Interface motion by interface diffusion driven by bulk energy: justification of a diffusive interface model

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Abstract

A diffusive interface model for interface motion by interface diffusion is justified. The diffusion is driven by bulk terms of the free energy and the volumes of the material phases are conserved. The model includes an evolution equation similar to the Cahn-Hilliard equation with an additional gradient term. To justify the model we show by formal asymptotics that solutions converge to solutions of a sharp interface model when a regularity parameter tends to zero. The gradient term ensures that the curvature does not appear in the limit model as driving force. We show how the sharp interface model is obtained from the second law of thermodynamics.

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1 Introduction and statement of results

The goal of this article is to justify a phase field model, or diffusive interface model, for interface motion by interface diffusion, which was formulated in [3]. This model is valid for diffusion, which is solely driven by the free energy of the bulk. It consists of a system of partial differential equations including an evolution equation for an order parameter, which is similar to the Cahn-Hilliard equation, but contains an additional gradient term. To justify the model we construct an asymptotic solution of this system, which converges to a solution of a sharp interface model when a regularity parameter in the evolution equation tends to zero.

It is essential that because of the gradient term in the evolution equation the curvature is not part of the driving force for the diffusion in the sharp interface limit. This is different from other models, where the curvature appears automatically as part of the driving force. We first explain the model background.

Diffusion of material along a surface of a solid body or along an interface within a solid body appears in the technological process of sintering, which serves to form mechanical components out of ceramic powders. The grains in the powder touch at parts of their boundaries and have free surfaces at voids between the grains. When heated to a high temperature below the melting point, material at the grain boundaries becomes mobile and diffuses along the free surfaces bounding the voids and along the adjacent boundaries of neighboring grains; the latter process is called grain boundary diffusion. Since the common boundaries of neighboring grains form an interface, we use the term interface diffusion for this process, to distinguish it from diffusion along free surfaces, which we term surface diffusion. A similar process is diffusion induced grain boundary motion, which appears when polycrystalline films are placed in vapor consisting of another metal. Atoms from the vapor diffuse into the film along the grain boundaries.

When atoms, which left the crystal lattice and became mobile at one part of the grain boundary, or which entered the grain boundary from outside, move by diffusion and are built in again into the crystal lattice at another part of the boundary, the grain boundary moves in normal direction and the shape of the grain changes.

These example shows that interface and surface diffusion are closely related phenomena. The models we consider describe interface motion by interface diffusion, though they could be modified to describe surface motion by surface diffusion; this remains to be done in the future. The two parts of the solid separated by the interface are called material phases. We assume that the two phases consist of atoms of different types; atoms, which become mobile on one side of the interface, are therefore deposited on the same side. The volumes, or better the masses, of both phases are thus conserved in time. This is different from the ordinary situation in sintering, where the atoms on both sides of the interface are of the same type and the volumes of the phases are not conserved.

A well known model both for surface and interface motion by diffusion is

$$s(t,x) = -c\,\Delta_{\Gamma(t)}\kappa(t,x), \tag{1.1}$$

formulated by Mullins, cf. [21, 11]. It is known that this model satisfies the second law of thermodynamics for a free energy concentrated on the interface; the diffusion along the interface is thus driven by the interface energy. Here $\Gamma(t) \subseteq \mathbb{R}^3$ is a two-dimensional manifold representing the moving interface at time t, $s(t,x)$ is the normal velocity of this grain 1

interface diffusion

grain 2

surface diffusion

interface at the point $x \in \Gamma(t)$, the constant c is positive, κ is twice the mean curvature of $\Gamma(t)$, and $\Delta_{\Gamma(t)}$ denotes the surface Laplacian of $\Gamma(t)$.

In general however, the free energy does not only have an interface part, but has also a bulk part, which is given by the energy stored in the elastic deformations of the solid caused by stresses. These stresses influence the interface movement when the elastic properties of the two material phases are different. A more general model for interface motion by interface diffusion should therefore also account for the bulk part of the free energy. In Section 7 it is shown how such a general model is obtained from the second law of thermodynamics. The special form of the model obtained when the free energy only consists of a bulk term is stated below in (1.3) – (1.7). Just as the model (1.1), the general model describes the interface as a two-dimensional manifold. It is thus of sharp interface type.

In many situations it is advantageous to work with a diffusive interface model instead of a sharp interface model. A diffusive interface model corresponding to the model (1.1) was formulated in [9]. It consists of the Cahn-Hilliard equation

$$S_t = -\mathrm{div}_x\big(M(S)\nabla_x(\nu\Delta_x S - \hat{\psi}'(S))\big) \tag{1.2}$$

with a degenerate mobility function $M(S) = 1 - S^2$. Here S is a smooth order parameter, which characterizes the two material phases. At the point x at time t the material is in phase 1 or 2 if the value $S(t,x) \in \mathbb{R}$ is near to zero or one. $\hat{\psi}$ is a temperature dependent potential with two minima and ν is a positive parameter. Since $M(0) = M(1) = 1$, the mobility differs from zero by a sizeable amount only in a narrow band in the neighborhood of the interface, where S runs from 0 to 1. To justify (1.2) as a phase field model it was shown in [9] by formal asymptotics that for $\nu \to 0$ and under some assumptions for $\hat{\psi}$ the solution S approaches the characteristic function of a region bounded by the manifold $\Gamma(t)$ moving with normal velocity s given by (1.1), where $c = \nu\frac{\pi^2}{16}$.

