditions of Theorem 2.7, that u_0, u_1 are given by (2.78) – (2.80) and that S_0, S_1 satisfy the differential equations (2.50), (2.51) with g_1 and ω given by (2.52) – (2.56). Suppose that the normal velocity s satisfies (2.3) with ω_1 and B given in (2.82) and (2.83). Then the equation*

$$\begin{aligned}
& \partial_t S^{(\nu)} + f(\psi_S - \nu \Delta_x S^{(\nu)}) |\nabla_x S^{(\nu)}| \\
&= \nu \omega^2 R_f \partial_\xi S^{(\nu)} \\
&\quad + \nu^{1/2} \left(S_{1,t} - \zeta \partial_t n \cdot \nabla_\eta S^{(\nu)} - \frac{S_{0,t}}{S'_0} S'_1 \right) \\
&\quad + \nu R_f \partial_\xi S^{(\nu)} + f(\psi_S - \nu \Delta_x S^{(\nu)}) (|\nabla_x S^{(\nu)}| - \partial_\xi S^{(\nu)}), \tag{3.66}
\end{aligned}$$

holds on $\Gamma_k[\nu]$, where

$$R_{f'}(\nu, t, \eta) = \frac{1}{\nu^{1/2}\omega} \left(f'(n \cdot [\hat{C}]n) - f'(n \cdot [\hat{C}]n + \vartheta\nu^{1/2}\omega) \right),$$

with a suitable function $\vartheta : \Gamma \rightarrow (0, 1)$. With the local Lipschitz constant \mathcal{L} of f' we have for all $\nu \in (0, \nu_0]$ and all $(t, \eta) \in \Gamma$ that

$$|R_{f'}(\nu, t, \eta)| \leq \mathcal{L}. \quad (3.67)$$

Proof: Since $\varphi_\nu(t, \eta, \zeta) = 1$ for $(t, \eta, \zeta) \in \Gamma_{k,\nu}[a, b]$, by (2.58), it follows from the definition of (...) in (3.58) and from (2.51), (2.52) that for such (t, η, ζ)

$$\left(\frac{S_{0,t}}{f'(n \cdot [\hat{C}]n) S'_0} + (\dots) \right) (t, \eta, \zeta) = (\tilde{\psi}_{SS}(S_0)S_1 - S''_1 - g_1)(t, \eta, \zeta) = \omega(t, \eta).$$

Thus, by the mean value theorem the first term on the right hand side of (3.64) is equal to

$$\left(-s + f(n \cdot [\hat{C}]n + \nu^{1/2}\omega) + \nu^{1/2}\omega \left(f'(n \cdot [\hat{C}]n) - f'(n \cdot [\hat{C}]n + \vartheta\nu^{1/2}\omega) \right) \right) \partial_\xi S^{(\nu)}. \quad (3.68)$$

Since ω satisfies (2.81) and s satisfies (2.3), we obtain $-s + f(n \cdot [\hat{C}]n + \nu^{1/2}\omega) = 0$. Insertion of this equation into (3.68) shows that (3.64) reduces to (3.66). By assumption, f belongs to $C^3(\mathbb{R})$, hence f' is locally Lipschitz continuous. The estimate (3.67) is obvious from this Lipschitz continuity of f' . \blacksquare

3.3.3 End of the proof of Theorem 2.7

To prove (2.89), note first that there is a constant K_1 such that the term $R_{\text{div}+b}$ defined in (3.39) satisfies for all $0 < \nu \leq \nu_0$ and $(t, \eta, \xi) \in \Gamma[\nu]$

$$|R_{\text{div}+b}(\nu, t, \eta, \xi)| \leq K_1. \quad (3.69)$$

To see this, we observe that the operators ∇_{Γ_ξ} , div_{Γ_ξ} and $\text{div}_{\Gamma,\xi}$ all are bounded functions of the operator ∇_η and thus do not contain derivatives with respect to ξ , which is shown by the definitions (2.13) – (2.16) and the transformation equations (3.29) – (3.33). Thus, if we employ the definition of R_v in (3.37) and remember that $|\xi/\nu^{1/2}| \leq C$, which holds by (3.26), we find that

$$\left| \text{div}_{\Gamma,\xi} T_0(t, \eta, \xi/\nu^{1/2}) + \text{div}_{\Gamma_\xi} T_1(t, \eta, \xi/\nu^{1/2}) + R_v(t, \eta, \xi, \xi/\nu^{1/2}) \right| \leq C_1$$

and

$$\left| \nu^{1/2} \text{div}_x \left(D\varepsilon(\nabla_\Gamma u_0(t, \eta, \xi/\nu^{1/2}) R_A(t, \eta, \xi, \xi/\nu^{1/2}) + \nabla_{\Gamma_\xi} u_1(t, \eta, \xi/\nu^{1/2})) \right) \right| \leq C_2,$$

for all $(t, \eta, \xi) \in \Gamma[\nu]$. Together these two estimates imply (3.69). We use (3.69) to infer from (3.38) that

$$\left| \text{div}_x T^{(\nu)}(t, x) + \mathbf{b}(t, x) \right| \leq K_1 \nu^{1/2}, \quad (t, x) \in \Gamma[\nu]. \quad (3.70)$$

Next, from (2.36), (2.37) and (2.63) we obtain

$$\begin{aligned} u^{(\nu)}(t, x) &= \hat{u}(t, x), & (t, x) \in Q \setminus \mathcal{U}, \\ u^{(\nu)}(t, x) &= \hat{u}(t, x) + \nu c_+(t, \eta) 1^+(\xi) \phi(t, x), & (t, x) \in \mathcal{U} \setminus \Gamma[\nu]. \end{aligned}$$

Using (2.42), we thus infer from (2.39) that

$$T^{(\nu)}(t, x) = \begin{cases} \hat{T}(t, x), & (t, x) \in Q \setminus \mathcal{U}, \\ \hat{T}(t, x) + \nu D\varepsilon\left(\nabla_x(c_+(t, \eta) 1^+(\xi) \phi(t, x))\right), & (t, x) \in \mathcal{U} \setminus \Gamma[\nu]. \end{cases} \quad (3.71)$$

Since $c_+(t, \eta) 1^+(\xi) \phi(t, x)$ is independent of ν , we have

$$\left| \operatorname{div}_x D\varepsilon\left(\nabla_x(c_+(t, \eta) 1^+(\xi) \phi(t, x))\right) \right| \leq K_2$$

with a suitable constant K_2 independent of ν , whence, together with (3.71), (2.1) and (2.2),

$$\left| \operatorname{div}_x T^{(\nu)}(t, x) - \mathbf{b}(t, x) \right| \leq \begin{cases} 0, & (t, x) \in Q \setminus \mathcal{U}, \\ \nu K_2, & (t, x) \in \mathcal{U} \setminus \Gamma[\nu]. \end{cases}$$

The inequality (2.89) follows from this estimate and from (3.70).

To prove (2.90) we use the auxilliary estimates proved in Lemma 3.7 following below. Note first that $S^{(\nu)}$ is constant equal to 0 in $\gamma \setminus \Gamma[\nu]$ and equal to 1 in $\gamma' \setminus \Gamma[\nu]$, by (2.38) and (2.40), which implies that

$$\partial_t S^{(\nu)} + f(\psi_S(\varepsilon(\nabla_x u^{(\nu)}), S^{(\nu)}) - \nu \Delta_x S^{(\nu)}) |\nabla_x S^{(\nu)}| = 0$$

in $Q \setminus \Gamma[\nu]$. Hence, (2.90) holds for $V = Q \setminus \Gamma[\nu]$.

The asymptotic expansion (3.56) implies that there is a constant $C_1 > 0$, which is independent of $\nu \in (0, \nu_0]$, such that on $\Gamma[\nu]$ the inequality

$$\left| f(\psi_S(\varepsilon(\nabla_x u^{(\nu)}), S^{(\nu)}) - \nu \Delta_x S^{(\nu)}) \right| \leq C_1 \quad (3.72)$$

holds. This inequality and (3.77) together yield

$$\left\| \partial_t S^{(\nu)} + f(\psi_S(\varepsilon(\nabla_x u^{(\nu)}), S^{(\nu)}) - \nu \Delta_x S^{(\nu)}) |\nabla_x S^{(\nu)}| \right\|_{L^\infty(\tilde{\Gamma}_k[\nu])} \leq \hat{K}_4 + C_1 \hat{K}_4 = K_4,$$

which shows that the the estimate (2.90) holds for $V = \tilde{\Gamma}_k[\nu]$.

To verify this estimate for $V = \Gamma_k[\nu]$, we employ the asymptotic expansion (3.66), which is valid on $\Gamma_k[\nu]$: By (3.57), the term $R_f(\nu, t, \eta, \xi, \frac{\xi}{\nu^{1/2}})$ in (3.66) is bounded on $\Gamma[\nu]$, uniformly with respect to ν . Therefore we obtain from (3.67) and from the auxilliary estimate (3.74) that on $\Gamma[\nu]$

$$\nu |\omega^2 R_{f'} \partial_\xi S^{(\nu)}| + \nu |R_f \partial_\xi S^{(\nu)}| \leq C_2 \nu^{1/2}. \quad (3.73)$$

Furthermore, combination of (2.77), (3.72) with the auxilliary estimates (3.75), (3.78) shows that on $\Gamma_k[\nu]$

$$\left| \nu^{1/2} \left(S_{1,t} - \zeta \partial_t n \cdot \nabla_\eta S^{(\nu)} - \frac{S_{0,t}}{S'_0} S'_1 \right) + f(\psi_S - \nu \Delta_x S^{(\nu)}) (|\nabla_x S^{(\nu)}| - \partial_\xi S^{(\nu)}) \right| \leq C_3 \nu^{1/2}.$$

If we use this inequality and (3.73) to estimate the right hand side of (3.66), we see that (2.90) holds also for $V = \Gamma_k[\nu]$. The proof of Theorem 2.7 is complete. \blacksquare

3.4 Auxiliary estimates

In the following lemmas we collect estimates needed in Sections 3.1 and 3.3.3.

Lemma 3.7 *There are constants $k > 0$, $\hat{K}_1, \dots, \hat{K}_5 > 0$ and $\nu_0 > 0$ such that for all ν with $0 < \nu \leq \nu_0$ and for the sets $\Gamma_k[\nu]$, $\tilde{\Gamma}_k[\nu]$ defined in (2.88) we have*

$$|\partial_\xi S^{(\nu)}(t, x)| \leq \hat{K}_1 \nu^{-1/2}, \quad (t, x) \in \Gamma[\nu], \quad (3.74)$$

$$\left| \frac{\partial_t S_0}{S_0'}(t, \eta, \zeta) \right| \leq \hat{K}_2, \quad (t, \eta, \zeta) \in \Gamma[a, b], \quad (3.75)$$

$$\left| \frac{\nabla_{\Gamma_\xi} S^{(\nu)}}{\nu^{1/2} \partial_\xi S^{(\nu)}}(t, x) \right| \leq \hat{K}_3, \quad (t, x) \in \Gamma_k[\nu], \quad (3.76)$$

$$|\nabla_x S^{(\nu)}(t, x)|, |\partial_t S^{(\nu)}(t, x)| \leq \hat{K}_4, \quad (t, x) \in \tilde{\Gamma}_k[\nu], \quad (3.77)$$

$$|(|\nabla_x S^{(\nu)}| - \partial_\xi S^{(\nu)})(t, x)| \leq \hat{K}_5 \nu^{1/2}, \quad (t, x) \in \Gamma_k[\nu]. \quad (3.78)$$

Proof: (3.74) follows immediately from (3.65). To prove the remaining estimates we define a function $\chi : \Gamma[a, b] \rightarrow [0, \infty)$, which can be used to bound the derivatives of S_0 below and above. To this end note that by the assumptions 1. – 3. for $\tilde{\psi}$ in Theorem 2.3 there are constants $c_1, c_2 > 0$ such that

$$\partial_S \tilde{\psi}(t, \eta, S) \begin{cases} \geq c_0/2, & \text{for } (t, \eta) \in \Gamma, 0 \leq S \leq c_1 \\ \leq -c_0/2, & \text{for } (t, \eta) \in \Gamma, 1 - c_1 \leq S \leq 1, \end{cases} \quad (3.79)$$

$$\tilde{\psi}(t, \eta, S) \geq c_2, \quad \text{for } (t, \eta) \in \Gamma, c_1 \leq S \leq 1 - c_1. \quad (3.80)$$

Here $c_0 > 0$ is the constant from assumption 3 in Theorem 2.3. Let

$$\begin{aligned} V_1 &= \Gamma[a, b] \cap S_0^{-1}([0, c_1]), \\ V_2 &= \Gamma[a, b] \cap S_0^{-1}([c_1, 1 - c_1]), \\ V_3 &= \Gamma[a, b] \cap S_0^{-1}((1 - c_1, 1]), \end{aligned}$$

where $S_0^{-1}(U)$ denotes the inverse image of a set $U \subseteq \mathbb{R}$. Since S_0 is continuous on $\Gamma[a, b]$, since S_0 vanishes on the surface $l_a = \{(t, \eta, \zeta) \mid \zeta = a(t, \eta)\}$ and since S_0 is equal to 1 on the surface $l_b = \{(t, \eta, \zeta) \mid \zeta = b(t, \eta)\}$, it follows that $l_a \subseteq V_1$, $l_b \subseteq V_3$ and that the compact set V_2 has a positive distance d_1 from $l_a \cup l_b$. We now define χ by

$$\chi(t, \eta, \zeta) = \begin{cases} \frac{c_0}{2}(\zeta - a(t, \eta)), & (t, \eta, \zeta) \in V_1, \\ \sqrt{2c_2}, & (t, \eta, \zeta) \in V_2, \\ \frac{c_0}{2}(b(t, \eta) - \zeta), & (t, \eta, \zeta) \in V_3. \end{cases} \quad (3.81)$$

With this function we can bound the derivatives of S_0 . Namely, there are constants C_1, \dots, C_3 such that on $\Gamma[a, b]$

$$\chi \leq S_0' \leq C_1 \chi, \quad (3.82)$$

$$|\partial_t S_0| \leq C_2 \chi, \quad |\nabla_\eta S_0| \leq C_3 \chi. \quad (3.83)$$

To see this observe that (3.79) and the differential equation (2.50) together imply

$$S_0''(t, \eta, \zeta) \begin{cases} \geq c_0/2, & (t, \eta, \zeta) \in V_1 \\ \leq -c_0/2, & (t, \eta, \zeta) \in V_3. \end{cases}$$

If we integrate these inequalities, use that $S_0'(t, \eta, a(t, \eta)) = S_0'(t, \eta, b(t, \eta)) = 0$, which holds by (2.69), and note the definition of χ in (3.81), we see that S_0' can be bounded below by χ on $V_1 \cup V_3$. That S_0' can be bounded below by χ on V_2 follows from (3.80) and the differential equation (2.66), which together yield

$$S_0'(t, \eta, \zeta) \geq \sqrt{2c_2} = \chi(t, \eta, \zeta), \quad \text{for } (t, \eta, \zeta) \in V_2.$$

To prove that S_0' can be bounded above by $C_1\chi$ with a sufficiently large constant C_1 it suffices to remark that S_0' is continuously differentiable, by Theorem 2.3, which implies that S_0' is uniformly Lipschitz continuous, and that S_0' vanishes on $l_a \cup l_b$. This proves (3.82).

Equation (3.83) follows by the same reasoning as in the proof of the second inequality in (3.82), since $\frac{\partial}{\partial t}S_0$ and $\nabla_\eta S_0$ are continuously differentiable on the compact set $\Gamma[a, b]$ and vanish on $l_a \cup l_b$, by (2.70).

After these preparations we can prove (3.75) – (3.78). The estimate (3.75) follows immediately from (3.82) and (3.83), which yield

$$\left| \frac{\partial_t S_0}{S_0'} \right| \leq \frac{C_2 \chi}{\chi} = \hat{K}_2.$$

To prove (3.76) define $c_4 = \sup_{\Gamma[a, b]} |S_1'|$. Then (3.65) and (3.82) imply for all $(t, x) \in \Gamma[\nu]$ that

$$\nu^{-1/2} \chi(t, x) - c_4 \leq \partial_\xi S^{(\nu)}(t, x) \leq \nu^{-1/2} C_1 \chi(t, x) + c_4, \quad (3.84)$$

where $\chi(t, x) = \chi(t, \eta, \frac{\xi}{\nu^{1/2}})$, as usual. Moreover, since by (3.30)

$$\nabla_{\Gamma_\xi} S^{(\nu)}(t, x) = A^T(t, \eta, \xi) \nabla_\eta (S_0 + \nu^{1/2} S_1)(t, \eta, \frac{\xi}{\nu^{1/2}}),$$

we obtain from (3.83) that

$$|\nabla_{\Gamma_\xi} S^{(\nu)}(t, x)| \leq C_4 \chi(t, x) + c_5 \nu^{1/2}, \quad (3.85)$$

with suitable constants $C_4, c_5 > 0$. Now choose $\nu_0 \leq \left(\frac{1}{2c_4} \sqrt{2c_2}\right)^2$ and set

$$k = 4 \frac{c_4}{c_0}. \quad (3.86)$$

The definition of χ in (3.81) then yields for $0 < \nu \leq \nu_0$ and for ζ satisfying $a(t, \eta) + k\nu^{1/2} \leq \zeta \leq b(t, \eta) - k\nu^{1/2}$ that

$$\frac{1}{2} \chi(t, \eta, \zeta) \geq c_4 \nu^{1/2},$$

which is equivalent to $\frac{1}{2} \chi(t, x) \geq c_4 \nu^{1/2}$ for all $(t, x) \in \Gamma_k[\nu]$, by definition of $\Gamma_k[\nu]$ in (2.88). Combination of this inequality with (3.84) yields

$$\nu^{1/2} \partial_\xi S^{(\nu)} \geq \frac{1}{2} \max(\chi, c_4 \nu^{1/2}), \quad \text{on } \Gamma_k[\nu]. \quad (3.87)$$

From this estimate and from (3.85) we conclude that

$$\left| \frac{\nabla_{\Gamma_\xi} S(\nu)}{\nu^{1/2} \partial_\xi S(\nu)} \right| \leq 2 \frac{C_4 \chi + c_5 \nu^{1/2}}{\max(\chi, c_4 \nu^{1/2})} \leq \hat{K}_3, \quad (3.88)$$

on $\Gamma_k[\nu]$. This is (3.76) with $\hat{K}_3 = 2(C_4 + \frac{c_5}{c_4})$ and k defined in (3.86).