The question arises whether a diffusive interface model corresponding to the sharp interface model (1.3) – (1.7) for diffusion driven solely by bulk terms of the free energy can be found. Based on investigations in [1, 2], we formulated in [3] a system of partial differential equations and conjectured, that it forms such a diffusive interface model. This system, which is stated below in (1.10) – (1.12), contains an evolution equation similar to (1.2), but with $M(S)$ replaced by $|\nabla_x S|$. The conjecture was based on the asymptotic behavior of plane traveling wave solutions, which converge to solutions of the sharp interface model for $\nu \to 0$. To definitely justify the model it remains to exclude the possibility, that only plane waves show this behavior. This justification is given here. To this end we assume that a smooth, but otherwise arbitrary solution of the sharp interface model exists and use it to construct an asymptotic solution of the diffusive interface model, which approaches the sharp interface solution when ν tends to zero.

In [4] it was shown that solutions of (1.10) – (1.12) exist in "$1\frac{1}{2}$–space dimensions". A proof for the existence of solutions in higher space dimensions is not available. This is different for the model (1.2), for which existence of solutions was proved in [12]. Other investigations related to this and to similar models can be found in [5, 6, 23, 28, 29] and in the references cited therein. For the sharp interface model (1.1) existence, regularity and asymptotic behavior of a family of smooth manifolds, whose evolution is governed by the sharp interface model (1.1) or by an alternative evolution law proposed in [11], are investigated in [13, 14, 15]. We are not aware of such investigations for the sharp interface problem (1.3) – (1.7).

Models for interface diffusion problems, where diffusing atoms can be deposited on both sides of the interface and the volume of the phases is not conserved in time, have been proposed and investigated in [10, 16, 17, 19, 24, 26, 27].

Following the work in [22], the sharp interface limit has been determined for several models; we mention the investigations in [7, 9, 16, 18, 20, 28], for example. Whereas these investigations are based on formal asymptotics, the asymptotic limit has been determined rigorously in [8, 25].

In the remainder of this introduction we first formulate the sharp and diffusive interface models and explain the construction of the asymptotic solution of the diffusive interface model. The main convergence result is stated in Theorem 1.3 at the end of the introduction. The diffusive interface model contains a double well potential. Our construction of the asymptotic solution yields conditions for the form of this double well potential, which can be interpreted physically. We study these conditions and give the interpretation in Section 2. Sections 3 – 6 contain the proof of Theorem 1.3. In the final Section 7 we show how the sharp interface model is obtained from the second law of thermodynamics.

Sharp interface model. Let Ω be an open subset in $\mathbb{R}^3$. It represents the material points of a solid body. Let $0 \le t_1 < t_2 < \infty$ 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

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

embedded in Ω. The two different phases are characterized by the values of the order parameter $\hat{S}$, which in this model is piecewise constant and only takes the values 0 or 1 with a jump along the interface Γ separating the phases. The sharp interface model determines the unknown position of the interface, the unknown displacement $\hat{u}(t, x) \in \mathbb{R}^3$ and the unknown Cauchy stress tensor $\hat{T}(t, x) \in \mathcal{S}^3$. Here $\mathcal{S}^3$ denotes the set of symmetric 3×3-matrices. The model consists of the equations

$$-\mathrm{div}_x \hat{T} = b, \tag{1.3}$$

$$\hat{T} = D(\varepsilon(\nabla_x \hat{u}) - \bar{\varepsilon}\hat{S}), \tag{1.4}$$

$$s = -c\,\Delta_\Gamma(n \cdot [\hat{C}]n), \tag{1.5}$$

$$[\hat{u}] = 0, \tag{1.6}$$

$$[\hat{T}]n \quad = \quad 0, \tag{1.7}$$

and of suitable boundary and initial conditions. (1.3) and (1.4) must hold on $Q \setminus \Gamma$, the jump conditions (1.5) – (1.7) are given on Γ. Here $\nabla_x u$ denotes the 3×3–matrix of first order derivatives of u, the deformation gradient, and

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

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 $D : \mathcal{S}^3 \to \mathcal{S}^3$ is a linear, symmetric, positive definite mapping, $c > 0$ is a given constant and $b : [0, \infty) \times \Omega \to \mathbb{R}^3$ is the given volume force.

The unit normal vector $n(t, x) \in \mathbb{R}^3$ to $\Gamma(t)$ at $x \in \Gamma(t)$ points into the region where $\hat{S} = 1$, and $s(t, x) \in \mathbb{R}$ is the normal speed of $\Gamma(t)$ at $x \in \Gamma(t)$ in direction $n(t, x)$. Also, $\Delta_\Gamma = \Delta_{\Gamma(t)}$ is the surface Laplacian introduced in (1.1). In the following we use this simpler notation for the surface Laplacian, since no confusion is possible. $[\hat{u}], [\hat{T}], [\hat{C}]$ denote the jumps of $\hat{u}, \hat{T}$ and of the Eshelby tensor

$$\hat{C}(\nabla_x u, \hat{S}) = \psi(\varepsilon(\nabla_x \hat{u}), \hat{S})I - (\nabla_x \hat{u})^T \hat{T} \tag{1.8}$$

across Γ, where I is the 3×3–unit matrix, where $(\nabla_x \hat{u})^T \hat{T}$ denotes the matrix product, and where

$$\psi(\varepsilon, S) = \frac{1}{2}\big(D(\varepsilon - \bar{\varepsilon}S)\big) \cdot (\varepsilon - \bar{\varepsilon}S) + \hat{\psi}(S), \tag{1.9}$$

is the free energy. Here the scalar product of two matrices is denoted by $A \cdot B = \sum a_{ij} b_{ij}$, and $\hat{\psi} : \mathbb{R} \to [0, \infty)$ is a double well potential. Of course, for the sharp interface problem only the values of $\hat{\psi}$ at $\hat{S} = 0$ and $\hat{S} = 1$ do matter, but the values of $\hat{\psi}(S)$ for all $S \in [0, 1]$ become important in the diffusive interface problem, where the discontinuous order parameter $\hat{S}$ is replaced by a smooth order parameter S.

Precisely, for a function w defined in a neighborhood of $\Gamma(t)$ and for $x \in \Gamma(t)$ we define

$$[w] = \lim_{\xi \searrow 0} \big(w(x + n(t, x)\xi) - w(x - n(t, x)\xi)\big).$$

The evolution law (1.5) describes motion of the interface $\Gamma(t)$ due to diffusion of atoms along the interface. The flux is given by $-c\nabla_\Gamma\,(n \cdot [\hat{C}]n)$ with the surface gradient $\nabla_\Gamma = \nabla_{\Gamma(t)}$. It is not difficult to see that because of the presence of the surface Laplacian in (1.5) the integral $\int_\Omega \hat{S}(t, x)dx$ is constant in time, hence the volume of the phases is preserved in time. The equations (1.3) and (1.4), which differ from the system of linear elasticity only by the term $\bar{\varepsilon}\hat{S}$, determine the elastic properties of the two phases characterized by the values $\hat{S} = 0$ or $\hat{S} = 1$: In the first phase the material is stress free at the strain state $\varepsilon(\nabla_x u) = 0$, in the other phase at $\varepsilon(\nabla_x u) = \bar{\varepsilon}$. This corresponds to different crystal structures of the phases. The elasticity tensor D has the same value at both phases, but it would be important for applications to study the case where D is a function of $\hat{S}$ with $D[0] \neq D[1]$.

Diffusive interface model. In this model the material at the point $x \in \Omega$ at time t is in phase 1 or 2 if the value $S(t, x) \in \mathbb{R}$ of the smooth order parameter S is near to zero or one. The other unknowns are the displacement $u(t,x) \in \mathbb{R}^3$ and the Cauchy stress tensor $T(t,x) \in \mathcal{S}^3$. The unknowns must satisfy the quasi-static equations

$$-\operatorname{div}_x T(t,x) = b(t,x), \tag{1.10}$$

$$T(t,x) = D\big(\varepsilon(\nabla_x u) - \bar{\varepsilon} S\big)(t,x), \tag{1.11}$$

$$S_t(t,x) = c \operatorname{div}_x \Big(\nabla_x \big(\psi_S(\varepsilon(\nabla_x u), S) - \nu \Delta_x S\big) |\nabla_x S|\Big)(t,x), \tag{1.12}$$

for $(t,x) \in (0,\infty) \times \Omega$. Here $\nu > 0$ is a small parameter of regularization, D, $\bar{\varepsilon}$, c and b are defined as in (1.3) – (1.5), and $\psi_S = \frac{\partial}{\partial S}\psi$ is the partial derivative of the free energy given in (1.9), whence

$$\psi_S(\varepsilon, S) = -T \cdot \bar{\varepsilon} + \hat{\psi}'(S). \tag{1.13}$$

The double well potential $\hat{\psi}$ must satisfy conditions, which are discussed in Section 2.