To prove (3.77) note that χ defined in (3.81) vanishes on $l_a \cup l_b$ and grows linearly with slope $\partial_\zeta \chi = \pm \frac{c_0}{2}$ on the set $V_1 \cup V_3$, which is a neighborhood of $l_a \cup l_b$ relative to $\Gamma[a, b]$. Therefore $\chi(t, x) = \chi(t, \eta, \frac{\xi}{\nu^{1/2}})$ grows linearly with slope

$$\partial_\xi \chi = \pm \frac{c_0}{2\nu^{1/2}} \quad (3.89)$$

on the set

$$U[\nu] = \left\{ (t, \eta, \xi) \mid (t, \eta, \frac{\xi}{\nu^{1/2}}) \in V_1 \cup V_3 \right\} \subseteq \Gamma[\nu].$$

Since $V_1 \cup V_3$ contains all points (t, η, ζ) with $\min(\zeta - a(t, \eta), b(t, \eta) - \zeta) < d_1$, where d_1 is the distance of V_2 from $l_a \cup l_b$, it follows that $U[\nu]$ contains all points (t, η, ξ) with $\min(\xi - \nu^{1/2} a(t, \eta), \nu^{1/2} b(t, \eta) - \xi) < \nu^{1/2} d_1$. Using this relation and the definition of $\Gamma_k[\nu]$ and $\tilde{\Gamma}_k[\nu]$ in (2.88), we see that if we choose $\nu_0 > 0$ sufficiently small such that

$$k\nu_0^{1/2} < d_1,$$

then we have $\tilde{\Gamma}_k[\nu] \subseteq U[\nu]$ for all $0 < \nu \leq \nu_0$. Consequently, (3.89) holds on $\tilde{\Gamma}_k[\nu]$, which together with (2.88) implies that $\chi \leq k \frac{c_0}{2} \nu^{1/2}$ on $\tilde{\Gamma}_k[\nu]$. Using this and (3.84), (3.85), we compute

$$\begin{aligned} |\nabla_x S(\nu)| &= \sqrt{(\partial_\xi S(\nu))^2 + |\nabla_{\Gamma_\xi} S(\nu)|^2} \leq \partial_\xi S(\nu) + |\nabla_{\Gamma_\xi} S(\nu)| \\ &\leq \nu^{-1/2} C_1 \chi(t, x) + c_4 + C_4 \chi(t, x) + c_5 \nu^{1/2} \leq C_1 k \frac{c_0}{2} + c_6 = \hat{K}_4, \end{aligned}$$

which is the first estimate in (3.77). The estimate for $\partial_t S(\nu)$ in (3.77) is proved in the same way using (3.59).

To prove (3.78) we note that on the set $\Gamma_k[\nu]$ we have $\partial_\xi S(\nu) > 0$, by (3.87), whence

$$|\nabla_x S(\nu)| = \sqrt{(\partial_\xi S(\nu))^2 + |\nabla_{\Gamma_\xi} S(\nu)|^2} = \partial_\xi S(\nu) \sqrt{1 + \left(\frac{|\nabla_{\Gamma_\xi} S(\nu)|}{\partial_\xi S(\nu)} \right)^2}.$$

On the set $\Gamma_k[\nu]$ we thus infer from the mean value theorem and from (3.76) that

$$\begin{aligned} |\nabla_x S(\nu)| - \partial_\xi S(\nu) &= \frac{1}{2} \partial_\xi S(\nu) \frac{1}{1 + \vartheta \left(\frac{|\nabla_{\Gamma_\xi} S(\nu)|}{\partial_\xi S(\nu)} \right)^2} \left(\frac{|\nabla_{\Gamma_\xi} S(\nu)|}{\partial_\xi S(\nu)} \right)^2 \\ &\leq \frac{1}{2} \partial_\xi S(\nu) \nu K_3^2 \leq \nu^{1/2} \frac{1}{2} \hat{K}_1 \hat{K}_3^2, \end{aligned}$$

where $0 < \vartheta < 1$ is suitable. To get the last estimate we employed (3.74). This proves (3.78) with $\hat{K}_5 = \frac{1}{2} \hat{K}_1 \hat{K}_3^2$ and completes the proof of Lemma 3.7. \blacksquare

Lemma 3.8 *Let $f \in C^3(\mathbb{R}, \mathbb{R})$ satisfy $f'(r) \geq c_1 > 0$ for all $r \in \mathbb{R}$ and let $\varphi_\nu \in C_0^\infty(\Gamma[\nu])$ satisfy (2.58). For $(t, \eta, \zeta) \in \Gamma[a, b]$ let d denote the distance of ζ to the boundary of the interval $[a(t, \eta), b(t, \eta)]$. Then for $i = 1, 2$*

$$\left| \nabla_\eta^i \left(\frac{\partial_t S_0 \varphi_\nu}{f'(n \cdot [\hat{C}]n) S'_0} \right) \right| \leq \begin{cases} K_1 d^{-i}, & \text{on } \Gamma_{k,\nu}[a, b], \\ K_1 d^{-(i-1)} \nu^{-1/2}, & \text{on } \tilde{\Gamma}_{k,\nu}[a, b], \end{cases} \quad (3.90)$$

$$\left| \partial_t \left(\frac{\partial_t S_0 \varphi_\nu}{f'(n \cdot [\hat{C}]n) S'_0} \right) \right| \leq \begin{cases} K_2 d^{-1}, & \text{on } \Gamma_{k,\nu}[a, b], \\ K_2 \nu^{-1/2}, & \text{on } \tilde{\Gamma}_{k,\nu}[a, b]. \end{cases} \quad (3.91)$$

Proof: Let τ_1, τ_2 be orthogonal unit tangent vectors to Γ . Then we have

$$\begin{aligned} \partial_{\tau_i} \left(\frac{\partial_t S_0}{f' S'_0} \right) &= \frac{\partial_{\tau_i} \partial_t S_0}{f' S'_0} - \frac{\partial_t S_0}{S'_0} \frac{\partial_{\tau_i} (f' S'_0)}{(f')^2 S'_0}, \\ \partial_{\tau_j} \partial_{\tau_i} \frac{\partial_t S_0}{f' S'_0} &= \frac{\partial_{\tau_j} \partial_{\tau_i} \partial_t S_0}{f' S'_0} - \frac{\partial_{\tau_i} \partial_t S_0 \partial_{\tau_j} (f' S'_0) + \partial_{\tau_j} (\partial_t S_0 \partial_{\tau_i} (f' S'_0))}{(f' S'_0)^2} \\ &\quad + 3 \frac{\partial_t S_0}{S'_0} \frac{\partial_{\tau_i} (f' S'_0) \partial_{\tau_j} (f' S'_0)}{(f')^3 (S'_0)^2}. \end{aligned}$$

Since $S_0, S'_0 \in C^3(\Gamma[a, b])$, by Theorem 2.3, and since by assumption $f' \geq c_1 > 0$, we infer from these equations and from (3.75) and (3.82) that on $\Gamma_{k,\nu}[a, b]$ the inequalities

$$\left| \partial_{\tau_i} \frac{\partial_t S_0}{f' S'_0} \right| \leq C_1 d^{-1}, \quad \left| \partial_{\tau_i} \partial_{\tau_j} \frac{\partial_t S_0}{f' S'_0} \right| \leq C_2 d^{-2}$$

hold. Using Leibniz' rule, we obtain (3.90) by combination of these inequalities with the estimates for the derivatives of φ_ν stated in (2.58). The estimate (3.91) is proved in the same manner. We leave this proof to the reader. \blacksquare

4 Asymptotic solution for the Allen-Cahn model

In this section we construct a family $(u^{(\mu)}, T^{(\mu)}, S^{(\mu)})$ of asymptotic solution of first order to the rescaled Allen-Cahn model (1.20) – (1.22) for $\mu \rightarrow 0$. Section 4.1 contains the construction of this family, the main results are stated in Section 4.2. In particular, the estimate for the residue, with which the asymptotic solutions satisfy the model equations, is stated in Theorem 4.3. The proofs of the main results are given in Section 5.

Though our construction of the asymptotic solutions follows the well known procedure, we give not only the formal inner and outer asymptotic expansions, but a complete proof of the residue estimate. We hope that this is justified, since, as discussed in the introduction, to compare the Allen-Cahn and hybrid model we need to know the behavior of the asymptotic solution and of the residue not only with respect to the parameter μ , but also with respect to the parameter λ . The behavior of the asymptotic solution with respect to this second parameter is not usually discussed in investigations of phase field models containing the Allen-Cahn equation.

Our investigations are general also with respect to the constitutive function f in (1.22), which can be nonlinear. It will be seen that differently from the hybrid model, the nonlinearity f in the evolution equation for the order parameter in the Allen-Cahn model and the nonlinearity g in the sharp interface limit problem are not the same, but are connected by an integral operator.

The notations used in this and the following section are similar to the notations in the previous sections, but do not always coincide.

4.1 Construction of the asymptotic solution of first order

The construction of the asymptotic solution is based on a given solution of the sharp interface model

$$-\operatorname{div}_x \hat{T} = \mathbf{b}, \quad (4.1)$$

$$\hat{T} = D(\varepsilon(\nabla_x \hat{u}) - \bar{\varepsilon} \hat{S}), \quad (4.2)$$

$$s = g(n \cdot [\hat{C}]n + \lambda^{1/2} c_1 \kappa_\Gamma), \quad (4.3)$$

$$[\hat{u}] = 0, \quad (4.4)$$

$$[\hat{T}]n = 0, \quad (4.5)$$

where $\kappa_\Gamma(t, x)$ denotes twice the mean curvature of the phase interface $\Gamma(t)$ at $x \in \Gamma(t)$ and where the constant $c_1 > 0$ is given by (1.27). The function $g : \mathbb{R} \rightarrow \mathbb{R}$ depends on the constitutive function f and on the double well potential $\hat{\psi}$ in (1.22). It is defined as follows. We assume that $f : \mathbb{R} \rightarrow \mathbb{R}$ is strictly increasing and that $\hat{\psi}(r) \geq 0$ for all $r \in \mathbb{R}$. For simplicity assume that f is surjective, hence the inverse f^{-1} is defined on all of \mathbb{R} . Define the inverse $g^{-1} : \mathbb{R} \rightarrow \mathbb{R}$ of g by

$$g^{-1}(r) = \int_0^1 f^{-1}(r \sqrt{2\hat{\psi}(\zeta)}) d\zeta. \quad (4.6)$$

Note that g^{-1} is strictly increasing since f^{-1} is strictly increasing, whence the inverse g of g^{-1} exists. From (4.6) we see immediately that if f is equal to the linear function (1.25), then the kinetic relation (4.3) takes the form (1.26).

In the following we assume that $(\hat{u}, \hat{T}, \hat{S}, \Gamma)$ is solution of (4.1) – (4.5), which has the regularity properties stated in the following assumption. As in Section 2.2 we denote by γ the set of all $(t, x) \in Q \setminus \Gamma$ with $\hat{S}(t, x) = 0$ and by γ' is the set of all $(t, x) \in Q \setminus \Gamma$ with $\hat{S}(t, x) = 1$. This implies that $Q \setminus \Gamma = \gamma \cup \gamma'$.

Assumption C. Let Γ be a three-dimensional C^4 -manifold embedded in Q , such that the set Γ is a compact subset of Q and the two-dimensional manifold $\Gamma(t)$ does not have a boundary for every $t \in [t_1, t_2]$. Suppose that the function (\hat{u}, \hat{T}) belongs to the space $C^4(\gamma \cup \gamma') \times C^3(\gamma \cup \gamma')$ and that the derivatives of \hat{u} up to order four and the derivatives of \hat{T} up to order three have continuous extensions from γ to $\gamma \cup \Gamma$ and from γ' to $\gamma' \cup \Gamma$.

Now we can state the ansatz for the asymptotic solution $(u^{(\mu)}, T^{(\mu)}, S^{(\mu)})$ of (1.20) – (1.22). To this end let the set $\mathcal{U} \subset Q$ and the mapping $(t, \eta, \xi) \mapsto (t, x) : \Gamma \times (-\delta, \delta) \rightarrow \mathcal{U}$ be defined by (2.6). With u^* given in (2.19) and ξ^+ given in (2.18) define the function $v : \mathcal{U} \rightarrow \mathbb{R}^3$ by

$$\hat{u}(t, x) = u^*(t, \eta)\xi^+ + v(t, x), \quad (4.7)$$

where (t, η, ξ) are the new coordinates of the point $(t, x) \in \mathcal{U}$. Then it follows as in Lemma 2.2 that for $i + j \leq 3$ and $i + j + l \leq 4$ the derivatives $\partial_t^i \nabla_{\Gamma\xi}^j \partial_\xi^l v$ exist in $\gamma \cup \gamma'$ and are bounded and continuous. For $i + j \leq 3$ and $l \leq 1$ these derivatives can be joined continuously across Γ , whence these derivatives exist in Q and are continuous.

With $\hat{\phi} \in C_0^\infty((-2, 2))$ satisfying

$$\hat{\phi}(r) = 1, \quad \text{for } |r| \leq 1.$$

and with a constant $a > 0$, which will be fixed later, we set

$$S^{(\mu)}(t, x) = S_1^{(\mu)}(t, x) \hat{\phi}\left(\frac{a\xi}{|(\mu\lambda)^{1/2} \ln \mu|}\right) + S_2^{(\mu)}(t, x) \left(1 - \hat{\phi}\left(\frac{a\xi}{|(\mu\lambda)^{1/2} \ln \mu|}\right)\right), \quad (4.8)$$

$$u^{(\mu)}(t, x) = u_1^{(\mu)}(t, x) \hat{\phi}\left(\frac{a\xi}{|(\mu\lambda)^{1/2} \ln \mu|}\right) + u_2^{(\mu)}(t, x) \left(1 - \hat{\phi}\left(\frac{a\xi}{|(\mu\lambda)^{1/2} \ln \mu|}\right)\right), \quad (4.9)$$

$$T^{(\mu)}(t, x) = D(\varepsilon(\nabla_x u^{(\mu)}(t, x)) - \bar{\varepsilon} S^{(\mu)}(t, x)), \quad (4.10)$$

where

$$S_1^{(\mu)}(t, x) = S_0\left(\frac{\xi}{(\mu\lambda)^{1/2}}\right) + \mu^{1/2} S_1\left(t, \eta, \frac{\xi}{(\mu\lambda)^{1/2}}\right), \quad (4.11)$$

$$S_2^{(\mu)}(t, x) = \hat{S}(t, x) + \mu^{1/2} \tilde{S}_1(t, x) + \mu \tilde{S}_2(t, x), \quad (4.12)$$

$$u_1^{(\mu)}(t, x) = (\mu\lambda)^{1/2} u_0\left(t, \eta, \frac{\xi}{(\mu\lambda)^{1/2}}\right) + v(t, x), \quad (4.13)$$

$$u_2^{(\mu)}(t, x) = \hat{u}(t, x) + \mu^{1/2} \tilde{u}_1(t, x), \quad (4.14)$$

with

$$u_0(t, \eta, \zeta) = u^*(t, \eta) \int_{-\infty}^{\zeta} S_0(\vartheta) d\vartheta. \quad (4.15)$$

We also use the notation

$$T_i^{(\mu)}(t, x) = D(\varepsilon(\nabla_x u_i^{(\mu)}) - \bar{\varepsilon} S_i^{(\mu)}), \quad \text{for } i = 1, 2. \quad (4.16)$$

We partition Q into the three sets

$$\Gamma_i[\mu, \lambda] = \left\{ (t, \eta, \xi) \in \mathcal{U} \mid |\xi| < \frac{(\mu\lambda)^{(1/2)} |\ln(\mu)|}{a} \right\}, \quad (4.17)$$

$$\Gamma_m[\mu, \lambda] = \left\{ (t, \eta, \xi) \in \mathcal{U} \mid \frac{(\mu\lambda)^{(1/2)} |\ln(\mu)|}{a} < |\xi| < 2 \frac{(\mu\lambda)^{(1/2)} |\ln(\mu)|}{a} \right\}, \quad (4.18)$$

$$\Gamma_o[\mu, \lambda] = Q \setminus (\Gamma_i[\mu, \lambda] \cup \Gamma_m[\mu, \lambda]). \quad (4.19)$$

From (4.8) and (4.9) we see that in the inner region $\Gamma_i[\mu, \lambda]$ the ansatz for $S^{(\mu)}$ and $u^{(\mu)}$ reduces to $S_1^{(\mu)}$ and $u_1^{(\mu)}$, and in the outer region $\Gamma_o[\mu, \lambda]$ to $S_2^{(\mu)}$ and $u_2^{(\mu)}$. In the matching region $\Gamma_m[\mu, \lambda]$ the expression $S_1^{(\mu)}$ must be matched with $S_2^{(\mu)}$ and $u_1^{(\mu)}$ must be matched with $u_2^{(\mu)}$. To find differential equations for the unknown functions S_0 and S_1 in (4.11) we insert $u_1^{(\mu)}$, $T_1^{(\mu)}$, $S_1^{(\mu)}$ into the equations (1.20) – (1.22), expand both sides of these equations into a truncated series of powers of μ and equate the coefficients. This calculation is carried out carefully in Section 5.2. If we set $\zeta = \frac{\xi}{(\mu\lambda)^{1/2}}$ and write w' , w'' for $\partial_\zeta w$, $\partial_\zeta^2 w$, we obtain from this calculation the recursively solvable system

$$\hat{\psi}'(S_0(\zeta)) - S_0''(\zeta) = 0, \quad (4.20)$$

$$\hat{\psi}''(S_0(\zeta)) S_1(t, \eta, \zeta) - S_1''(t, \eta, \zeta) = F_1(t, \eta, \zeta), \quad (4.21)$$

with the right hand side

$$F_1(t, \eta, \zeta) = \bar{\varepsilon} : [\hat{T}](t, \eta) S_0(\zeta) + \bar{\varepsilon} : \hat{T}^{(-)}(t, \eta) - \lambda^{1/2} \kappa_\Gamma(t, \eta) S_0'(\zeta) + f^{-1}(s(t, \eta) S_0'(\zeta)), \quad (4.22)$$

where $s(t, \eta)$ denotes the normal speed of Γ determined by (4.3). To see for what values of (t, η, ζ) the differential equations (4.20), (4.21) must be satisfied, note that $S_1^{(\mu)}$ contributes to $S^{(\mu)}$ only on the domain $\Gamma_i[\mu, \lambda] \cup \Gamma_m[\mu, \lambda]$; the point (t, η, ξ) belongs to this domain if $\frac{|a\xi|}{|(\mu\lambda)^{1/2} \ln \mu|} < 2$. This would imply that it suffices that the differential equations (4.20) and (4.21) hold for $(t, \eta, \zeta) \in \Gamma \times [-\frac{2}{a} |\ln \mu|, \frac{2}{a} |\ln \mu|]$. Yet, since we consider the limit $\mu \rightarrow 0$, the differential equations must hold on the union of these domains, which is $\Gamma \times \mathbb{R}$.