(1.12) is the evolution equation for the order parameter S, which is non-uniformly parabolic because of the regularizing term $c\nu \operatorname{div}_x\big(\nabla_x(\nu \Delta S)\,|\nabla_x S|\big)$. The system (1.10) – (1.12) of partial differential equations must be supplemented by boundary and initial conditions to complete the diffusive interface model. Yet, in our investigation these conditions do not play a role, since we construct asymptotic solutions of (1.10) – (1.12) in the interior of $(0,\infty) \times \Omega$. Only for completeness we mention that in [4] existence of weak solutions was proved for an initial-boundary value problem in "$1\frac{1}{2}$–space dimensions", which consists of the equations (1.10) – (1.12), of the boundary conditions

$$u(t,x) = \gamma(t,x), \quad \frac{\partial}{\partial n} S(t,x) = 0, \quad \frac{\partial}{\partial n}\big(\psi_S(\varepsilon, S) - \nu \Delta_x S\big) = 0$$

which must be satisfied for $(t,x) \in [0,\infty) \times \partial\Omega$, and of the initial condition

$$S(0,x) = S_0(x), \quad x \in \Omega.$$

Asymptotic solution. We aim to construct an asymptotic solution

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

of the system (1.10) – (1.12), which converges for $\nu \to 0$ to solutions of the sharp interface model (1.3) – (1.7). To construct the asymptotic solution we replace the jump function $\hat{S}$ from the sharp interface solution by a smooth transition profile $S^{(\nu)}$. To determine the transition profile we apply the usual procedure to make an asymptotic ansatz for $S^{(\nu)}$, insert the ansatz into (1.12) and equate coefficients in the resulting truncated series to zero. This yields a system of ordinary differential equations for the terms in the ansatz. However, in (1.12) not only S, but also u appears; we must therefore also determine an ansatz for the component $u^{(\nu)}$ of the asymptotic solution. To obtain this ansatz, we use the function $\hat{u}$ from the sharp interface solution. Essential for the ansatz is the behavior of $\hat{u}$ at the interface Γ. This function is continuous at Γ, but in general the gradient jumps. The ansatz for $u^{(\nu)}$ is obtained by modification of $\hat{u}$ in a neighborhood of Γ using an asymptotic series, which regularizes the singular behavior of $\nabla_x \hat{u}$. To explain this construction in detail we first introduce some notations and assumptions used throughout the paper.

We denote by $(\hat{u}, \hat{T}, \Gamma)$ a given solution of (1.3) – (1.7) in the set $Q = [t_1, t_2] \times \Omega$. Precisely, we require that this solution satisfies the following

Assumption A. Γ is a C^6–manifold embedded in Q, such that the set Γ is a compact subset of Q and such that the two-dimensional manifold $\Gamma(t)$ does not have a boundary for all $t \in [t_1, t_2]$. The set of all $(t, x) \in Q \backslash \Gamma$ with $\hat{S}(t, x) = 0$ is denoted by γ, and γ' is the set of all $(t, x) \in Q$ with $\hat{S}(t, x) = 1$. We assume that the functions $\hat{u}$ and $\hat{T}$ are six times continuously differentiable on γ and on γ' with six times continuously differentiable extensions from γ to $\gamma \cup \Gamma$ and from γ' to $\gamma' \cup \Gamma$.

The pairwise disjoint sets Γ, γ and γ' satisfy $\Gamma \cup \gamma \cup \gamma' = Q$. 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 $t \in [t_1, t_2]$. By choosing δ smaller if necessary, we can guarantee that

$$(\eta, \xi) \mapsto x(t, \eta, \xi) = \eta + n(t, \eta)\xi : \Gamma(t) \times (-\delta, \delta) \to \mathcal{U}(t) \tag{1.14}$$

defines a new coordinate system in this neighborhood for every $t \in [t_1, t_2]$. This implies that for ξ satisfying $-\delta < \xi < \delta$

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

is a C^5–parallel manifold of Γ embedded in $\mathcal{U}$, and

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

is a C^5–parallel manifold of $\Gamma(t)$ embedded in $\mathcal{U}(t)$. Twice the mean curvature of the manifold $\Gamma_\xi(t)$ at the point (η, ξ) is denoted by $\kappa(t, \eta, \xi)$. Let $\tau_1,\ \tau_2 \in \mathbb{R}^3$ be two orthogonal unit vectors tangent to Γ_ξ at $(\eta, \xi) \in \Gamma_\xi(t)$. For functions $w : \Gamma_\xi(t) \to \mathbb{R}$ and $W : \Gamma_\xi(t) \to \mathbb{R}^3$ we define the surface gradients

$$\nabla_{\Gamma_\xi} w = (\partial_{\tau_1} w)\tau_1 + (\partial_{\tau_2} w)\tau_2 \in \mathbb{R}^3, \tag{1.15}$$

$$\hat{\nabla}_{\Gamma_\xi} W = (\partial_{\tau_1} W) \otimes \tau_1 + (\partial_{\tau_2} W) \otimes \tau_2 \in \mathbb{R}^{3\times 3}, \tag{1.16}$$

where the argument of all functions is (η, ξ), and 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 $\nabla_\Gamma = \nabla_{\Gamma_0}$, $\hat{\nabla}_\Gamma = \hat{\nabla}_{\Gamma_0}$.

Following the ideas explained above we begin the construction of the ansatz for $u^{(\nu)}$ by splitting $\hat{u}$ into a leading term, whose gradient shows the same jump behavior as $\nabla_x \hat{u}$, but vanishes outside of $\mathcal{U}$, and into a term, which is continuously differentiable in Q. Note that since the derivatives of $\hat{u}$ have continuous extensions from γ to Γ and from γ' to Γ, equation (1.16) together with (1.6) implies

$$[\hat{\nabla}_\Gamma \hat{u}] = \hat{\nabla}_\Gamma [\hat{u}] = 0 \tag{1.17}$$

Therefore only the normal derivative jumps at Γ. With the notation

$$u^*(t, \eta) = [\partial_n \hat{u}](t, \eta). \tag{1.18}$$

we conclude from the equation $\nabla_x \hat{u} = \nabla_\Gamma \hat{u} + (\partial_n \hat{u}) \otimes n$ that

$$[\nabla_x \hat{u}] = u^* \otimes n. \tag{1.19}$$

Choose $\phi \in C^\infty(Q)$ such that $\phi = 0$ outside the set $\mathcal{U}$ and $\phi = 1$ in a neighborhood of Γ. The splitting of $\hat{u}$ is now given by

$$\begin{aligned} \hat{u}(t,x) &= u^*(t,\eta) \int_0^\xi \hat{S}(t, \eta + n(t,\eta)\zeta)\, d\zeta\, \phi(t,x) + v(t,x) \\ &= u^*(t,\eta)\, \langle \xi \rangle\, \phi(t,x) + v(t,x), \end{aligned} \tag{1.20}$$

where (η, ξ) are the new coordinates of $x \in \mathcal{U}(t)$ and where

$$\langle \xi \rangle = \begin{cases} \xi, & \xi \geq 0, \\ 0, & \xi < 0. \end{cases} \tag{1.21}$$

We have

$$[\nabla_x \hat{u}] = [\nabla_x (u^* \langle \xi \rangle)], \qquad [\nabla_x v] = 0. \tag{1.22}$$

The means that the first term in (1.20) has the same jump behavior at Γ as $\nabla_x \hat{u}$, and that the remainder term v in (1.20) is continuously differentiable at Γ. Hence, v is continuously differentiable in Q. To prove (1.22), note that an obvious computation yields for the inverse $x \mapsto (\eta(t,x), \xi(t,x))$ of $(\eta, \xi) \mapsto x(t, \eta, \xi)$, for $x_0 \in \Gamma(t)$ and for a vector $\tau \in \mathbb{R}^3$ tangent to $\Gamma(t)$ at x_0 that

$$\begin{aligned} \partial_\tau \xi(t, x_0) &= 0, \qquad & \partial_\tau \eta(t, x_0) &= \tau, \\ \partial_n \xi(t, x_0) &= 1, \qquad & \partial_n \eta(t, x_0) &= 0. \end{aligned}$$

We thus obtain for the directional derivative ∂_z with respect to a vector $z \in \mathbb{R}^3$ and for $x_0 \in \Gamma(t)$ that

$$\begin{aligned} \lim_{\substack{x \to x_0 \\ x \in \gamma'}} \partial_z (u^*(t,\eta)\, \xi\, \phi(t,x)) &= \lim_{\substack{x \to x_0 \\ x \in \gamma'}} \Big(\hat{\nabla}_\Gamma u^*(t,\eta)\, \partial_z \eta(t,x) \xi + u^*(t,\eta)\, \partial_z \xi(t,x) \Big) \\ &= \begin{cases} 0, & \text{if } z \text{ is tangential to } \Gamma(t) \text{ at } x_0\,, \\ u^*(t,x_0), & \text{if } z = n(t,x_0)\,. \end{cases} \end{aligned}$$

This yields $[\hat{\nabla}_\Gamma (u^* \langle \xi \rangle \phi)] = 0$ and $[\partial_n (u^* \langle \xi \rangle \phi)] = u^*$. Using the equation $\nabla_x W = \hat{\nabla}_\Gamma W + (\partial_n W) \otimes n$, applied to $W = u^* \langle \xi \rangle \phi$, we obtain together with (1.19) that

$$[\nabla_x (u^* \langle \xi \rangle \phi)] = u^* \otimes n = [\nabla_x \hat{u}].$$

This proves (1.22), since $\phi = 1$ in a neighborhood of Γ.

The ansatz for $u^{(\nu)}$ sought for is now obtained by replacing the jump function $\hat{S}$ in (1.20) with the smooth transition profile $S^{(\nu)}$. We thus want to find an asymptotic solution $(u^{(\nu)}, T^{(\nu)}, S^{(\nu)})$ of the system (1.10) – (1.12) with order parameter and displacement field of the form

$$
\begin{aligned}
S^{(\nu)}(t,\eta,\xi) &= S_0\big(t,\eta,\frac{\xi}{\nu^{1/2}}\big) + \nu^{1/2} S_1\big(t,\eta,\frac{\xi}{\nu^{1/2}}\big) + \nu S_2\big(t,\eta,\frac{\xi}{\nu^{1/2}}\big), && (1.23)\\
u^{(\nu)}(t,x) &= u^*(t,\eta)\int_0^\xi S^{(\nu)}(t,\eta,\zeta)\,d\zeta\,\phi(t,x) + v(t,x)\\
&= u^*(t,\eta)\,S^{(\nu)(-1)}(t,\eta,\xi)\,\phi(t,x) + v(t,x)\\
&= u^*(t,\eta)\sum_{i=0}^{2}\nu^{\frac{i+1}{2}} S_i^{(-1)}\big(t,\eta,\frac{\xi}{\nu^{1/2}}\big)\,\phi(t,x) + v(t,x). && (1.24)
\end{aligned}
$$