To find equations for the unknown functions \tilde{S}_1 , \tilde{S}_2 and \tilde{u}_1 in (4.12) and (4.14) we insert $u_2^{(\mu)}$, $T_2^{(\mu)}$ and $S_2^{(\mu)}$ into (1.20) – (1.22) and equate the coefficients of powers of μ . This computation, also carried out in Section 5.2, shows that the unknown functions together with a function \tilde{T}_1 must satisfy the system

$$-\operatorname{div}_x \tilde{T}_1 = 0, \quad (4.23)$$

$$\tilde{T}_1 = D(\varepsilon(\nabla_x \tilde{u}_1) - \bar{\varepsilon} \tilde{S}_1), \quad (4.24)$$

$$-\hat{T} : \bar{\varepsilon} + \hat{\psi}''(\hat{S}) \tilde{S}_1 = 0, \quad (4.25)$$

$$-\tilde{T}_1 : \bar{\varepsilon} + \frac{1}{2} \hat{\psi}'''(\hat{S}) \tilde{S}_1^2 + \psi''(\hat{S}) \tilde{S}_2 = 0. \quad (4.26)$$

To see for what (t, x) these equations must hold, observe that $S_2^{(\mu)}$ and $u_2^{(\mu)}$ contribute to $S^{(\mu)}$ and to $u^{(\mu)}$ only on the set $Q \setminus \Gamma_i[\mu, \lambda]$, hence (4.23) – (4.26) must hold on this set. Yet, since this must be true for all sufficiently small $\mu > 0$, these equations must hold on the union $\bigcup_{\mu > 0} (Q \setminus \Gamma_i[\mu, \lambda]) = \gamma \cup \gamma'$.

The equations (4.20) – (4.26) must be supplemented by boundary conditions and by conditions at infinity. These conditions are consequences of the matching conditions. To see what conditions are necessary, observe that since \hat{T} is known from the sharp interface problem and since \hat{S} is the characteristic function of the set γ' , (4.25) is an algebraic equation for \tilde{S}_1 , which yields

$$\tilde{S}_1(t, x) = \frac{\bar{\varepsilon} : \hat{T}(t, x)}{\hat{\psi}''(\hat{S}(t, x))}. \quad (4.27)$$

Therefore \tilde{S}_1 is known. Using this, we conclude from the requirement that $S_1^{(\mu)}$ and $S_2^{(\mu)}$ match in the domain $\Gamma_m[\mu, \lambda]$ that S_0 and S_1 must satisfy

$$\lim_{\zeta \rightarrow -\infty} S_0(\zeta) = 0, \quad \lim_{\zeta \rightarrow \infty} S_0(\zeta) = 1, \quad (4.28)$$

$$\lim_{\zeta \rightarrow -\infty} S_1(t, \eta, \zeta) = \tilde{S}_1^{(-)}(t, \eta) = \frac{\bar{\varepsilon} : \hat{T}^{(-)}(t, \eta)}{\hat{\psi}''(0)}, \quad (4.29)$$

$$\lim_{\zeta \rightarrow +\infty} S_1(t, \eta, \zeta) = \tilde{S}_1^{+}(t, \eta) = \frac{\bar{\varepsilon} : \hat{T}^{+}(t, \eta)}{\hat{\psi}''(1)}. \quad (4.30)$$

As we shall show, the functions S_0 and S_1 can be determined from the differential equations (4.20), (4.21) and from the conditions (4.28) – (4.30) at infinity.

Since \tilde{S}_1 is known, for every $t \in [t_1, t_2]$ the equations (4.23) and (4.24) form an elliptic system for the unknown functions \tilde{u}_1 and \tilde{T}_1 in the disjoint sets $\gamma(t)$ and in $\gamma'(t)$. To determine these functions uniquely we therefore need boundary conditions posed on $\partial\gamma(t) = \Gamma(t) \cup \partial\Omega$ and on $\partial\gamma'(t) = \Gamma(t)$. On $\Gamma(t)$ such conditions are yielded by the requirement that $(\lambda\mu)^{1/2}u^*S_0^{(-1)} + v$ and $\hat{u} + \mu^{1/2}\tilde{u}_1$ must match in $\Gamma_m[\mu, \lambda]$. It will be seen that the resulting conditions are

$$\tilde{u}_1^{(+)}(t, \eta) = \lambda^{1/2}u^*(t, \eta) \int_{-\infty}^{\infty} (S_0(\zeta) - 1^+)d\zeta, \quad (4.31)$$

$$\tilde{u}_1^{(-)}(t, \eta) = 0, \quad (4.32)$$

for $\eta \in \Gamma(t)$. We also require that

$$\tilde{u}_1|_{\partial\Omega} = 0. \quad (4.33)$$

(4.31) is the Dirichlet boundary condition for the elliptic system in $\gamma'(t)$, whereas (4.32) and (4.33) together define the Dirichlet boundary condition for the system in the domain $\gamma(t)$. The standard existence theory for the linear elliptic system (4.23), (4.24) shows that there is a unique solution $(\tilde{u}_1, \tilde{T}_1)$ of this system to the function \tilde{S}_1 given by (4.27) and to the boundary conditions (4.31) – (4.33). Therefore \tilde{u}_1, \tilde{T}_1 are known by now. Finally, (4.26) is an algebraic equation for the function \tilde{S}_2 and can be solved for this function, since all other functions in this equation have been determined already.

4.2 Main theorems

The preceding considerations show that all unknown functions in the ansatz (4.8) – (4.15) can be determined from the differential equations and the matching conditions, if the boundary value problems for the differential equations (4.20) and (4.21) can be solved. The next two theorems provide existence results for these boundary value problems.

Consider the initial boundary value problem

$$S_0'(\zeta) = \sqrt{2\hat{\psi}(S_0(\zeta))}, \quad S_0(0) = \frac{1}{2}. \quad (4.34)$$

By differentiation of the first order differential equation we see immediately that a two times differentiable solution is also a solution of (4.15). To solve the boundary value problem (4.20), (4.28) it therefore suffices to study this problem. We have

Theorem 4.1 *Assume that $\hat{\psi} \in C^3([0, 1], \mathbb{R})$ satisfies*

$$\hat{\psi}(r) > 0, \quad \text{for } 0 < r < 1, \quad (4.35)$$

$$\hat{\psi}(r) = \hat{\psi}'(r) = 0, \quad \text{for } r = 0, 1, \quad (4.36)$$

$$a = \min \left\{ \sqrt{\hat{\psi}''(0)}, \sqrt{\hat{\psi}''(1)} \right\} > 0. \quad (4.37)$$

Then there is a unique solution $S_0 \in C^4(\mathbb{R}, (0, 1))$ of the initial value problem (4.34). This solution is strictly increasing and satisfies (4.20) and (4.28). Moreover, there are constants $K_1, \dots, K_3 > 0$ such that

$$0 < S_0(\zeta) \leq K_1 e^{-a|\zeta|}, \quad -\infty < \zeta \leq 0, \quad (4.38)$$

$$1 - K_2 e^{-a\zeta} \leq S_0(\zeta) < 1, \quad 0 \leq \zeta < \infty, \quad (4.39)$$

$$|\partial^i S_0(\zeta)| \leq K_3 e^{-a|\zeta|}, \quad -\infty < \zeta < \infty, \quad i = 1, \dots, 4. \quad (4.40)$$

This theorem follows immediately from the standard theory of ordinary differential equations, and we omit the proof.

Theorem 4.2 *Assume that $\hat{\psi}$ belongs to $C^4([0, 1], \mathbb{R})$ and satisfies the assumptions (4.35) – (4.37), that f^{-1} exists and belongs to the space $C^2(\mathbb{R}, \mathbb{R})$, that $f(0) = 0$ and that g defined by (4.6) belongs to $C^2(\mathbb{R}, \mathbb{R})$. Suppose that $(\hat{u}, \hat{T}, \hat{S}, \Gamma)$ solves (4.1) – (4.5) and satisfies Assumption C. Let S_0 be the solution of the boundary value problem (4.20), (4.28). Then for every $(t, \eta) \in \Gamma$ there is a unique solution $\zeta \mapsto S_1(t, \eta, \zeta) : \mathbb{R} \rightarrow \mathbb{R}$ of the boundary value problem (4.21), (4.29), (4.30) with F_1 given by (4.22), which is orthogonal to the function S_0' :*

$$\int_{-\infty}^{\infty} S_1(t, \eta, \zeta) S_0'(\zeta) d\zeta = 0. \quad (4.41)$$

S_1 belongs to the space $C^2(\Gamma \times \mathbb{R})$. Moreover, with a defined in (4.37) there are constants $K_1 \dots K_4$ such that

$$\|D_{(t, \eta, \zeta)}^\alpha S_1\|_{L^\infty(\Gamma \times \mathbb{R})} \leq K_1, \quad |\alpha| \leq 2. \quad (4.42)$$

$$\left| S_1(t, \eta, \zeta) - \frac{\bar{\varepsilon} \hat{T}^{(+)}(t, \eta)}{\psi''(1)} \right| \leq K_2 e^{-a\zeta}, \quad (t, \eta, \zeta) \in \Gamma \times [0, \infty), \quad (4.43)$$

$$\left| S_1(t, \eta, \zeta) - \frac{\bar{\varepsilon} \hat{T}^{(-)}(t, \eta)}{\psi''(0)} \right| \leq K_3 e^{-a\zeta}, \quad (t, \eta, \zeta) \in \Gamma \times (-\infty, 0], \quad (4.44)$$

$$|\partial_\zeta^i S_1(t, \eta, \zeta)| \leq K_4 e^{-a|\zeta|}, \quad (t, \eta, \zeta) \in \Gamma \times \mathbb{R}, \quad i = 1, 2. \quad (4.45)$$

$$|\partial_t \partial_\zeta S_1(t, \eta, \zeta)|, |\nabla_\eta \partial_\zeta S_1(t, \eta, \zeta)| \leq K_5 e^{-a|\zeta|}, \quad (t, \eta, \zeta) \in \Gamma \times \mathbb{R}. \quad (4.46)$$

Before we prove this theorem in Section 5.1, we state the main results of this section in the following theorem and corollary:

Theorem 4.3 *Let the assumptions for $\hat{\psi}$ and f in Theorem 4.1 and Theorem 4.2 be satisfied. Assume in addition that f is Lipschitz continuous. Let $(\hat{u}, \hat{T}, \hat{S}, \Gamma)$ be a solution of (4.1) – (4.5) satisfying Assumption C. Let $S^{(\mu)}$, $u^{(\mu)}$ and $T^{(\mu)}$ be defined by (4.8) – (4.15) with the functions S_0, S_1 given in Theorems 4.1 and 4.2 and with the constant a defined by (4.37).*

Then the function $(u^{(\mu)}, T^{(\mu)}, S^{(\mu)})$ belongs to the space $C^2(Q) \times C^1(Q) \times C^2(Q)$, satisfies equation (1.21) identically and (1.20), (1.22) asymptotically for $\mu \rightarrow 0$. More precisely, let $1 > \mu_0 > 0$ and $\lambda_0 > 0$ be fixed. Then there are constants K_1, \dots, K_4 such that for all $\mu \in (0, \mu_0]$, $\lambda \in (0, \lambda_0]$

$$\|\operatorname{div}_x T^{(\mu)} + \mathbf{b}\|_{L^\infty(\Gamma_i[\mu, \lambda] \cup \Gamma_m[\mu, \lambda])} \leq \lambda^{-1/2} K_1, \quad (4.47)$$

$$\|\operatorname{div}_x T^{(\mu)} + \mathbf{b}\|_{L^\infty(\Gamma_o[\mu, \lambda])} \leq \mu K_2, \quad (4.48)$$

$$\left\| S_t^{(\mu)} + \frac{1}{(\mu\lambda)^{1/2}} f\left(W_S + \frac{1}{\mu^{1/2}} \hat{\psi}'(S^{(\mu)}) - \mu^{1/2} \lambda \Delta_x S^{(\mu)}\right) \right\|_{L^\infty(\Gamma_i[\mu, \lambda] \cup \Gamma_m[\mu, \lambda])} \leq |\ln \mu| \lambda^{-1/2} K_3, \quad (4.49)$$

$$\left\| S_t^{(\mu)} + \frac{1}{(\mu\lambda)^{1/2}} f\left(W_S + \frac{1}{\mu^{1/2}} \hat{\psi}'(S^{(\mu)}) - \mu^{1/2} \lambda \Delta_x S^{(\mu)}\right) \right\|_{L^\infty(\Gamma_o[\mu, \lambda])} \leq \mu^{1/2} \lambda^{-1/2} K_4, \quad (4.50)$$

where $W_S = W_S(\varepsilon(u^{(\nu)}), S^{(\nu)})$.

The **proof** of this theorem is given in Section 5.2.

The definitions (4.17) and (4.18) imply that there is a constant K_5 such that

$$\text{meas}(\Gamma_i[\mu, \lambda] \cup \Gamma_m[\mu, \lambda]) \leq (\mu\lambda)^{1/2} |\ln \mu| K_5.$$

This estimate and Theorem 4.3 immediately yield

Corollary 4.4 *There are constants $K_6, K_7 > 0$ such that for all $\mu, \lambda > 0$*

$$\|\text{div}_x T^{(\mu)} + \mathbf{b}\|_{L^1(Q)} \leq |\ln \mu| \mu^{1/2} K_6, \quad (4.51)$$

$$\left\| S_t^{(\mu)} + \frac{1}{(\mu\lambda)^{1/2}} f\left(W_S + \frac{1}{\mu^{1/2}} \hat{\psi}'(S^{(\mu)}) - \mu^{1/2} \lambda \Delta_x S^{(\mu)}\right)\right\|_{L^1(Q)} \leq |\ln \mu|^2 \left(\frac{\mu}{\lambda}\right)^{1/2} K_7. \quad (4.52)$$

Remarks. We call $(u^{(\mu)}, T^{(\mu)}, S^{(\mu)})$ asymptotic solution of first order, since the error, up to which the equations (1.20) and (1.22) are satisfied, tends to zero in the L^1 -norm with the order $|\ln \mu|^2 \mu^{1/2}$ for $\mu \rightarrow 0$. Here we follow the terminology introduced in Section 2.

The right hand sides of the equations (4.47) – (4.52) do not tend to zero for $\lambda \rightarrow 0$. We can understand the dependence of solutions of the Allen-Cahn model on the parameter λ , if with a solution (u, T, S) of (1.20) – (1.22) we introduce the functions

$$(\check{u}, \check{T}, \check{S})(t, x) = \left(\frac{u}{\lambda^{1/2}}, T, S\right)(\lambda^{1/2}t, \lambda^{1/2}x), \quad \check{\mathbf{b}}(t, x) = \lambda^{1/2} \mathbf{b}(\lambda^{1/2}t, \lambda^{1/2}x).$$

These functions satisfy the Allen-Cahn system

$$\begin{aligned} -\text{div}_x \check{T} &= \check{\mathbf{b}}, \\ \check{T} &= D(\varepsilon(\nabla_x \check{u}) - \bar{\varepsilon} \check{S}), \\ \partial_t \check{S} &= -\frac{1}{\mu^{1/2}} f(-\bar{\varepsilon} : \check{T} + \frac{1}{\mu^{1/2}} \hat{\psi}'(\check{S}) - \mu^{1/2} \Delta_x \check{S}), \end{aligned}$$

in the scaled domain $\Omega_\lambda = \frac{1}{\lambda^{1/2}} \Omega$. The parameter λ has been transformed away in this system. If we denote the level surface $\{S = \frac{1}{2}\}$ by Γ' and if $\kappa_{\Gamma'}$ is twice the mean curvature of Γ' , then $\check{\Gamma}' = \frac{1}{\lambda^{1/2}} \Gamma'$ is the level surface $\{\check{S} = \frac{1}{2}\}$ with twice the mean curvature $\kappa_{\check{\Gamma}'} = \lambda^{1/2} \kappa_{\Gamma'}$. Therefore the “curvature” of the diffusive interface for the transformed system tends to zero with the order $\lambda^{1/2}$. From this we can understand why the coefficient of the curvature term in the kinetic relation (4.3), which by our asymptotic results determines the speed of the level surface Γ' within the diffusive interface, is proportional to $\lambda^{1/2}$.

5 Proof of the main theorems from Section 4

5.1 Proof of Theorem 4.2

Choose $\varphi \in C^\infty(\mathbb{R})$ such that

$$\varphi(\zeta) = \begin{cases} 0, & \zeta \leq -1 \\ 1, & \zeta \geq 1, \end{cases}$$

and define

$$\varrho(t, \eta, \zeta) = \frac{\bar{\varepsilon} : \hat{T}^{(+)}(t, \eta)}{\hat{\psi}''(1)} \varphi(\zeta) + \frac{\bar{\varepsilon} : \hat{T}^{(-)}(t, \eta)}{\hat{\psi}''(0)} (1 - \varphi(\zeta)). \quad (5.1)$$

For the solution of (4.21), (4.29), (4.30) we make the ansatz

$$S_1(t, \eta, \zeta) = w(t, \eta, \zeta) + \varrho(t, \eta, \zeta). \quad (5.2)$$

Insertion of this ansatz into (4.21) shows that w must satisfy the differential equation

$$\hat{\psi}''(S_0(\zeta))w(\zeta) - \partial_\zeta^2 w(\zeta) = F_1(t, \eta, \zeta) + F_2(t, \eta, \zeta), \quad (5.3)$$

for all $\zeta \in \mathbb{R}$, where F_1 is given in (4.22) and where

$$F_2 = -(\hat{\psi}''(S_0) - \partial_\zeta^2)\varrho. \quad (5.4)$$

Comparison of (5.1), (5.2) and (4.29), (4.30) show that w must also satisfy

$$\lim_{\zeta \rightarrow \pm\infty} w(t, \eta, \zeta) = 0. \quad (5.5)$$

We apply the L^2 -theory of linear selfadjoint differential operators on \mathbb{R} to the symmetric operator $\hat{\psi}''(S_0) - \partial_\zeta^2$ to show that a solution w of the boundary value problem (5.3), (5.5) exists. S_1 given by (5.2) will then solve (4.21), (4.29), (4.30). To apply this theory it must be shown that the right hand side $F_1 + F_2$ belongs to $L^2(\mathbb{R})$. Since the operator $\hat{\psi}''(S_0) - \partial_\zeta^2$ has a non-zero kernel, as will be seen, we must also show that $F_1 + F_2$ is orthogonal to this kernel.