In the last two lines we used the notations

$$
\begin{aligned}
S_i^{(-1)}(t,\eta,\xi) &= \int_0^\xi S_i\big(t,\eta,\zeta\big)\,d\zeta\,, \qquad i=0,1,2, && (1.25)\\
S^{(\nu)(-1)}(t,\eta,\xi) &= \int_0^\xi S^{(\nu)}(t,\eta,\zeta)\,d\zeta \;=\; \sum_{i=0}^{2}\nu^{\frac{i+1}{2}} S_i^{(-1)}\big(t,\eta,\frac{\xi}{\nu^{1/2}}\big)\,. && (1.26)
\end{aligned}
$$

More precisely, we want that $S^{(\nu)}$ is a transition profile connecting the state $S^{(\nu)}=0$ with the state $S^{(\nu)}=1$. Therefore we require that there exist functions $a:\Gamma\to(-\infty,0)$, $d:\Gamma\to(0,\infty)$ such that

$$
S_0\big(t,\eta,\frac{\xi}{\nu^{1/2}}\big) + \nu^{1/2} S_1\big(t,\eta,\frac{\xi}{\nu^{1/2}}\big) + \nu S_2\big(t,\eta,\frac{\xi}{\nu^{1/2}}\big) = \begin{cases} 0, & \xi=\nu^{1/2}\,a(t,\eta),\\ 1, & \xi=\nu^{1/2}\,d(t,\eta). \end{cases} \qquad (1.27)
$$

If such functions a and d exist, then the set

$$
\Gamma[\nu] = \{(t,x(t,\eta,\xi)) \mid (t,\eta)\in\Gamma,\ \nu^{1/2}a(t,\eta)\le\xi\le\nu^{1/2}d(t,\eta)\}. \qquad (1.28)
$$

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 $\nu\to 0$. For fixed ν the thickness is not constant but depends on the point $(t,\eta)\in\Gamma$.

To find equations for the unknown functions S_0, S_1 and S_2 we insert (1.23) and (1.24) into the evolution equation (1.12), expand both sides of this equation into a truncated series of powers of $\nu^{1/2}$ and equate the coefficients of the powers $m=0,1,2$ to zero. This straightforward, but technically complicated procedure is carried out in Section 3. It leads to a recursively solvable system of ordinary differential equations for the functions

$$
\zeta\mapsto S_i(t,\eta,\zeta):[a(t,\eta),d(t,\eta)]\to\mathbb{R},\quad i=0,1,2.
$$

Here $\xi/\nu^{1/2}$ has been replaced by ζ. The functions depend on the parameter $(t,\eta)\in\Gamma$, since the system of differential equations depends on this parameter and must be satisfied for every value of the parameter. Therefore S_0, S_1 and S_2 are defined on the set

$$
\Gamma[a,b] = \{(t,\eta,\zeta) \mid (t,\eta)\in\Gamma,\ a(t,\eta)\le\zeta\le d(t,\eta)\}\,, \qquad (1.29)
$$

which we do not identify with a subset of $(t_1,t_2)\times\Omega$, differently from $\Gamma[\nu]$. Boundary conditions for S_i are obtained from (1.27).

To state the resulting system we sometimes drop the arguments t and η for simplicity, but all the functions in the system depend on these arguments. Differentiation with respect to ζ is denoted by '. The notation $S_i''(\zeta)$ thus means $\partial_\zeta^2 S_i(t,\eta,\zeta)$. It follows that S_0, S_1, S_2 must satisfy the differential equations

$$\tilde{\psi}_S(S_0(\zeta)) - S_0''(\zeta) = 0, \tag{1.30}$$

$$\tilde{\psi}_{SS}(S_0(\zeta))\, S_1(\zeta) - S_1''(\zeta) = f_1(t,\eta,\zeta) + C_1(t,\eta), \tag{1.31}$$

$$\tilde{\psi}_{SS}(S_0(\zeta))\, S_2(\zeta) - S_2''(\zeta) = f_2(t,\eta,\zeta) + C_2(t,\eta) \tag{1.32}$$

for $\zeta \in [a(t,\eta), d(t,\eta)]$, where

$$f_1(t,\eta,\zeta) = \kappa_0 S_0'(\zeta) + \dot{\sigma}(\zeta)\zeta + \overline{\varepsilon} \cdot D\varepsilon\Big(\hat{\nabla}_\Gamma\big(u^*\, S_0^{(-1)}(\zeta)\big)\Big), \tag{1.33}$$