We first show that the function $F_1 + F_2$ belongs to $C^2(\Gamma \times \mathbb{R})$ and decays exponentially for $\zeta \rightarrow \pm\infty$, which of course implies that $(\zeta \mapsto (F_1 + F_2)(t, \eta, \zeta)) \in L^2(\mathbb{R})$. To this end note that insertion of $[\hat{T}] = \hat{T}^{(+)} - \hat{T}^{(-)}$ into (4.22) yields

$$\begin{aligned} F_1(t, \eta, \zeta) &= \bar{\varepsilon} : \hat{T}^{(+)}(t, \eta) S_0(\zeta) + \bar{\varepsilon} : \hat{T}^{(-)}(t, \eta) (1 - S_0(\zeta)) \\ &\quad - \lambda^{1/2} \kappa_\Gamma(t, \eta) S_0'(\zeta) + f^{-1}(s(t, \eta) S_0'(\zeta)). \end{aligned}$$

Therefore we can decompose $F_1 + F_2$ in the form

$$F_1 + F_2 = \sum_{j=1}^4 I_j, \quad (5.6)$$

with

$$I_1 = f^{-1}(s S_0') - \lambda^{1/2} \kappa_\Gamma S_0', \quad (5.7)$$

$$I_2 = \bar{\varepsilon} : \hat{T}^{(+)} \left(S_0 - \frac{\hat{\psi}''(S_0)}{\hat{\psi}''(1)} \varphi \right), \quad (5.8)$$

$$I_3 = \bar{\varepsilon} : \hat{T}^{(-)} \left((1 - S_0) - \frac{\hat{\psi}''(S_0)}{\hat{\psi}''(0)} (1 - \varphi) \right), \quad (5.9)$$

$$I_4 = \left(\frac{\bar{\varepsilon} : \hat{T}^{(+)}}{\hat{\psi}''(1)} \varphi'' - \frac{\bar{\varepsilon} : \hat{T}^{(-)}}{\hat{\psi}''(0)} \varphi'' \right). \quad (5.10)$$

We investigate everyone of the terms I_1, \dots, I_4 separately. To study I_1 , note that by Assumption C we have that the curvature κ_Γ and the normal vector field n are two-times continuously differentiable on Γ . The same is true for $[\hat{C}]$. This follows from Assumption C and from the definitions of the Eshelby tensor \hat{C} in (1.19) and of ψ in (1.11). Hence the argument of the function g in (4.3) is two-times continuously differentiable on Γ . Since by assumption $g \in C^2(\mathbb{R})$, we conclude from (4.3) that $s \in C^2(\Gamma, \mathbb{R})$. Using that by Theorem 4.1 the function S_0 is four times differentiable and that $f^{-1} \in C^2(\mathbb{R})$, we therefore obtain from (5.7) that $I_1 \in C^2(\Gamma \times \mathbb{R})$. If we use that $f^{-1}(0) = 0$ and apply the mean value theorem to f^{-1} , we also obtain from (5.7) and (4.40) that

$$|I_1(t, \eta, \zeta)| \leq K e^{-a|\zeta|}, \quad (5.11)$$

with a suitable constant $K > 0$, which can be chosen independent of t and η . To study I_4 , remember that by assumption φ'' is infinitely differentiable and has compact support contained in $[-1, 1]$ and that $\hat{T}^{(+)}, \hat{T}^{(-)} \in C^2(\Gamma)$. From (5.10) we thus get

$$I_4 \in C^2(\Gamma \times \mathbb{R}), \quad I_4(t, \eta, \zeta) = 0 \quad \text{for } |\zeta| \geq 1. \quad (5.12)$$

Since by assumption $\hat{\psi} \in C^4$ we conclude from (5.8) by a similar reasoning that $I_2 \in C^2(\Gamma \times \mathbb{R})$. To study the behavior of I_2 for $\zeta \rightarrow \pm\infty$, note that the mean value theorem yields

$$\frac{|\hat{\psi}''(S_0(\zeta)) - \hat{\psi}''(1)|}{\hat{\psi}''(1)} \leq K |S_0(\zeta) - 1|,$$

with a suitable constant $K > 0$. Since $\varphi = 1$ on $[1, \infty)$, we infer from this inequality and from (4.39) that for $\zeta \geq 1$

$$\begin{aligned} |I_2| &= \left| \bar{\varepsilon} : \hat{T}^{(+)} \left(1 + (S_0 - 1) - \left(1 + \frac{\hat{\psi}''(S_0) - \hat{\psi}''(1)}{\hat{\psi}''(1)} \right) \varphi \right) \right| \\ &\leq |\bar{\varepsilon} : \hat{T}^{(+)}| (|S_0 - 1| + K |S_0 - 1|) \leq K' K_2 e^{-a|\zeta|}, \end{aligned} \quad (5.13)$$

where the constants K' and K_2 are independent of (t, η) . Since $\varphi = 0$ on $(-\infty, -1]$, we see from (4.38) and (5.8) that the estimate (5.13) holds for all $\zeta \in \mathbb{R}$. In the same way we see that $I_3 \in C^2(\Gamma \times \mathbb{R})$ and that

$$|I_3| \leq K e^{-a|\zeta|}, \quad \zeta \in \mathbb{R}. \quad (5.14)$$

Therefore everyone of the terms I_1, \dots, I_4 belongs to $C^2(\Gamma \times \mathbb{R})$. From (5.6) and (5.11) – (5.14) we thus conclude that $F_1 + F_2 \in C^2(\Gamma \times \mathbb{R})$ and that $F_1 + F_2$ decays exponentially, as we stated:

$$|(F_1 + F_2)(t, \eta, \zeta)| \leq K e^{-a|\zeta|}, \quad \text{for all } (t, \eta, \zeta) \in \Gamma \times \mathbb{R}, \quad (5.15)$$

where K is independent of (t, η, ζ) .

To show that the kernel of the operator $\hat{\psi}''(S_0) - \partial_\zeta^2$ is non-zero it suffices to differentiate (4.20), which yields

$$\hat{\psi}''(S_0) S_0' - \partial_\zeta^2 S_0' = 0.$$

Since S_0' decays to zero exponentially for $\zeta \rightarrow \pm\infty$, by (4.40), it follows that S_0' is an eigenfunction of the boundary value problem (5.3), (5.5) to the eigenvalue 0. From the

theory of ordinary differential equations we know that the eigenspace is one-dimensional. Therefore this boundary value problem has a solution w if the right hand side $F_1 + F_2$ of (5.3) is orthogonal to the eigenfunction S'_0 . To verify that $F_1 + F_2$ satisfies this orthogonality condition note first that since S'_0 decays exponentially we obtain from (5.4) by partial integration

$$\int_{-\infty}^{\infty} S'_0 F_2 d\zeta = - \int_{-\infty}^{\infty} S'_0 (\hat{\psi}''(S_0) - \partial_{\zeta}^2) \varrho d\zeta = \int_{-\infty}^{\infty} ((\hat{\psi}''(S_0) - \partial_{\zeta}^2) S'_0) \varrho d\zeta = 0. \quad (5.16)$$

Furthermore, the definition of F_1 in (4.22) and the differential equation (4.34) yield

$$\begin{aligned} & \int_{-\infty}^{\infty} S'_0 F_1 d\zeta \\ &= \int_{-\infty}^{\infty} \bar{\varepsilon} : [\hat{T}] S_0 S'_0 + \bar{\varepsilon} : \hat{T}^{(-)} S'_0 - \lambda^{1/2} \kappa_{\Gamma} (S'_0)^2 + f^{-1}(s S'_0) S'_0 d\zeta \\ &= \left[\bar{\varepsilon} : [\hat{T}] \frac{1}{2} S_0^2 + \bar{\varepsilon} : \hat{T}^{(-)} S_0 \right]_{-\infty}^{\infty} \\ &\quad + \int_{-\infty}^{\infty} \left(-\lambda^{1/2} \kappa_{\Gamma} \sqrt{2\hat{\psi}(S_0)} + f^{-1}(s \sqrt{2\hat{\psi}(S_0)}) \right) S'_0 d\zeta \\ &= \frac{1}{2} \bar{\varepsilon} : [\hat{T}] + \bar{\varepsilon} : \hat{T}^{(-)} - \lambda^{1/2} \kappa_{\Gamma} \int_0^1 \sqrt{2\hat{\psi}(r)} dr + \int_0^1 f^{-1}(s \sqrt{2\hat{\psi}(r)}) dr \\ &= -n \cdot [\hat{C}] n - \lambda^{1/2} c_1 \kappa_{\Gamma} + g^{-1}(s) = 0. \end{aligned} \quad (5.17)$$

To get the second last equality sign we employed (1.27) and (4.6). We also used (2.30), which implies

$$\frac{1}{2} \bar{\varepsilon} : [\hat{T}] + \bar{\varepsilon} : \hat{T}^{(-)} = \frac{1}{2} \bar{\varepsilon} : (\hat{T}^{(+)} + \hat{T}^{(-)}) = \bar{\varepsilon} : \langle \hat{T} \rangle = -n \cdot [\hat{C}] n.$$

The last equality sign in (5.17) is a consequence of (4.3).

(5.16) and (5.17) imply that the right hand side of (5.3) is orthogonal to S'_0 . Hence there is a solution $w(t, \eta, \cdot) \in L^2(\mathbb{R})$ of the boundary value problem (5.3), (5.5). All solutions are obtained by adding multiples of the eigenfunction S'_0 to w . In particular, we can select a suitable coefficient function $\alpha(t, \eta)$ such that $w(t, \eta, \cdot) + \alpha(t, \eta) S'_0(\cdot)$ is orthogonal to S'_0 for all $(t, \eta) \in \Gamma$. We denote this modified solution again by w . This solution satisfies

$$|\partial_{\zeta}^i w(t, \eta, \zeta)| \leq K e^{-a|\zeta|}, \quad \text{for all } (t, \eta, \zeta) \in \Gamma \times \mathbb{R} \text{ and } i = 0, \dots, 2, \quad (5.18)$$

with K independent of (t, η, ζ) and with a defined in (4.37). This follows by standard techniques for linear ordinary differential equations, using that the coefficient function $\hat{\psi}''(S_0)$ in the differential equation (5.3) satisfies

$$\lim_{\zeta \rightarrow \infty} \hat{\psi}''(S_0(\zeta)) = \hat{\psi}''(1) \geq a^2 > 0, \quad \lim_{\zeta \rightarrow -\infty} \hat{\psi}''(S_0(\zeta)) = \hat{\psi}''(0) \geq a^2 > 0,$$

and that the right hand side of this differential equation satisfies the exponential estimate (5.15). Moreover, since $F_1 + F_2$ belongs to the space $C^2(\Gamma \times \mathbb{R})$, we know from the standard theory of eigenspaces of parameter dependent self adjoint differential operators [36] that also $w \in C^2(\Gamma \times \mathbb{R})$ and that w is bounded in $C^2(\Gamma \times \mathbb{R})$. From the definition of ρ in

(5.1) and from the properties of w , which we have verified by now, we immediately see that the function S_1 defined by (5.2) solves (4.21), (4.29), (4.30), belongs to $C^2(\Gamma \times \mathbb{R})$ and satisfies the estimate (4.42). The exponential estimates (4.43) – (4.45) are immediate consequences of (5.1) and (5.18). To prove (4.46) note that by (5.1) and (5.4) the functions $\partial_t \partial_\zeta \rho$ and $\partial_t \partial_\zeta F_2$ vanish for $|\zeta| \geq 1$. By differentiation of (5.3) we see that $\partial_t \partial_\zeta w$ is a solution of the linear differential equation

$$\hat{\psi}''(S_0(\zeta)) \partial_t \partial_\zeta w(\zeta) - \partial_\zeta^2 \partial_t \partial_\zeta w(\zeta) = \partial_t \partial_\zeta F_1(t, \eta, \zeta) + \partial_t \partial_\zeta F_2(t, \eta, \zeta) - \hat{\psi}'''(S_0) S_0' \partial_t w. \quad (5.19)$$

For the right hand side of this equation we have

$$|\partial_t \partial_\zeta F_1(t, \eta, \zeta) + \partial_t \partial_\zeta F_2(t, \eta, \zeta) - \hat{\psi}'''(S_0) S_0' \partial_t w| \leq K e^{-a|\zeta|}. \quad (5.20)$$

To show this note that w is bounded in $C^2(\Gamma \times \mathbb{R})$, hence $\partial_t w$ is bounded. If we differentiate (4.22) and use (4.40) we thus obtain

$$|\partial_t \partial_\zeta F_1(t, \eta, \zeta) - \hat{\psi}'''(S_0) S_0' \partial_t w| \leq K e^{-a|\zeta|},$$

which implies (5.20), since F_2 vanishes for $|\zeta| \geq 1$. Thus, (5.19) is a differential equation of the same type as (5.3) with an exponentially decaying right hand side. Therefore similar arguments as in the proof of (5.18) yield $|\partial_t \partial_\zeta w| \leq K e^{-a|\zeta|}$. This inequality and (5.2) together imply the estimate for $\partial_t \partial_\zeta S_1$ in (4.46), again using that $\partial_t \partial_\zeta \rho$ vanishes for $|\zeta| \geq 1$. The corresponding estimate for $\nabla_\eta \partial_\zeta S_1$ in (4.46) is proved in the same way.

To assure that (4.41) holds, we can add a multiple of S_0' to S_1 . Since S_0' satisfies (4.40), the new function, which we again denote by S_1 , has all the properties, which we just verified for S_1 . The proof is complete. \blacksquare

5.2 Proof of Theorem 4.3

To prove this theorem we compute in Section 5.2.1 an asymptotic expansion for the term $\operatorname{div}_x T^{(\mu)} + \mathbf{b}$ in powers of $\mu^{1/2}$. In Section 5.2.2 we derive such expansions for the term $S_t + (\mu\lambda)^{-1/2} f(W_S + \frac{1}{\mu^{1/2}} \hat{\psi}' - \mu^{1/2} \lambda \Delta_x S)$. The leading terms in these latter expansions vanish if (4.20), (4.21) and (4.25), (4.26) hold, for the higher order terms we derive estimates. In Section 5.2.3 we prove auxiliary estimates, which are needed to verify the inequalities (4.47) and (4.49) in the matching region $\Gamma_m[\mu, \lambda]$. Finally, in Section 5.2.4 we put all these results together to finish the proof of the inequalities (4.47) – (4.50).

5.2.1 Asymptotic expansion for $\operatorname{div}_x T^{(\mu)} + \mathbf{b}$

In the following we use the notation

$$T_0(t, \eta, \zeta) = D\left(\varepsilon(u^*(t, \eta) \otimes n(t, \eta)) - \bar{\varepsilon}\right) S_0(\zeta). \quad (5.21)$$

From (2.22) we see that $T_0(t, \eta, \zeta) = [\hat{T}](t, \eta) S_0(\zeta)$.

Lemma 5.1 *Assume that $(u_i^{(\mu)}, T_i^{(\mu)}, S_i^{(\mu)})$ is given by (4.11) – (4.16) for $i = 1, 2$, let T_0 be defined by (5.21) and set $\zeta^+ = \frac{\xi^+}{(\mu\lambda)^{1/2}}$, with ξ^+ defined in (2.18). Then we have in $Q \setminus \Gamma$ that*

$$T_2^{(\mu)} = \hat{T} + \mu^{1/2} \tilde{T}_1 - \mu D \bar{\varepsilon} \tilde{S}_2, \quad (5.22)$$

and in \mathcal{U} that

$$\hat{T} = [\hat{T}]\hat{S} + (\mu\lambda)^{1/2}D\varepsilon(\nabla_{\Gamma_\xi}u^*)\zeta^+ + D\varepsilon(\nabla_x v), \quad (5.23)$$

$$T_1^{(\mu)} = T_0 + \mu^{1/2}D(\lambda^{1/2}\varepsilon(\nabla_{\Gamma_\xi}u_0) - \bar{\varepsilon}S_1) + D\varepsilon(\nabla_x v), \quad (5.24)$$

$$\begin{aligned} W_S(\varepsilon(\nabla_x u_1^{(\mu)}), S_1^{(\mu)}) &= -\bar{\varepsilon} : T_1^{(\mu)} \\ &= -\bar{\varepsilon} : [\hat{T}]S_0 - \sigma_1 - \mu^{1/2}\bar{\varepsilon} : D(\lambda^{1/2}\varepsilon(\nabla_{\Gamma_\xi}u_0) - \bar{\varepsilon}S_1), \end{aligned} \quad (5.25)$$

where $\sigma_1(t, x) = \bar{\varepsilon} : D\varepsilon(\nabla_x v(t, x))$.

Proof: We insert (4.12) and (4.14) into (4.16) to obtain

$$\begin{aligned} T_2^{(\mu)} &= D\left(\varepsilon(\nabla_x(\hat{u} + \mu^{1/2}\tilde{u}_1)) - \bar{\varepsilon}(\hat{S} + \mu^{1/2}\tilde{S}_1 + \mu\tilde{S}_2)\right) \\ &= D(\varepsilon(\nabla_x\hat{u}) - \bar{\varepsilon}\hat{S}) + \mu^{1/2}D(\varepsilon(\nabla_x\tilde{u}_1) - \bar{\varepsilon}\tilde{S}_1) - \mu D\bar{\varepsilon}\tilde{S}_2. \end{aligned}$$

(5.22) is a consequence of this equation and of (4.2), (4.24). To prove (5.23) we insert (4.7) into (4.2) and remember (2.11). This yields

$$\begin{aligned} \hat{T} &= D(\varepsilon(\nabla_x(u^*\xi^+) + \nabla_x v) - \bar{\varepsilon}\hat{S}) \\ &= D\left(\varepsilon(u^* \otimes n \partial_\xi \xi^+ + (\mu\lambda)^{1/2}\nabla_{\Gamma_\xi}u^*\zeta^+) - \bar{\varepsilon}\hat{S}\right) + D\varepsilon(\nabla_x v). \end{aligned}$$

We use that $\partial_\xi \xi^+ = 1^+ = \hat{S}$ and employ (2.22) to obtain (5.23). Similarly, insertion of (4.11) and (4.13) into (4.16) yields

$$\begin{aligned} T_1^{(\mu)} &= D\left(\varepsilon((\mu\lambda)^{1/2}\nabla_x u_0 + \nabla_x v) - \bar{\varepsilon}(S_0 + \mu^{1/2}S_1)\right) \\ &= D\left(\varepsilon(\partial_\zeta u_0 \otimes n + (\mu\lambda)^{1/2}\nabla_{\Gamma_\xi}u_0) - \bar{\varepsilon}S_0 - \mu^{1/2}\bar{\varepsilon}S_1\right) + D\varepsilon(\nabla_x v). \end{aligned}$$

We use (4.15), which yields $\partial_\zeta u_0 = u^*S_0$, and employ (5.21) to get (5.24). Equation (5.25) is a direct consequence of (1.24) and (5.24). \blacksquare

Corollary 5.2 *We have*

$$(\operatorname{div}_x T_2^{(\mu)} + \mathbf{b})(t, x) = -\mu \operatorname{div}_x(D\bar{\varepsilon}\tilde{S}_2), \quad \text{in } Q \setminus \Gamma, \quad (5.26)$$

$$(\operatorname{div}_x T_1^{(\mu)} + \mathbf{b})(t, \eta, \xi) = R_{\operatorname{div}+\mathbf{b}}(\mu, t, \eta, \xi), \quad \text{in } \mathcal{U}, \quad (5.27)$$

where

$$R_{\operatorname{div}+\mathbf{b}} = \operatorname{div}_{\Gamma_\xi}[\hat{T}](S_0 - \hat{S}) + \mu^{1/2}\operatorname{div}_x D\left(\lambda^{1/2}\varepsilon(\nabla_{\Gamma_\xi}(u_0 - u^*\zeta^+)) - \bar{\varepsilon}S_1\right). \quad (5.28)$$

Proof: (5.26) is an immediate consequence of (5.22), (4.1) and (4.23). To prove (5.27) we conclude from (4.1) that

$$\operatorname{div}_x T_1^{(\mu)} + \mathbf{b} = \operatorname{div}_x(T_1^{(\mu)} - \hat{T}). \quad (5.29)$$

Since $T_0 = [\hat{T}]S_0$, we obtain from (5.23) and (5.24) for the difference on the right hand side of this equation that

$$T_1^{(\mu)} - \hat{T} = [\hat{T}](S_0 - \hat{S}) + \mu^{1/2}D\left(\lambda^{1/2}\varepsilon(\nabla_{\Gamma_\xi}(u_0 - u^*\zeta^+)) - \bar{\varepsilon}S_1\right).$$

(5.27) results by insertion of this equation into (5.29) and by noting that (2.12) and (4.5) together yield

$$\operatorname{div}_x([\hat{T}](S_0 - \hat{S})) = \partial_\xi(S_0 - \hat{S})[\hat{T}]n + \operatorname{div}_{\Gamma_\xi}[\hat{T}](S_0 - \hat{S}) = \operatorname{div}_{\Gamma_\xi}[\hat{T}](S_0 - \hat{S}).$$

This completes the proof of the corollary. \blacksquare

5.2.2 Asymptotic expansions and estimates for $S_t + (\mu\lambda)^{-1/2}f$

To prove the inequalities (4.49) and (4.50) we need estimates for the term $S_t^{(\mu)} + (\mu\lambda)^{-1/2}f(W_S + \frac{1}{\mu^{1/2}}\hat{\psi}' - \mu^{1/2}\lambda\Delta_x S^{(\mu)})$ on the left hand sides of these inequalities with $(u^{(\mu)}, S^{(\mu)})$ replaced by the function $(u_1^{(\mu)}, S_1^{(\mu)})$ and by $(u_2^{(\mu)}, S_2^{(\mu)})$, respectively, where $u_i^{(\mu)}$ and $S_i^{(\mu)}$ are defined in (4.11) – (4.14). These estimates are derived in this subsection. The proof of the estimates is based on asymptotic expansions in powers of $\mu^{1/2}$.

We begin by deriving the estimate for $(u_1^{(\mu)}, S_1^{(\mu)})$. Note first that

$$\begin{aligned} & \left| \partial_t S_1^{(\mu)} + \frac{1}{(\mu\lambda)^{1/2}} f\left(W_S + \frac{1}{\mu^{1/2}}\hat{\psi}' - \mu^{1/2}\lambda\Delta_x S_1^{(\mu)}\right) \right| \\ &= \frac{1}{(\mu\lambda)^{1/2}} \left| -f\left(f^{-1}(-(\mu\lambda)^{1/2}\partial_t S_1^{(\mu)})\right) + f\left(W_S + \frac{1}{\mu^{1/2}}\hat{\psi}' - \mu^{1/2}\lambda\Delta_x S_1^{(\mu)}\right) \right| \\ &\leq \frac{L_f}{(\mu\lambda)^{1/2}} \left| W_S + \frac{1}{\mu^{1/2}}\hat{\psi}' - \mu^{1/2}\lambda\Delta_x S_1^{(\mu)} - f^{-1}\left(-(\mu\lambda)^{1/2}\partial_t S_1^{(\mu)}\right) \right|, \end{aligned} \quad (5.30)$$

where $L_f > 0$ denotes the Lipschitz constant of f . Here we used that by assumption $f(0) = 0$. To estimate the absolute value term on the right hand side of this inequality we derive an asymptotic expansion for this term and estimate the remainder term. To this end we first observe that (3.45) is also valid in the present situation. This follows from the definition of v in (4.7). From this equation and the mean value theorem we obtain

$$\sigma_1(t, \eta, \xi) = \bar{\varepsilon} : \hat{T}^{(-)}(t, \eta) + (\sigma_1(t, \eta, \xi) - \sigma(t, \eta, 0)) = \bar{\varepsilon} : \hat{T}^{(-)}(t, \eta) + \sigma^*(t, \eta, \xi)\xi.$$

Insertion of this equation into (5.25) yields

$$W_S(\varepsilon(\nabla_x u_1^{(\mu)}), S_1^{(\mu)}) = -\bar{\varepsilon} : [\hat{T}]S_0 - \bar{\varepsilon} : \hat{T}^{(-)} - \mu^{1/2}R_W, \quad (5.31)$$

with the remainder term

$$R_W(t, \eta, \xi, \zeta) = \lambda^{1/2}\sigma^*(t, \eta, \xi)\zeta + \bar{\varepsilon} : D\left(\lambda^{1/2}\varepsilon(\nabla_{\Gamma_\xi} u_0(t, \eta, \zeta)) - \bar{\varepsilon}S_1(t, \eta, \zeta)\right).$$

Here we set $\zeta = \frac{\xi}{(\mu\lambda)^{1/2}}$, as always. Since σ^* is bounded on the neighborhood \mathcal{U} of Γ and since $|\zeta| \leq \frac{2|\ln \mu|}{a}$ for $(t, \eta, \xi) \in (\Gamma_i[\mu, \lambda] \cup \Gamma_m[\mu, \lambda])$, by (4.17) and (4.18), we see that if we choose $\mu_0, \lambda_0 > 0$ sufficiently small such that $\Gamma_i[\mu_0, \lambda_0] \cup \Gamma_m[\mu_0, \lambda_0] \subseteq \mathcal{U}$, then this remainder term satisfies the estimate

$$|R_W(t, \eta, \xi, \zeta)| \leq K_1 \frac{2|\ln \mu|}{a} + K_2, \quad (5.32)$$

for all $\mu \in (0, \mu_0]$, $\lambda \in (0, \lambda_0]$ and all $(t, \eta, \xi) \in \Gamma_i[\mu, \lambda] \cup \Gamma_m[\mu, \lambda]$.

Next we use Taylor's formula as in (3.48) to compute an expansion for $\hat{\psi}'(S_1^{(\mu)})$ and proceed as in (3.50) – (3.52) to derive an expansion of $\Delta_x S_1^{(\mu)}$. The result is

$$\begin{aligned} & \frac{1}{\mu^{1/2}}\hat{\psi}'(S_1^{(\mu)}) - \mu^{1/2}\lambda\Delta_x S_1^{(\mu)} \\ &= \frac{1}{\mu^{1/2}}\left(\hat{\psi}'(S_0(\zeta)) - S_0''(\zeta)\right) + \left(\hat{\psi}''(S_0(\zeta))S_1(\zeta) - S_1''(\zeta) + \lambda^{1/2}\kappa_\Gamma S_0'(\zeta)\right) \\ & \quad + \mu^{1/2}R_{\hat{\psi}'-\Delta}(\mu, \lambda, t, \eta, \xi, \zeta), \end{aligned} \quad (5.33)$$

with

$$\begin{aligned} |R_{\hat{\psi}'-\Delta}(\mu, \lambda, t, \eta, \xi, \zeta)| &= \left| \frac{1}{2} \hat{\psi}^{(III)}(S_0 + \vartheta \mu^{1/2} S_1) S_1^2 \right. \\ &\quad \left. + \lambda \kappa^*(\xi) \zeta S_0' + \lambda^{1/2} \kappa_{\Gamma_\xi} S_1' - \lambda \Delta_{\Gamma_\xi} S_1^{(\mu)} \right| \leq K_3 \frac{2|\ln \mu|}{a} + K_4, \end{aligned} \quad (5.34)$$

for $(\mu, \lambda) \in (0, \mu_0] \times (0, \lambda_0]$ and $(t, \eta, \xi) \in \Gamma_i[\mu, \lambda] \cup \Gamma_m[\mu, \lambda]$.

Equation (3.59), which also holds for $S_1^{(\mu)}$ instead of $S^{(\nu)}$, yields

$$\begin{aligned} &(\mu\lambda)^{1/2} \partial_t S_1^{(\mu)}(t, \eta, \xi) \\ &= (\mu\lambda)^{1/2} \left(S_{1,t}^{(\mu)}(t, \eta, \xi) - \xi \partial_t n(t, \eta) \cdot \nabla_\eta S_1^{(\mu)}(t, \eta, \xi) - s(t, \eta) \partial_\xi S_1^{(\mu)}(t, \eta, \xi) \right) \\ &= -s(t, \eta) S_0'(\zeta) + \mu^{1/2} R_{\partial_t}(\mu, \lambda, t, \eta, \xi). \end{aligned} \quad (5.35)$$

The estimates (4.42) implies that there is a constant K_5 such that for all $(\mu, \lambda) \in (0, \mu_0] \times (0, \lambda_0]$ and $(t, \eta, \xi) \in \Gamma_i[\mu, \lambda] \cup \Gamma_m[\mu, \lambda]$ the remainder term satisfies

$$|R_{\partial_t}(\mu, \lambda, t, \eta, \xi)| = |(\mu\lambda)^{1/2} (S_{1,t} - \xi \partial_t n \cdot \nabla_\eta S_1) - s S_1'| \leq K_5. \quad (5.36)$$

We apply the mean value theorem to f^{-1} and obtain from (5.35), (5.36) that

$$f^{-1}(-(\mu\lambda)^{1/2} \partial_t S_1^{(\mu)}) = f^{-1}(s(t, \eta) S_0'(\zeta)) + \mu^{1/2} R_f(\mu, \lambda, t, \eta, \xi), \quad (5.37)$$

with

$$|R_f(\mu, \lambda, t, \eta, \xi)| = |(f^{-1})'(s S_0' - \vartheta \mu^{1/2} R_{\partial_t}) R_{\partial_t}(\mu, \lambda, t, \eta, \xi)| \leq K_6. \quad (5.38)$$

Combination of (5.31), (5.33) and (5.37) results in the asymptotic expansion

$$\begin{aligned} &W_S(\varepsilon(\nabla_x u_1^{(\mu)}), S_1^{(\mu)}) + \frac{1}{\mu^{1/2}} \hat{\psi}'(S_1^{(\mu)}) - \mu^{1/2} \lambda \Delta_x S_1^{(\mu)} - f^{-1}(-(\mu\lambda)^{1/2} \partial_t S_1^{(\mu)}) \\ &= \frac{1}{\mu^{1/2}} \left(\hat{\psi}'(S_0) - S_0'' \right) \\ &\quad + \left(\hat{\psi}''(S_0) S_1 - S_1'' + \lambda^{1/2} \kappa_{\Gamma} S_0' - \bar{\varepsilon} : [\hat{T}] S_0 - \bar{\varepsilon} : \hat{T}^{(-)} - f^{-1}(s S_0') \right) \\ &\quad + \mu^{1/2} (-R_W + R_{\hat{\psi}'-\Delta} - R_f). \end{aligned} \quad (5.39)$$

Corollary 5.3 *If S_0 and S_1 satisfy (4.20), (4.21) with F_1 given by (4.22), then*

$$\begin{aligned} &\left| \partial_t S_1^{(\mu)} + \frac{1}{(\mu\lambda)^{1/2}} f \left(W_S(\varepsilon(\nabla_x u_1^{(\mu)}), S_1^{(\mu)}) + \frac{1}{\mu^{1/2}} \hat{\psi}'(S_1^{(\mu)}) - \mu^{1/2} \lambda \Delta_x S_1^{(\mu)} \right) \right| \\ &\leq \frac{L_f}{\lambda^{1/2}} |(-R_W + R_{\hat{\psi}'-\Delta} - R_f)| \leq \frac{K L_f}{\lambda^{1/2}} \left(\frac{|\ln \mu|}{a} + 1 \right), \end{aligned} \quad (5.40)$$

for all $\mu \in (0, \mu_0]$, $\lambda \in (0, \lambda_0]$ and $(t, \eta, \xi) \in \Gamma_i[\mu, \lambda] \cup \Gamma_m[\mu, \lambda]$. Here L_f denotes the Lipschitz constant of f .

Proof: If (4.20) and (4.21) hold, then the right hand side of (5.39) reduces to $\mu^{1/2}(-R_W + R_{\hat{\psi}'-\Delta} - R_f)$. Consequently (5.40) follows by insertion of (5.39) into (5.30), noting the estimates (5.32), (5.34) and (5.38). \blacksquare

To derive the estimate for the left hand side of (4.49) and (4.50) with $(u^{(\mu)}, S^{(\mu)})$ replaced by $(u_2^{(\mu)}, S_2^{(\mu)})$ note that $W_S(\varepsilon(\nabla_x u_2^{(\mu)}), S_2^{(\mu)}) = -\bar{\varepsilon} : T_2^{(\mu)}$, by (1.24). From this equation and from (4.12), (5.22) we obtain by a straightforward computation using Taylor's theorem that in the domain $\gamma \cup \gamma'$

$$\begin{aligned} & W_S(\varepsilon(\nabla_x u_2^{(\mu)}), S_2^{(\mu)}) + \frac{1}{\mu^{1/2}} \hat{\psi}'(S_2^{(\mu)}) - \mu^{1/2} \lambda \Delta_x S_2^{(\mu)} \\ &= \frac{1}{\mu^{1/2}} \hat{\psi}'(\hat{S}) - \bar{\varepsilon} : \hat{T} + \hat{\psi}''(\hat{S}) \tilde{S}_1 + \mu^{1/2} (-\bar{\varepsilon} : \tilde{T}_1 + \hat{\psi}''(\hat{S}) \tilde{S}_2 + \frac{1}{2} \hat{\psi}'''(\hat{S}) \tilde{S}_1^2) \\ & \quad + \mu R_1(\mu, \lambda, t, x), \end{aligned} \tag{5.41}$$

where

$$\begin{aligned} R_1(\mu, \lambda, t, x) &= \hat{\psi}'''(\hat{S})(\tilde{S}_1 \tilde{S}_2 + \mu^{1/2} \frac{1}{2} \tilde{S}_2^2) \\ & \quad + \frac{1}{6} \hat{\psi}^{(IV)}(\hat{S} + \vartheta(\mu^{1/2} \tilde{S}_1 + \mu \tilde{S}_2))(\tilde{S}_1 + \mu^{1/2} \tilde{S}_2)^3 - \lambda \Delta_x (\tilde{S}_1 + \mu^{1/2} \tilde{S}_2) + \bar{\varepsilon} : D \bar{\varepsilon} \tilde{S}_2. \end{aligned}$$

Furthermore, since $\partial_t \hat{S}(t, x) = 0$ for $(t, x) \in (\gamma \cup \gamma')$, we have in the domain $\gamma \cup \gamma'$

$$\partial_t S_2^{(\mu)} = \partial_t (\hat{S} + \mu^{1/2} \tilde{S}_1 + \mu \tilde{S}_2) = \mu^{1/2} R_2(\mu, t, x), \tag{5.42}$$

where $R_2(\mu, t, x) = \partial_t \tilde{S}_1 + \mu^{1/2} \tilde{S}_2$. With these preparatory results we obtain

Corollary 5.4 *Let L_f be the Lipschitz constant of f . If \tilde{S}_1 and \tilde{S}_2 satisfy (4.25) and (4.26), then the inequality*

$$\begin{aligned} & \left| \partial_t S_2^{(\mu)} + \frac{1}{(\mu\lambda)^{1/2}} f \left(W_S(\varepsilon(\nabla_x u_2^{(\mu)}), S_2^{(\mu)}) + \frac{1}{\mu^{1/2}} \hat{\psi}'(S_2^{(\mu)}) - \mu^{1/2} \lambda \Delta_x S_2^{(\mu)} \right) \right| \\ & \leq \mu^{1/2} (|R_2| + \frac{L_f}{\lambda^{1/2}} |R_1|) \leq \mu^{1/2} \frac{L_f}{\lambda^{1/2}} K, \end{aligned} \tag{5.43}$$

holds for all $\mu \in (0, \mu_0]$, $\lambda \in (0, \lambda_0]$ and all $(t, x) \in (\gamma \cup \gamma')$.