$$\begin{aligned} f_2(t,\eta,\zeta) &= \kappa_0 S_1'(\zeta) + \kappa_1 \zeta S_0'(\zeta) + \frac{1}{2}\ddot{\sigma}(\zeta)\zeta^2 \\ &\quad + \overline{\varepsilon} \cdot D\varepsilon\Big(\hat{\nabla}_\Gamma\big(u^*\, S_1^{(-1)}(\zeta)\big) + \zeta\, \hat{\nabla}_\Gamma\big(u^*\, S_0^{(-1)}(\zeta)\big) A_1\Big) \\ &\quad + \Delta_\Gamma S_0(\zeta) - \frac{1}{2}\tilde{\psi}_{SSS}(S_0(\zeta))\, S_0(\zeta)^2, \end{aligned} \tag{1.34}$$

and the boundary conditions

$$S_0(t,\eta,a(t,\eta)) = 0, \quad S_0(t,\eta,d(t,\eta)) = 1, \tag{1.35}$$

$$S_i(t,\eta,a(t,\eta)) = S_i(t,\eta,d(t,\eta)) = 0, \qquad i = 1,2. \tag{1.36}$$

The coefficient functions in these equations have the following meaning:

$$\tilde{\psi}(t,\eta,S) = \hat{\psi}(S) - \hat{\psi}(0)(1-S) - \hat{\psi}(1)S + \frac{1}{2}\overline{\varepsilon} \cdot [\hat{T}](t,\eta)S(1-S) \tag{1.37}$$

with $\hat{\psi}$ defined in (1.9) is the effective free energy. $\tilde{\psi}_S$, $\tilde{\psi}_{SS}$ $\tilde{\psi}_{SSS}$ are the partial derivatives, $C_1(t,\eta), C_2(t,\eta)$ are functions constant with respect to ζ. The procedure described above does not determine these constants, but to guarantee existence of the solutions S_1, S_2, they must be chosen in a unique way. The condition for these constants is stated in Theorem 1.2 below. The stress field $D\varepsilon(\nabla_x v)$ generated by the regular part v in (1.20) influences the transition profile via the component

$$\sigma = \overline{\varepsilon} \cdot D\varepsilon(\nabla_x v). \tag{1.38}$$

As shown by (1.22), $\overline{\varepsilon} \cdot D\varepsilon(\nabla_x\, v)$ is continuous across Γ, but the derivatives $\partial_\xi^i \sigma(\xi) = \partial_\xi^i \sigma(t,\eta,\xi)$ can have jumps at $\xi = 0$ for $i \geq 1$. We thus set

$$\dot{\sigma}(\xi) = \partial_\xi \sigma(\pm 0), \quad \ddot{\sigma}(\xi) = \partial_\xi^2 \sigma(\pm 0), \tag{1.39}$$

where we choose the $+$ sign for $\xi > 0$ and the $-$ sign for $\xi < 0$. With twice the mean curvature $\kappa(t,\eta,\xi)$ of $\Gamma_\xi(t)$ at (η,ξ) we define

$$\kappa_i(t,\eta) = \partial_\xi^i \kappa(t,\eta,0), \quad i = 0,1. \tag{1.40}$$

To define A_1, let t and ξ be fixed and consider the mapping $\mathcal{T}_{t,\xi} : \Gamma(t) \to \Gamma_\xi(t)$ defined by

$$\mathcal{T}_{t,\xi}(\eta) = \eta + n(t,\eta)\xi.$$

This mapping has an inverse $\mathcal{T}_{t,\xi}^{-1}$. For every $\hat{\eta} \in \Gamma_\xi(t)$ there is a linear mapping $d\mathcal{T}_{t,\xi}^{-1}(\hat{\eta}) \in L(\mathbb{R}^3, \mathbb{R}^3)$, which we represent as a matrix in $\mathbb{R}^{3\times 3}$, such that for every $W : \Gamma(t) \mapsto \mathbb{R}^3$ the equation

$$\hat{\nabla}_{\Gamma_\xi}(W \circ \mathcal{T}_{t,\xi}^{-1}) = \big((\hat{\nabla}_\Gamma W) \circ \mathcal{T}_{t,\xi}^{-1}\big) d\mathcal{T}_{t,\xi}^{-1} \tag{1.41}$$

holds. The usual matrix product on the right hand side of this equation is written without a dot. $d\mathcal{T}_{t,\xi}^{-1}$ is the matrix representation of the differential of $\mathcal{T}_{t,\xi}^{-1}$. Of course, we have $d\mathcal{T}_{t,0}^{-1}(\hat{\eta}) = I$, where $I \in \mathbb{R}^{3\times 3}$ denotes the identity. Now consider $A(t,\eta,\xi) = d\mathcal{T}_{t,\xi}^{-1} \circ \mathcal{T}_{t,\xi}(\eta)$. From (1.41) we have

$$\hat{\nabla}_{\Gamma_\xi}(W \circ \mathcal{T}_{t,\xi}^{-1}) \circ \mathcal{T}_{t,\xi} = (\hat{\nabla}_\Gamma W)A. \tag{1.42}$$

The role of A therefore is to express the gradient tangential to $\Gamma_\xi(t)$ as gradient tangential to $\Gamma(t)$. We set

$$A_1(t,\eta) = \partial_\xi A(t,\eta,0) \in \mathbb{R}^{3\times 3}. \tag{1.43}$$

A_1 coincides essentially with the shape-operator (Weingarten-Abbildung) in differential geometry. This completes the construction of the asymptotic solution.