Proof: Observe that $\hat{\psi}'(\hat{S}) = 0$ in $\gamma \cup \gamma'$, since $\hat{\psi}'(0) = \hat{\psi}'(1) = 0$ and since \hat{S} takes only the values 0 or 1. Thus, if \tilde{S}_1 and \tilde{S}_2 satisfy the equations (4.25) and (4.26), then the right hand side of (5.41) reduces to μR_1 . From (5.41) and (5.42) we thus infer that the left hand side of (5.43) is equal to $|\mu^{1/2} R_2 + \frac{1}{(\mu\lambda)^{1/2}} f(\mu R_1)|$. This implies (5.43), since R_1 is bounded on $(0, \mu_0] \times (0, \lambda_0] \times (\gamma \cup \gamma')$, since R_2 is bounded on $(0, \mu_0] \times (\gamma \cup \gamma')$ and since $f(0) = 0$. \blacksquare

5.2.3 Auxiliary estimates

The following estimates are needed to prove (4.47) and (4.49) in the matching region $\Gamma_m[\mu, \lambda]$:

Lemma 5.5 *The functions $S_1^{(\mu)}$, $S_2^{(\mu)}$, $u_1^{(\mu)}$ and $u_2^{(\mu)}$ defined in (4.11) – (4.14) satisfy*

$$\|S_1^{(\mu)} - S_2^{(\mu)}\|_{L^\infty(\Gamma_m[\mu, \lambda])} \leq K\mu |\ln \mu| \quad (5.44)$$

$$\|D_x^\alpha(S_1^{(\mu)} - S_2^{(\mu)})\|_{L^\infty(\Gamma_m[\mu, \lambda])} \leq K\lambda^{-\frac{|\alpha|}{2}} \mu^{\frac{2-|\alpha|}{2}}, \quad 1 \leq |\alpha| \leq 2, \quad (5.45)$$

$$\|\partial_t(S_1^{(\mu)} - S_2^{(\mu)})\|_{L^\infty(\Gamma_m[\mu, \lambda])} \leq K\lambda^{-1/2} \mu^{1/2} \quad (5.46)$$

$$\|u_1^{(\mu)} - u_2^{(\mu)}\|_{L^\infty(\Gamma_m[\mu, \lambda])} \leq K\mu \frac{|\ln \mu| \lambda^{1/2}}{a}, \quad (5.47)$$

$$\|\nabla_x(u_1^{(\mu)} - u_2^{(\mu)})\|_{L^\infty(\Gamma_m[\mu, \lambda])} \leq K\mu^{1/2}, \quad (5.48)$$

$$\|T_1^{(\mu)} - T_2^{(\mu)}\|_{L^\infty(\Gamma_m[\mu, \lambda])} \leq K\mu^{1/2}, \quad (5.49)$$

$$\|D_x^\alpha \nabla_{\Gamma_\xi}(u_1^{(\mu)} - \hat{u})\|_{L^\infty(\Gamma_i[\mu, \lambda] \cup \Gamma_m[\mu, \lambda])} \leq K, \quad |\alpha| = 1, \quad (5.50)$$

for all $\mu \in (0, \mu_0]$, $\lambda \in (0, \lambda_0]$. Here α denotes multi-indices.

Proof: To prove (5.44) note that

$$\begin{aligned} |S_1^{(\mu)} - S_2^{(\mu)}| &= |S_0 + \mu^{1/2} S_1 - \hat{S} - \mu^{1/2} \tilde{S}_1 - \mu \tilde{S}_2| \\ &\leq |S_0 - \hat{S}| + \mu^{1/2} |S_1 - \tilde{S}_1| + \mu |\tilde{S}_2|. \end{aligned} \quad (5.51)$$

First we estimate the term $|S_0 - \hat{S}|$. By definition in (4.18) we have for $(t, \eta, \xi) \in \Gamma_m[\mu, \lambda]$ that

$$\frac{|\ln \mu|}{a} \leq \left| \frac{\xi}{(\mu\lambda)^{1/2}} \right| \leq 2 \frac{|\ln \mu|}{a}. \quad (5.52)$$

Since $\hat{S}(t, x) = \hat{S}(\xi) = 1^+(\xi)$, we infer from (4.38), (4.39) and (5.52) that for $(t, \eta, \xi) \in \Gamma_m[\mu, \lambda]$

$$|S_0\left(\frac{\xi}{(\mu\lambda)^{1/2}}\right) - \hat{S}(\xi)| \leq K_1 e^{-a|\xi/(\mu\lambda)^{1/2}|} \leq K_1 e^{-|\ln \mu|} = K_1 \mu. \quad (5.53)$$

To estimate the term $|S_1 - \tilde{S}_1|$ we first consider $(t, \eta, \xi) \in \Gamma_m[\mu, \lambda]$ with $\xi > 0$. Since by assumption \hat{T} is continuously differentiable on $\overline{\gamma'}$, we can use the mean value theorem and (4.27), (5.52) to conclude that

$$\begin{aligned} &\left| \tilde{S}_1\left(t, \eta, \frac{\xi}{(\mu\lambda)^{1/2}}\right) - \frac{\bar{\varepsilon} : \hat{T}^{(+)}(t, \eta)}{\hat{\psi}''(1)} \right| \\ &= \left| \frac{\bar{\varepsilon} : \hat{T}(t, \eta, \xi) - \bar{\varepsilon} : \hat{T}^{(+)}(t, \eta)}{\hat{\psi}''(1)} \right| \leq R_1(t, \eta, \xi) \xi \leq \frac{K_2}{a} (\mu\lambda)^{1/2} |\ln \mu|. \end{aligned}$$

This inequality, (4.43) and (5.52) together yield for such (t, η, ξ)

$$\begin{aligned} &|S_1(t, \eta, \xi) - \tilde{S}_1(t, \eta, \xi)| \\ &\leq \left| S_1(t, \eta, \xi) - \frac{\bar{\varepsilon} : \hat{T}^{(+)}(t, \eta)}{\hat{\psi}''(1)} \right| + \left| \tilde{S}_1(t, \eta, \xi) - \frac{\bar{\varepsilon} : \hat{T}^{(+)}(t, \eta)}{\hat{\psi}''(1)} \right| \\ &\leq K_3 e^{-a|\xi/(\mu\lambda)^{1/2}|} + \frac{K_2}{a} (\mu\lambda)^{1/2} |\ln \mu| \\ &\leq K_3 \mu + \frac{K_2}{a} (\mu\lambda)^{1/2} |\ln \mu|. \end{aligned} \quad (5.54)$$

The same estimate is obtained for $(t, \eta, \xi) \in \Gamma_m[\mu, \lambda]$ with $\xi < 0$ if we use (4.44) instead of (4.43) in the proof. The inequality (5.44) follows by insertion of (5.53) and (5.54) into (5.51).

To verify (5.45) observe that for $1 \leq |\alpha| \leq 2$

$$\begin{aligned} |D_x^\alpha(S_1^{(\mu)} - S_2^{(\mu)})| &= |D_x^\alpha(S_0 + \mu^{1/2}S_1) + D_x^\alpha(\hat{S} + \mu^{1/2}\tilde{S}_1 + \mu\tilde{S}_2)| \\ &\leq |D_x^\alpha S_0| + \mu^{1/2}|D_x^\alpha S_1| + \mu^{1/2}|D_x^\alpha(\tilde{S}_1 + \mu^{1/2}\tilde{S}_2)| \\ &\leq |D_x^\alpha S_0| + \mu^{1/2}|D_x^\alpha S_1| + \mu^{1/2}K_4. \end{aligned} \quad (5.55)$$

To estimate the first term on the right hand side remember that $S_0 = S_0(\frac{\xi}{(\mu\lambda)^{1/2}})$. We thus infer from (4.40) and (5.52) that

$$\begin{aligned} |D_x^\alpha S_0(\frac{\xi}{(\mu\lambda)^{1/2}})| &\leq C \sum_{i=1}^{|\alpha|} \frac{1}{(\mu\lambda)^{i/2}} |\partial_\zeta^i S_0(\zeta)| \\ &\leq C \sum_{i=1}^{|\alpha|} \frac{1}{(\mu\lambda)^{i/2}} e^{-|\ln \mu|} \leq \frac{K_5}{\lambda^{|\alpha|/2}} \mu^{\frac{2-|\alpha|}{2}}, \end{aligned} \quad (5.56)$$

for $(t, \eta, \xi) \in \Gamma_m[\mu, \lambda]$. Moreover, the estimates (4.42), (4.45), (4.46) and (5.52) imply

$$\begin{aligned} |D_x^\alpha S_1(t, \eta, \frac{\xi}{(\mu\lambda)^{1/2}})| &\leq C \sum_{1 \leq i+j \leq |\alpha|} \frac{1}{(\mu\lambda)^{i/2}} |\nabla_\eta^j \partial_\zeta^i S_1(t, \eta, \zeta)| \\ &\leq C_1 \left(1 + \sum_{i=1}^{|\alpha|} \frac{1}{(\mu\lambda)^{i/2}} e^{-a|\xi/(\mu\lambda)^{1/2}|} \right) \leq \frac{K_6}{\lambda^{|\alpha|/2}} (1 + \mu^{\frac{2-|\alpha|}{2}}). \end{aligned}$$

Combination of this estimate with (5.55) and (5.56) yields (5.45). Inequality (5.46) is proved in the same way using that $\partial_t S_i = S_{i,t} + (\mu\lambda)^{-1/2} \xi_t \partial_\zeta S_i$ and that $\xi_t = -s$, by (3.63).

Next we prove (5.47). By (4.7) and (4.13) – (4.15) we have with $\zeta = \frac{\xi}{(\mu\lambda)^{1/2}}$

$$\begin{aligned} u_1^{(\mu)} - u_2^{(\mu)} &= (\mu\lambda)^{1/2} u_0 + v - \hat{u} - \mu^{1/2} \tilde{u}_1 \\ &= (\mu\lambda)^{1/2} u_0 + v - (\mu\lambda)^{1/2} u^* \zeta^+ - v - \mu^{1/2} \tilde{u}_1 \\ &= (\mu\lambda)^{1/2} u^* \int_{-\infty}^{\zeta} (S_0(\vartheta) - 1^+(\vartheta)) d\vartheta - \mu^{1/2} \tilde{u}_1. \end{aligned} \quad (5.57)$$

Now consider $(t, \eta, \xi) \in \Gamma_m[\mu, \lambda]$ with $\xi < 0$. Since $1^+(\vartheta) = 0$ for $\vartheta < 0$, we infer from (4.38) and (5.52) that

$$\begin{aligned} |u^*(t, \eta) \int_{-\infty}^{\zeta} (S_0(\vartheta) - 1^+(\vartheta)) d\vartheta| &\leq |u^*(t, \eta)| \int_{-\infty}^{\zeta} S_0(\vartheta) d\vartheta \\ &\leq |u^*(t, \eta)| \int_{-\infty}^{\zeta} K_1 e^{a\vartheta} \leq K_2 e^{a\zeta} \leq K_2 e^{-|\ln \mu|} = K_2 \mu. \end{aligned} \quad (5.58)$$

Furthermore, (4.18), (4.32) and the mean value theorem yield

$$|\tilde{u}_1(t, \eta, \xi)| = |\tilde{u}_1(t, \eta, \xi) - \tilde{u}_1^{(-)}(t, \eta)| \leq R(t, \eta, \xi) |\xi| \leq R(t, \eta, \xi) \frac{2}{a} (\mu\lambda)^{1/2} |\ln \mu|. \quad (5.59)$$

Since $\Gamma_m[\mu, \lambda] \subseteq \mathcal{U}$ for all $\mu \in (0, \mu_0]$ and $\lambda \in (0, \lambda_0]$, it follows that $R(t, \eta, \xi) \leq K_3$ for all such μ, λ and $(t, \eta, \xi) \in \Gamma_m[\mu, \lambda]$. Combination of (5.57) – (5.59) yields

$$|(u_1^{(\mu)} - u_2^{(\mu)})(t, \eta, \xi)| \leq \mu^{3/2} \lambda^{1/2} K_2 + \mu |\ln \mu| \lambda^{1/2} \frac{2}{a} K_3, \quad (5.60)$$

for $(t, \eta, \xi) \in \Gamma_m[\mu, \lambda]$ with $\xi < 0$. To study the case $\xi > 0$, we subtract and add the term $(\mu\lambda)^{1/2} u^* \int_{-\infty}^{\infty} (S_0(\vartheta) - 1^+(\vartheta)) d\vartheta$ to the right hand side of (5.57). This yields

$$u_1^{(\mu)} - u_2^{(\mu)} = -(\mu\lambda)^{1/2} u^* \int_{\zeta}^{\infty} (S_0(\vartheta) - 1^+(\vartheta)) d\vartheta - \mu^{1/2} (\tilde{u}_1 - \tilde{u}_1^+),$$

where we also employed (4.31). Using the estimate (4.39) and the mean value theorem we see that the estimate (5.60) also holds for $(t, \eta, \xi) \in \Gamma_m[\mu, \lambda]$ with $\xi > 0$. Inequality (5.47) is a consequence of (5.60).

To prove (5.48) we infer from (5.57) with the splitting (2.11) of the gradient that

$$\begin{aligned} \nabla_x(u_1^{(\mu)} - u_2^{(\mu)}) &= (u^* \otimes n) (S_0 - \hat{S}) \\ &+ (\mu\lambda)^{1/2} (\nabla_{\Gamma_\xi} u^*) \int_{-\infty}^{\zeta} (S_0(\vartheta) - 1^+(\vartheta)) d\vartheta - \mu^{1/2} \nabla_x \tilde{u}_1. \end{aligned} \quad (5.61)$$

The estimates (4.38), (4.39) imply

$$\left| \int_{-\infty}^{\zeta} (S_0(\vartheta) - 1^+(\vartheta)) d\vartheta \right| \leq \max(K_1, K_2) \int_{-\infty}^{\infty} e^{-a|\vartheta|} d\vartheta \leq C. \quad (5.62)$$

We employ this inequality and the inequality (5.53) to estimate the terms on the right hand side of (5.61) and obtain (5.48). The inequality (5.49) is an immediate consequence of (4.16), (5.44) and (5.48). Finally, to prove (5.50) observe that (4.7) and (4.13), (4.15) imply

$$\nabla_{\Gamma_\xi}(u_1^{(\mu)} - \hat{u}) = (\mu\lambda)^{1/2} \nabla_{\Gamma_\xi}(u_0 - u^* \zeta^+) = (\mu\lambda)^{1/2} (\nabla_{\Gamma_\xi} u^*) \int_{-\infty}^{\zeta} (S_0(\vartheta) - 1^+(\vartheta)) d\vartheta.$$

Differentiation of this equation and application of the estimate (5.62) yields (5.50). We leave the details to the reader. \blacksquare

5.2.4 End of the proof of Theorem 4.3

We start with the proof of (4.47) and (4.48). Equation (4.9) yields

$$\nabla_x u^{(\mu)} = \nabla_x u_1^{(\mu)} \hat{\phi} + \nabla_x u_2^{(\mu)} (1 - \hat{\phi}) + (u_1^{(\mu)} - u_2^{(\mu)}) \otimes \nabla_x \hat{\phi}.$$

We insert this equation into (4.10) and use (4.8) and (4.16) to obtain

$$T^{(\mu)} = T_1^{(\mu)} \hat{\phi} + T_2^{(\mu)} (1 - \hat{\phi}) + D\varepsilon((u_1^{(\mu)} - u_2^{(\mu)}) \otimes \nabla_x \hat{\phi}). \quad (5.63)$$

The argument of $\hat{\phi}$ in (4.9) is $\frac{a\xi}{|(\lambda\mu)^{1/2} \ln \mu|}$. Therefore we have

$$\nabla_x \hat{\phi} = \frac{a}{|(\lambda\mu)^{1/2} \ln \mu|} \hat{\phi}' n, \quad (5.64)$$

with the unit normal vector n to $\Gamma(t)$. From this equation and from (5.63) we compute

$$\begin{aligned} \operatorname{div}_x T^{(\mu)} + \mathbf{b} &= (\operatorname{div}_x T_1^{(\mu)} + \mathbf{b})\hat{\phi} + (\operatorname{div}_x T_2^{(\mu)} + \mathbf{b})(1 - \hat{\phi}) \\ &+ \left((T_1^{(\mu)} - T_2^{(\mu)})n + \operatorname{div}_x D\varepsilon((u_1^{(\mu)} - u_2^{(\mu)}) \otimes n) \right) \frac{a}{|(\lambda\mu)^{1/2} \ln \mu|} \hat{\phi}' \\ &+ \left(D\varepsilon((u_1^{(\mu)} - u_2^{(\mu)}) \otimes n) \right) n \frac{a^2}{|(\lambda\mu)^{1/2} \ln \mu|^2} \hat{\phi}'' . \end{aligned} \quad (5.65)$$

Inequality (4.48) is an immediate consequence of this equation and of (5.26), since $\hat{\phi} = 0$ in $\Gamma_o[\lambda, \mu]$. The proof of the inequality (4.47) is more involved, since we must estimate every term on the right hand side of (5.65). To estimate $\operatorname{div}_x T_1^{(\mu)} + \mathbf{b}$ note that (5.50) yields

$$\begin{aligned} |(\mu\lambda)^{1/2} \operatorname{div}_x D\varepsilon(\nabla_{\Gamma_\xi}(u_0 - u^* \zeta^+))| &= |\operatorname{div}_x D\varepsilon(\nabla_{\Gamma_\xi}(u_1^{(\mu)} - \hat{u}))| \\ &\leq C \sum_{|\alpha|=1} |D_x^\alpha \nabla_{\Gamma_\xi}(u_1^{(\mu)} - \hat{u})| \leq K, \end{aligned} \quad (5.66)$$

and that

$$\left| \mu^{1/2} \operatorname{div}_x D\bar{\varepsilon} S_1(t, \eta, \frac{\xi}{(\mu\lambda)^{1/2}}) \right| = \mu^{1/2} \left| (D\bar{\varepsilon}) \nabla_x S_1(t, \eta, \frac{\xi}{(\mu\lambda)^{1/2}}) \right| \leq K\lambda^{-1/2}. \quad (5.67)$$

With (5.66), (5.67) we estimate the right hand side $R_{\operatorname{div}+\mathbf{b}}$ of (5.27) given in (5.28) and obtain

$$\|\operatorname{div}_x T_1^{(\mu)} + \mathbf{b}\|_{L^\infty(\Gamma_i[\mu, \lambda] \cup \Gamma_m[\mu, \lambda])} \leq K\lambda^{-1/2}, \quad \mu \in (0, \mu_0], \lambda \in (0, \lambda_0]. \quad (5.68)$$

Moreover, observe that

$$|\operatorname{div}_x D\varepsilon((u_1^{(\mu)} - u_2^{(\mu)}) \otimes n)| \leq C(|\nabla_x(u_1^{(\mu)} - u_2^{(\mu)})| + |u_1^{(\mu)} - u_2^{(\mu)}|). \quad (5.69)$$

(4.47) is obtained by estimating the right hand side of (5.65) using (5.68), (5.69), (5.26) and (5.47) – (5.49).

We next proof (4.49) and (4.50). The inequality (4.50) follows immediately from (5.43), since $S^{(\mu)} = S_2^{(\mu)}$ on $\Gamma_o[\mu, \lambda]$, by (4.8) and (4.19), and since $\Gamma_o[\mu, \lambda] \subseteq \gamma \cup \gamma'$. It remains to verify (4.48). Since $W_S(\varepsilon(\nabla_x u), S) = -T : \bar{\varepsilon}$ by (1.24), it follows from (5.63) that

$$\begin{aligned} W_S(\varepsilon(\nabla_x u^{(\mu)}), S^{(\mu)}) - W_S(\varepsilon(\nabla_x u_1^{(\mu)}), S_1^{(\mu)}) &= -\bar{\varepsilon} : (T^{(\mu)} - T_1^{(\mu)}) \\ &= -\bar{\varepsilon} : (T_2^{(\mu)} - T_1^{(\mu)})(1 - \hat{\phi}) - \bar{\varepsilon} : D\varepsilon((u_1^{(\mu)} - u_2^{(\mu)}) \otimes \nabla_x \hat{\phi}). \end{aligned}$$

The mean value theorem and (4.8) imply

$$\begin{aligned} \hat{\psi}'(S^{(\mu)}) - \hat{\psi}'(S_1^{(\mu)}) &= \hat{\psi}'' \left(S_1^{(\mu)} + \vartheta(S_2^{(\mu)} - S_1^{(\mu)})(1 - \hat{\phi}) \right) (S_2^{(\mu)} - S_1^{(\mu)})(1 - \hat{\phi}), \\ &\text{for a suitable } 0 < \vartheta(t, x) < 1, \\ \Delta_x S^{(\mu)} - \Delta_x S_1^{(\mu)} &= \Delta_x (S_2^{(\mu)} - S_1^{(\mu)})(1 - \hat{\phi}) + 2\nabla_x (S_1^{(\mu)} - S_2^{(\mu)}) \cdot \nabla_x \hat{\phi} \\ &+ (S_1^{(\mu)} - S_2^{(\mu)}) \Delta_x \hat{\phi}. \end{aligned}$$

The right hand side of the last three equations vanishes on the set $\Gamma_i[\mu, \lambda]$, since $\hat{\phi} = 1$ on this set. To estimate the right hand sides on the set $\Gamma_m[\mu, \lambda]$ we use (5.44), (5.45), (5.47), (5.49), (5.64) and the equation $\Delta_x \hat{\phi} = \frac{a^2}{|(\lambda\mu)^{1/2} \ln \mu|^2} \hat{\phi}''$. Together we obtain that on $\Gamma_i[\mu, \lambda] \cup \Gamma_m[\mu, \lambda]$ the inequality

$$\begin{aligned} & \left| \left(W_S(\varepsilon(\nabla_x u^{(\mu)}), S^{(\mu)}) + \frac{1}{\mu^{1/2}} \hat{\psi}'(S^{(\mu)}) - \mu^{1/2} \lambda \Delta_x S^{(\mu)} \right) \right. \\ & \quad \left. - \left(W_S(\varepsilon(\nabla_x u_1^{(\mu)}), S_1^{(\mu)}) + \frac{1}{\mu^{1/2}} \hat{\psi}'(S_1^{(\mu)}) - \mu^{1/2} \lambda \Delta_x S_1^{(\mu)} \right) \right| \\ & \leq K \mu^{1/2} (|\ln \mu| \lambda^{1/2} + 1 + |\ln \mu| + \frac{1}{|\ln \mu|}) \leq K \mu^{1/2} |\ln \mu| \end{aligned} \quad (5.70)$$

holds. Similarly, (4.8) implies

$$\partial_t S^{(\mu)} - \partial_t S_1^{(\mu)} = \partial_t (S_2^{(\mu)} - S_1^{(\mu)}) (1 - \hat{\phi}) + (S_1^{(\mu)} - S_2^{(\mu)}) \partial_t \hat{\phi}.$$

The right hand side of this equation vanishes on $\Gamma_i[\mu, \lambda]$. To estimate the right hand side on the set $\Gamma_m[\mu, \lambda]$ we use the inequalities (5.44), (5.46) and the equation

$$\partial_t \hat{\phi} = \frac{a \partial_t \xi}{(\mu\lambda)^{1/2} |\ln \mu|} \hat{\phi}' = - \frac{as}{(\mu\lambda)^{1/2} |\ln \mu|} \hat{\phi}',$$

which follows from (3.63). The result is

$$|\partial_t S^{(\mu)} - \partial_t S_1^{(\mu)}| \leq K \lambda^{-1/2} \mu^{1/2}, \quad \text{on } \Gamma_i[\mu, \lambda] \cup \Gamma_m[\mu, \lambda]. \quad (5.71)$$

By combination of (5.40), (5.70) and (5.71) we see that

$$\begin{aligned} & \left| \partial_t S^{(\mu)} + \frac{1}{(\mu\lambda)^{1/2}} f \left(W_S(\varepsilon(\nabla_x u^{(\mu)}), S^{(\mu)}) + \frac{1}{\mu^{1/2}} \hat{\psi}'(S^{(\mu)}) - \mu^{1/2} \lambda \Delta_x S^{(\mu)} \right) \right| \\ & \leq \left| \partial_t S_1^{(\mu)} + \frac{1}{(\mu\lambda)^{1/2}} f \left(W_S(\varepsilon(\nabla_x u_1^{(\mu)}), S_1^{(\mu)}) + \frac{1}{\mu^{1/2}} \hat{\psi}'(S_1^{(\mu)}) - \mu^{1/2} \lambda \Delta_x S_1^{(\mu)} \right) \right| \\ & \quad + K \lambda^{-1/2} \mu^{1/2} + L_f K \lambda^{-1/2} |\ln \mu| \\ & \leq \frac{K L_f}{\lambda^{1/2}} \left(\frac{|\ln \mu|}{a} + 1 \right) + K \frac{\mu^{1/2}}{\lambda^{1/2}} + L_f K \frac{|\ln \mu|}{\lambda^{1/2}} \leq K_1 (1 + L_f) \frac{|\ln \mu|}{\lambda^{1/2}} \end{aligned}$$

holds on the set $\Gamma_i[\mu, \lambda] \cup \Gamma_m[\mu, \lambda]$, where L_f is the Lipschitz constant of f . This proves (4.49). The proof of Theorem 4.3 is complete. \blacksquare

6 Numerical results

In this section we present and compare results of numerical experiments for the Allen-Cahn model and the hybrid model. These results illustrate the theoretical convergence results from Theorem 2.7 and Theorem 4.3. We do not study the different behavior of the models with respect to the nonlinearity of the function f ; instead, we assume that f in (1.3) and (1.22) is linear and concentrate on the comparison of the numerical efficiency of the models in simulations of physical situations, where the movement of the phase interface is only or mainly driven by the jump of the Eshelby tensor and where the influence of the curvature on this movement is small. In such situations the interface should essentially be stationary on the time scale considered when the jump of the Eshelby tensor vanishes.

6.1 Setting of the problem

For both models we compute the evolution in time of the order parameter S in two space dimensions. However, for simplicity we do not solve the full models (1.1) – (1.3) and (1.20) – (1.22). Instead, to simplify the computation we solve the evolution equations (1.3) or (1.22) but avoid to solve the elasticity equations (1.1), (1.2). To achieve this we determine the stress field T appearing in these evolution equations by an approximation procedure, which we explain first.

Following the analysis of the stress field $T^{(\nu)}$ in Sections 2 and 3 we decompose in this procedure the stress field T into a leading term, which can be determined exactly without solving the elasticity equations, and into a second term, which mainly, but not completely, depends on the given volume force \mathbf{b} and the given boundary data for the displacement or the stress field. This second term can be determined largely by prescribing these data suitably. Therefore we prescribe this term arbitrarily.

To explain the decomposition, note that by (3.34) the leading term of $T^{(\nu)}$ is T_0 . Using (3.41) and (2.22), (2.26) we obtain

$$T_0 = D(\varepsilon(u^* \otimes n) - \bar{\varepsilon})S_0 = [\hat{T}]S_0 = D(P_n - I)\bar{\varepsilon}S_0,$$

where n denotes the normal vector field of the manifold $\Gamma(t)$ given by the interface of the sharp interface problem. A stress field T obtained by determining an exact solution (u, T, S) of one of the phase field models (1.1) – (1.3) or (1.20) – (1.22) is not related to such a sharp interface problem. For an analogous decomposition of T we therefore need to define the normal vector field n independently of the sharp interface problem. It suggests itself to replace Γ by the three dimensional manifold Γ' formed by the level set $\{S = \frac{1}{2}\}$ and to choose for n the unit normal vector to $\Gamma'(t)$. With this vector field we introduce the decomposition

$$T = D(P_n - I)\bar{\varepsilon}S + w. \tag{6.1}$$

w is the solution of a boundary value problem for the elasticity equations. We sketch the derivation of this boundary value problem. Let Γ'_ξ be the three-dimensional manifold formed by the level set $\{S = \frac{1}{2} + \xi\}$. We define a coordinate system (η, ξ) in a neighborhood of $\Gamma'(t) = \Gamma'_0(t)$ such that ξ is constant on $\Gamma'_\xi(t)$ and such that $\partial_\xi x(t, \eta, \xi) \in \mathbb{R}^3$ is the unit normal vector to $\Gamma'_\xi(t)$. By definition of P_n there is a vector u^* such that $P_n \bar{\varepsilon} = \varepsilon(u^* \otimes n)$. Similarly as in (2.94), (2.99), with this new coordinate system we decompose u in the form

$$u(t, x) = u^*(t, \eta) \int_0^\xi S(t, \eta, \theta) d\theta + v(t, x).$$

Insertion of this decomposition into the elasticity equations (1.1), (1.2) yields the boundary value problem for w . The computations needed to derive this boundary value problem are technical because derivatives of $u^*(t, \eta)\xi^+$ tangential to Γ'_ξ appear. We do not need the exact form of the boundary value problem and therefore only state it for the case of one space dimension, where terms containing such tangential derivatives are not present. In this case the form of the boundary value problem can be read of from [3, Lemma 3], where an explicit solution is given for the Dirichlet boundary value problem to the

elasticity system (1.2), (1.3) when all variables only depend on (t, x_1) with x_1 varying in the interval $[\alpha, \beta]$. From this formula we see that v and w must solve the equations

$$\begin{aligned} -\partial_{x_1} w_1 &= \mathbf{b}, \\ w &= D\varepsilon(v_{x_1} \otimes (1, 0, 0)), \\ v(t, \alpha) &= v_-(t), \\ v(t, \beta) &= v_+(t). \end{aligned}$$

where $w_1(t, x_1)$ denotes the first column of the matrix $w(t, x_1)$ and v_-, v_+ are suitable boundary data, which, in fact, depend on the mean value $\int_{\alpha}^{\beta} S(t, x_1) dx_1$.

This boundary value problem shows that in one space w can be determined completely by choosing a suitable volume force and suitable boundary data. Therefore w can be given arbitrarily if one is only interested in comparing the different properties of the evolution equations (1.3) and (1.22). Although the situation is slightly less simple in higher space dimensions, we use the idea also in the two-dimensional computations and prescribe w in the decomposition (6.1) arbitrarily. More precisely, since not the complete function w appears in the evolution equations for S but only the scalar component $\bar{\varepsilon} : w$, we prescribe this scalar function arbitrarily. Of course, our computations do not accurately reflect the evolution of the phase interface in an elastic solid, but we believe that they faithfully show the properties of the two different phase field models we compare.

The stress field T enters the evolution equations (1.3) and (1.22) via the derivatives ψ_S and W_S . If we insert (6.1) into (1.8) and (1.24) we obtain

$$\psi_S = -\bar{\varepsilon} : D(P_n - I)\bar{\varepsilon}S - \bar{\varepsilon} : w + \hat{\psi}'(S), \quad (6.2)$$

$$W_S = -\bar{\varepsilon} : D(P_n - I)\bar{\varepsilon}S - \bar{\varepsilon} : w. \quad (6.3)$$

The coefficient $\bar{\varepsilon} : D(P_n - I)\bar{\varepsilon}$ of S in these equations is a function of the normal vector n to the phase interface alone. To simplify the computations further we consider a situation where this coefficient is a constant. This is the case when the transformation strain is a multiple of the identity matrix and the material is isotropic. We thus assume that

$$\bar{\varepsilon} = dI \quad \text{and} \quad D\sigma = \nu_1\sigma + \nu_2 \text{trace}(\sigma)I, \quad \text{for all } \sigma \in \mathcal{S}^3, \quad (6.4)$$

with constants $d \in \mathbb{R}$ and ν_1, ν_2 satisfying $\nu_1 > 0$ and $\nu_1 + 3\nu_2 > 0$. Using the definition of P_n in Lemma 2.2 we obtain under these assumptions by some computations that

$$P_n \bar{\varepsilon} = d \frac{\nu_1 + 3\nu_2}{\nu_1 + \nu_2} n \otimes n, \quad (6.5)$$

$$L_1 := \bar{\varepsilon} : D(P_n - I)\bar{\varepsilon} = d^2(\nu_1 + 3\nu_2) \left(\frac{\nu_1 + 3\nu_2}{\nu_1 + \nu_2} - 3 \right) \leq 0. \quad (6.6)$$

The last inequality sign in (6.6) follows from the properties of ν_1 and ν_2 and is in accordance with (2.29). Obviously, L_1 is constant and we can give it any nonpositive value by varying the coefficients ν_1, ν_2, d .

The two evolution equations, which we solve numerically, are obtained by insertion of (6.2) into (1.3) and by insertion of (6.3) into (1.22). If we also note (6.6), the resulting equations are

$$\partial_t S = -f_1(-\bar{\varepsilon} : w - L_1 S + \hat{\psi}'_1(S) - \nu \Delta_x S) |\nabla_x S|, \quad (6.7)$$

$$\partial_t S = -\frac{1}{(\mu\lambda)^{1/2}} f_2(-\bar{\varepsilon} : w - L_1 S + \frac{1}{\mu^{1/2}} \hat{\psi}'_2(S) - \mu^{1/2} \lambda \Delta_x S), \quad (6.8)$$

with functions $f_1, f_2 : \mathbb{R} \rightarrow \mathbb{R}$, which we both choose to be linear. Precisely, we choose $f_1(r) = r$ and $f_2(r) = \tilde{c}r$ with a suitable positive constant \tilde{c} . We want that the propagation speeds of the interfaces modelled by the asymptotic solutions constructed in Sections 2 and 4 coincide. The propagation speeds are determined by the kinetic relations (2.3) and (4.3). Therefore we must choose the constants \tilde{c} and λ such that these two relations become the same. This is possible because of the following result:

Lemma 6.1 *If D and $\bar{\varepsilon}$ satisfy (6.4), then the operator $B(n)$ in (2.3) is equal to zero.*

Proof: It suffices to show that the function σ_2 in the definition (2.83) of $B(n)$ vanishes. To this end we prove that the right hand side of (2.54) is equal to zero. Observe first that the effective potential $(n, S) \mapsto \tilde{\psi}(n, S)$ defined in (2.47) is actually a function $((n, S) \mapsto \tilde{\psi}(p(n), S)$ with p defined in (2.27), hence (2.66) implies $S_0(n, \zeta) = S_0(p(n), \zeta)$, whence (2.45) yields $S_0^{(-1)}(t, \eta, \zeta) = S_0^{(-1)}(p(t, \eta), \zeta)$. By (2.27) we have

$$p(n) = \bar{\varepsilon} : [\hat{T}] = \bar{\varepsilon} : D(P_n - I)\bar{\varepsilon} = L_1 = \text{const.} \quad (6.9)$$

Hence, $S_0^{(-1)}$ depends on ζ but is independent (t, η) , which implies that $\nabla_\eta S_0^{(-1)} = 0$. Therefore (2.55) yields $\partial_\zeta u_{11} = 0$.

Moreover, from (2.78) we infer that

$$\bar{\varepsilon} : D\varepsilon(a^* S_0^{(-1)} \otimes n + \nabla_\eta u_0) = \bar{\varepsilon} : D\varepsilon(a^* \otimes n + \nabla_\eta u^*) S_0^{(-1)}.$$

Consequently, the statement of the lemma follows if we show that $\bar{\varepsilon} : D\varepsilon(a^* \otimes n + \nabla_\eta u^*) = 0$. To this end we determine u^* and a^* . By (2.22), (2.26) and (6.5) we have $\varepsilon(u^* \otimes n) = c^* n \otimes n$ with the constant $c^* = d \frac{\nu_1 + 3\nu_2}{\nu_1 + \nu_2}$, thence $u^* = c^* n$. With this information we compute the right hand side of (2.24) to find a^* . In these computations we use that the matrix $\nabla_\Gamma n$ is symmetric and that if τ_1, τ_2 are orthogonal unit tangential vectors to Γ in the principle directions of curvature and if $\kappa_{\tau_1}, \kappa_{\tau_2}$ are the principle curvatures, then we have

$$\nabla_\Gamma n = \kappa_{\tau_1} \tau_1 \otimes \tau_1 + \kappa_{\tau_2} \tau_2 \otimes \tau_2, \quad \text{div}_\Gamma n = \sum_{i=1}^2 \tau_i \cdot (\nabla_\Gamma n) \tau_i = \kappa_{\tau_1} + \kappa_{\tau_2} = \kappa_\Gamma,$$

where in the last equation we used (2.9).

Thus, from (6.4) we infer that

$$\begin{aligned} \text{div}_\Gamma D\varepsilon(u^* \otimes n) &= c^* \text{div}_\Gamma D(n \otimes n) = c^* \text{div}_\Gamma (\nu_1(n \otimes n) + \nu_2 \text{trace}(n \otimes n) I) \\ &= c^* \nu_1 ((\nabla_\Gamma n)n + n(\text{div}_\Gamma n)) + c^* \text{div}_\Gamma (\nu_2 I) \\ &= c^* \nu_1 (\text{div}_\Gamma n)n = \nu_1 \kappa_\Gamma c^* n, \end{aligned} \quad (6.10)$$

and

$$\begin{aligned} D\varepsilon(\nabla_\Gamma u^*)n &= c^* D(\nabla_\Gamma n)n = c^* (\nu_1 (\nabla_\Gamma n)n + \nu_2 \text{trace}(\nabla_\Gamma n) In) \\ &= c^* \nu_2 \kappa_\Gamma n, \end{aligned} \quad (6.11)$$

$$\begin{aligned} (D\varepsilon(a^* \otimes n))n &= \frac{\nu_1}{2} (a^* \otimes n + n \otimes a^*)n + \nu_2 \text{trace}(a^* \otimes n) In \\ &= \frac{\nu_1}{2} a^* + \left(\frac{\nu_1}{2} + \nu_2\right) (a^* \cdot n) n. \end{aligned} \quad (6.12)$$

Insertion of (6.10) – (6.12) into (2.24) yields

$$\frac{\nu_1}{2}a^* + \left(\frac{\nu_1}{2} + \nu_2\right)(a^* \cdot n) + (\nu_1 + \nu_2)c^*\kappa_\Gamma n = 0.$$

Scalar multiplication of this equation with n yields $a^* \cdot n = -c^*\kappa_\Gamma$, whence $a^* = -\kappa_\Gamma c^*n$. With these values of u^* and a^* we finally compute

$$\begin{aligned} \bar{\varepsilon} : D\varepsilon(a^* \otimes n + \nabla_\eta u^*) &= c^*\bar{\varepsilon} : D\varepsilon(-\kappa_\Gamma n \otimes n + \nabla_\Gamma n) \\ &= c^*\bar{\varepsilon} : \left(\nu_1(-\kappa_\Gamma n \otimes n + \nabla_\Gamma n) + \nu_2(-\kappa_\Gamma + \text{trace}(\nabla_\Gamma n))I\right) \\ &= c^*d\nu_1(-\kappa_\Gamma(n \cdot n) + I : (\kappa_{\tau_1}\tau_1 \otimes \tau_1 + \kappa_{\tau_2}\tau_2 \otimes \tau_2)) + c^*\nu_2(-\kappa_\Gamma + \kappa_\Gamma)\bar{\varepsilon} : I \\ &= c^*d(-\kappa_\Gamma + \kappa_{\tau_1} + \kappa_{\tau_2}) = 0. \end{aligned}$$

This proves the lemma. ■

From this lemma, from the assumptions for f_1 and f_2 and from the fact that (4.3) is equal to (1.26) when f_2 is linear, we see that the kinetic relations (2.3) and (4.3) take the form

$$s = n \cdot [\hat{C}]n + \nu^{1/2}\omega_1\kappa_\Gamma, \quad (6.13)$$

$$s = \frac{\tilde{c}}{c_1}(n \cdot [\hat{C}]n + \lambda^{1/2}c_1\kappa_\Gamma), \quad (6.14)$$

with $\omega_1 = \int_0^1 \sqrt{2\tilde{\psi}_1(\theta)}d\theta$ and $c_1 = \int_0^1 \sqrt{2\hat{\psi}_2(\theta)}d\theta$. The potential $\hat{\psi}_1$, which we use in the numerical computations, satisfies $\hat{\psi}_1(0) = \hat{\psi}_1(1) = 0$. By (2.47) and (6.9) we therefore have

$$\tilde{\psi}_1(S) = \hat{\psi}_1(S) + \frac{1}{2}L_1S(1 - S). \quad (6.15)$$

The kinetic relations (6.13) and (6.14) coincide if we choose

$$\tilde{c} = c_1, \quad \lambda = \left(\frac{\omega_1}{c_1}\right)^2 \nu. \quad (6.16)$$

We insert these values into (6.7) and (6.8). This yields the initial-boundary value problems, which we solve numerically. They consist of either one of the two evolution equations

$$\partial_t S = (\bar{\varepsilon} : w + L_1S - \hat{\psi}'_1(S) + \nu\Delta_x S)|\nabla_x S|, \quad (6.17)$$

$$\partial_t S = \frac{c_1}{(\mu\lambda)^{1/2}}(\bar{\varepsilon} : w + L_1S - \frac{1}{\mu^{1/2}}\hat{\psi}'_2(S) + \mu^{1/2}\lambda\Delta_x S), \quad (6.18)$$

with λ given by (6.16), and of the boundary and initial conditions

$$S(t, x) = 0, \quad \text{for } x \in \partial\Omega, \quad (6.19)$$

$$S(0, x) = \bar{S}(x). \quad (6.20)$$

We can prescribe the boundary condition (6.19), since we only consider initial data \bar{S} vanishing in a neighborhood of the boundary $\partial\Omega$, and we stop the computation at a time before the phase interface reaches the boundary. For the double well potentials we choose

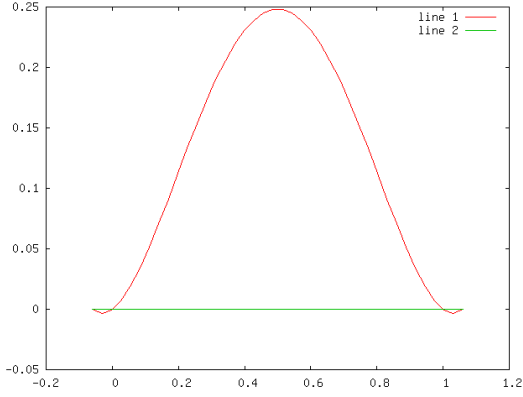


Fig. 1: Potential $\hat{\psi}_1$, hybrid model

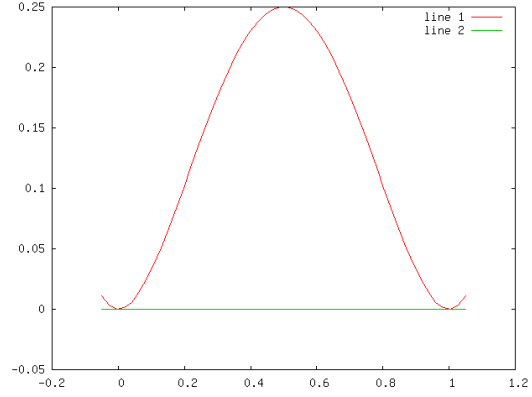


Fig. 2: Potential $\hat{\psi}_2$, Allen-Cahn model

$$\hat{\psi}_1(S) = \frac{S(S-1)(S-N_1)(S-(1-N_1))}{(\frac{1}{2}-N_1)^2}, \quad N_1 = -.06, \quad (6.21)$$

$$\hat{\psi}_2(S) = 4S^2(1-S)^2. \quad (6.22)$$

The graphs of these double well potentials are displayed in Figures 1 and 2. The potential $\hat{\psi}_2$ satisfies the conditions (4.35) – (4.37), and by an easy consideration we see that the hypotheses 1. – 4. of Theorem 2.3 hold for the effective potential $\tilde{\psi}_1$ given in (6.15) if

$$0 \geq L_1 > -2\hat{\psi}_1'(0) = -0.405.$$

If we therefore prescribe the constant L_1 in this range then the convergence results stated in Theorems 2.7 and 4.3 are valid. For the potentials $\hat{\psi}_1$ and $\hat{\psi}_2$ from (6.21), (6.22) the constants ω_1 and c_1 have the values

$$\omega_1 = 0.42147, \quad c_1 = 0.47084, \quad \text{hence } \lambda = \left(\frac{0.42147}{0.47084}\right)^2 \nu \approx 0.80 \nu.$$

Since we want to test the suitability of the phase field models to simulate material behavior where the curvature has little influence on the movement of the phase interface, we must choose the parameter $\nu > 0$ in the hybrid model small enough such that the term $\nu^{1/2}\omega_1\kappa_\Gamma$ in the kinetic relation (6.13) contributes little to the movement of the interface Γ in the range of time considered and such that the sharp interface solution to this kinetic relation is approximated well enough by the solution of the hybrid model. The choice of ν also fixes the value of λ in the Allen-Cahn model. Depending on λ , the parameter μ must be chosen small enough such that the Allen-Cahn solution approximates the sharp interface solution to the kinetic relation (6.14), which coincides with (6.13), well enough.

6.2 Discussion of the numerical results

We used implicit difference schemes to solve both initial-boundary value problems (6.17), (6.19), (6.20) and (6.18), (6.19), (6.20). The numerical procedures were not designed for optimal speed, but to make the results for both problems comparable. We used octave for the computations. Using Matlab instead yields the same results with very similar computation times. In all computations we choose the quadratic domain $\Omega = [-d, d] \times [-d, d]$ with $d = 0.35\pi$.

Figure 3 is a contour plot of the initial data \bar{S} used in all computations discussed here. Inside the region bounded by the innermost contour line the value of \bar{S} is 1, in the region between the boundary $\partial\Omega$ and the outermost contour line the value is 0. Figures 4 – 8 are contour plots of the solution S computed numerically with different choices of parameters. These five plots all show the respective solutions $x \mapsto S(t, x) : \Omega \rightarrow \mathbb{R}$ at time $t = 0.8$. The number t_{comp} is the time needed to compute the solution. $n_g \times m_g$ gives the numbers of grid lines in the x_1 and x_2 directions used in the computation to discretize the solution. Of course, n_g and m_g must be chosen large enough to resolve the transition of S from zero to one across the interface and the time steps must be chosen small enough such that the iteration converges.

To compute the solution shown in Figures 4 and 5 we chose $L_1 = 0$ and $\bar{\varepsilon} : w = 0$, hence $\bar{\varepsilon} : T = 0$, by (6.1) and (6.6). This corresponds to the choice $\bar{\varepsilon} = 0$, which means that the material behaves in both phases in the same way, i.e. there is actually only one material phase present. From (2.30) we obtain $n \cdot [\hat{C}]n = 0$, which means that in the sharp interface model (1.14) – (1.18) the interface is stationary. Figure 3 is computed using the hybrid model setting $\nu = 0.00125$, Figure 5 is computed using the Allen-Cahn model, where for λ we chose the corresponding value $\lambda = 0.8\nu = 0.001$. The two solutions coincide well, though for the Allen-Cahn model the transition of the order parameter at the phase interface is much steeper, in accordance with the theoretical results stated in Sections 2 and 4. As a consequence, the computing time for the Allen-Cahn model is about 100 times as large as for the hybrid model.

Comparing the computed solutions with the star shaped initial data displayed in Figure 3 we see that the interface is not stationary, but that the wiggling interface boundary of the initial data has been smoothed out and the variation of the curvature has been reduced. A closer investigation shows that also the mean diameter of the star shaped region did shrink. Therefore the values of ν and λ should be chosen even smaller to approximate the solution of the sharp interface model (1.14) – (1.18) on the time interval $[0, 0.8]$ for the given initial data, which contain large values of the curvature. This would however lead to an even larger ratio between the computing times for the hybrid model and the Allen-Cahn model.

Figures 6 and 7 represent the solution at time $t = 0.8$, again to the initial data in Figure 3, but with $L_1 = -0.4$ and $\bar{\varepsilon} : w = -0.3 + 0.1 \sin(7(x_1 + x_2))$. Figure 6 is computed with the hybrid model, Figure 7 with the Allen-Cahn model. The results agree quite well; this is seen from Figure 9, where the results of both computations are overlaid. The computation time for the Allen-Cahn model is about 50 times larger than for the hybrid model. In the Allen-Cahn model we chose $\mu = 0.2$ to guarantee that the solution of this model is close enough to the solution of the sharp interface model (6.14). For a larger value of μ the transition of the order parameter would be less steep and we could choose a coarser grid, which would reduce the time of computation. However, from Figure 8, which shows the result of the computation with the Allen-Cahn model for $\mu = 0.7$, we see that the solution obtained differs by a sizeable amount from the solution to $\mu = 0.2$ and thus is not close to the solution of the sharp interface model (6.14). This is clearly shown by Figure 10, where Figures 6, 7 and 8 are overlaid. For an accurate computation we therefore cannot increase the value of $\mu = 0.2$ much.

Figures 11 - 13 are plots of the function $x_1 \rightarrow S(t, x_1, 0) : [-a/2, a/2] \rightarrow \mathbb{R}$ with $t = 0.12$. Thus, these plots show cross sections of the solution along the line of symmetry $[-a/2, a/2] \times \{0\}$ of the domain $\Omega = [-a/2, a/2] \times [-a/2, a/2]$. In Figure 11 the function

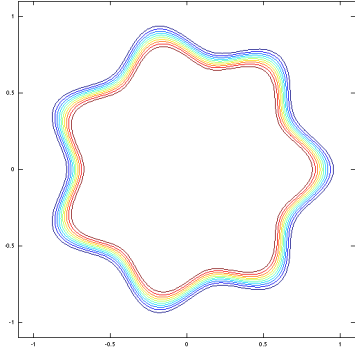


Fig. 3: Initial data
 $t = 0$

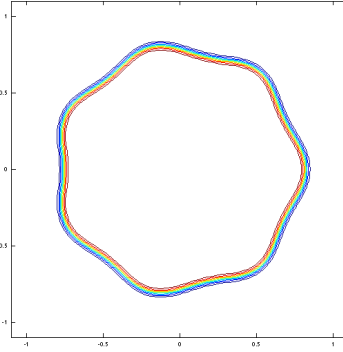


Fig. 4: Hybrid model
 $\nu = 0.00125$,
 $n_g \times m_g = 100 \times 100$,
time steps = 20,
 $t_{\text{comp}} = 2.29$ sec

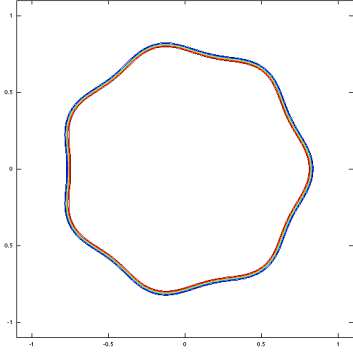


Fig. 5: Allen-Cahn model
 $\lambda = 0.001$, $\mu = 0.2$,
 $n_g \times m_g = 250 \times 250$,
time steps = 100,
 $t_{\text{comp}} = 243$ sec

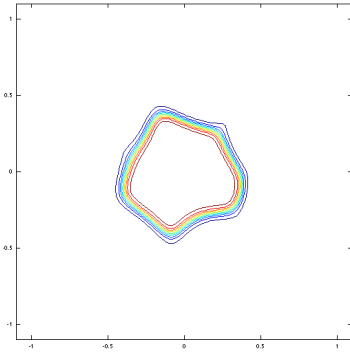


Fig. 6: Hybrid model
 $\nu = 0.00125$,
 $n_g \times m_g = 100 \times 100$,
time steps = 20,
 $t_{\text{comp}} = 6.03$ sec

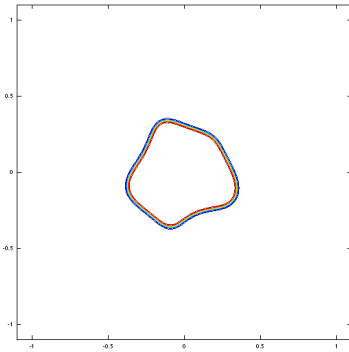


Fig. 7: Allen-Cahn model
 $\lambda = 0.001$, $\mu = 0.2$,
 $n_g \times m_g = 260 \times 260$,
time steps = 100,
 $t_{\text{comp}} = 310$ sec

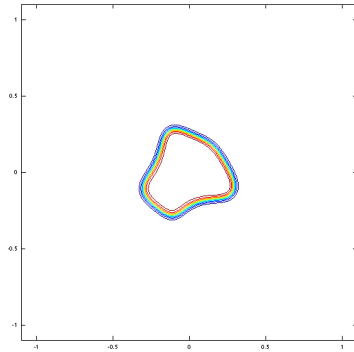


Fig. 8: Allen-Cahn model
 $\lambda = 0.001$, $\mu = 0.7$,
 $n_g \times m_g = 200 \times 200$,
time steps = 100,
 $t_{\text{comp}} = 169$ sec

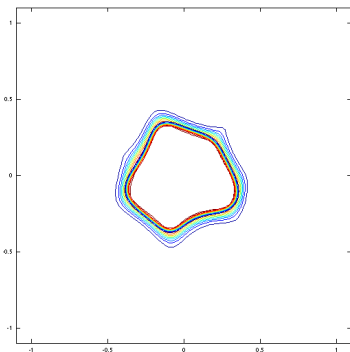


Fig. 9:
figures 6 and 7 overlaid

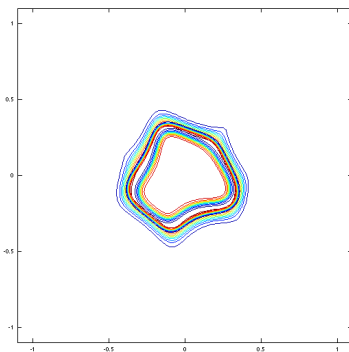


Fig. 10:
figures 6, 7 and 8 overlaid

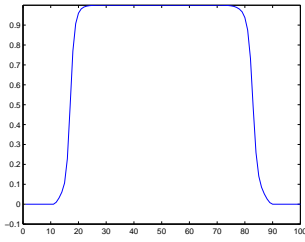


Fig. 11: Cross section,
hybrid model, $t = 0.12$

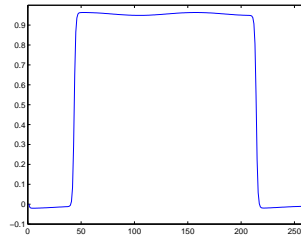


Fig. 12: Cross section,
Allen-Cahn model, $\mu = 0.2$,
 $t = 0.12$

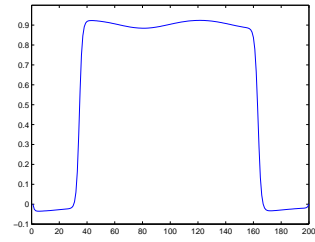


Fig. 13: Cross section,
Allen-Cahn model, $\mu = 0.7$,
 $t = 0.12$

S is computed with the hybrid model using the data and parameters of the computation to Figure 6, Figure 12 is computed with the Allen-Cahn model using the data and parameters of the computation to Figure 7, and Figure 13 is computed with the Allen-Cahn model using the same data and parameters as in Figure 8. In these figures the x_1 -axis is labeled with the number of the grid line. In figure 13 we see that the values of S in phase 2 differ from 1 by almost 0.1 and that the variation of the function $\bar{\varepsilon} : w$ is strongly visible. This is another hint that the value $\mu = 0.7$, which is used in the computation of this figure, is too large to get a good approximation of the sharp interface problem.

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