Main results. Existence of solutions of the coupled boundary value problems (1.30) – (1.36) is studied in Section 4. To state the existence result for the nonlinear boundary value problem (1.30), (1.35) proved there, consider the initial value problem

$$S_0'(t,\eta,\zeta) = \sqrt{2\tilde{\psi}(t,\eta,S_0(t,\eta,\zeta))}, \qquad S_0(t,\eta,0) = \frac{1}{2}. \tag{1.44}$$

By differentiation of this first order differential equation with respect to ζ we see immediately that a two-times differentiable solution is also a solution of the second order differential equation (1.30). Therefore it suffices to study this initial value problem.

Theorem 1.1 *Suppose that the function $\tilde{\psi} : \Gamma \times \mathbb{R}$ defined in* (1.37) *has the following prperties:*
1. $(S \mapsto \tilde{\psi}(t,\eta,S)) \in C^7(\mathbb{R},\mathbb{R})$, $\tilde{\psi}_S \in C^6(\Gamma \times \mathbb{R}, \mathbb{R})$,
2. $\tilde{\psi}(t,\eta,S) > 0$ *for* $0 < S < 1$, $(t,\eta) \in \Gamma$,
3. there is $c_0 > 0$ *such that for all* $(t,\eta) \in \Gamma$

$$\partial_S\tilde{\psi}(t,\eta,0) \geq c_0, \qquad \partial_S\tilde{\psi}_S(t,\eta,1) \leq -c_0. \tag{1.45}$$

Then the following assertions hold:
(i) For all $(t,\eta) \in \Gamma$ *there exist numbers* $-\infty < a = a(t,\eta) < 0 < d = d(t,\eta) < \infty$ *and a unique solution* $\zeta \mapsto S_0(t,\eta,\zeta) : [a,d] \to [0,1]$ *of* (1.44)*, which is strictly increasing and satisfies*

$$S_0(t,\eta,a) = 0, \quad S_0(t,\eta,b) = 1, \quad S_0'(t,\eta,a) = S_0'(t,\eta,d) = 0. \tag{1.46}$$

S_0 has continuous derivatives up to sixth order with respect to all variables on the set $\Gamma[a,b]$ defined in (1.29). *Hence, these derivatives are bounded. Moreover, the solution satisfies* (1.30) *and*

$$\nabla_\eta S_0(t,\eta,\zeta)_{|\zeta=a(t,\eta)} = 0, \quad \nabla_\eta S_0(t,\eta,\zeta)_{|\zeta=d(t,\eta)} = 0.$$

(ii) The functions $(t,\eta) \mapsto a(t,\eta)$, $(t,\eta) \mapsto d(t,\eta)$ are five times continuously differentiable. All derivatives are bounded.

Insertion of the function S_0 from this theorem into the coefficient functions of the differential equations (1.31), (1.32) yields two linear boundary value problems for S_1 and S_2, which can be solved recursively. In Section 4 we prove the following existence result for these boundary value problems.

Theorem 1.2 *Assume that C_1, C_2 on the right hand side of* (1.31), (1.32) *satisfy the conditions*

$$C_i(t,\eta) = -\int_{a(t,\eta)}^{d(t,\eta)} f_i(t,\eta,\zeta) S_0'(t,\eta,\zeta)\, d\zeta, \quad i = 1,2, \tag{1.47}$$

with f_i given by (1.33), (1.34). *Then there are unique solutions $S_1, S_2 : \Gamma[a,d] \to \mathbb{R}$ of the differential equations* (1.31), (1.32) *and of the boundary conditions* (1.36), *which satisfy the orthogonality relation*

$$\int_{a(t,\eta)}^{d(t,\eta)} S_i(t,\eta,\zeta) S_0'(t,\eta,\zeta)\, d\zeta = 0.$$

Moreover, we have $S_1 \in C^5(\Gamma[a,d])$ and $S_2 \in C^4(\Gamma[a,d])$. In particular, the derivatives of S_1 up to order 5 *and of S_2 up to order four with respect to all variables are bounded.*

We denote the scalar product on $L^2(Q)$ by

$$(v,w)_Q = \int_Q v(t,x) w(t,x) d(t,x).$$

To state the main convergence result we need the space $\mathfrak{R}(Q)$ of Radon measures on Q. Since this space is isomorphic to the space of bounded linear functionals on $C_0(Q)$, the weak divergence $\text{div}_x W$ of a vector field $W \in L^2(Q,\mathbb{R}^3)$ is a Radon measure on Q, if there is $C > 0$ such that

$$|(W, \nabla_x \varphi)_Q| \le C \sup_{(t,x)\in Q} |\varphi(t,x)| = C\|\varphi\|_{C(Q)},$$

for all $\varphi \in C_0^1(\Omega)$. The norm of $\text{div}_x W$ in $\mathfrak{R}(Q)$ is

$$\|\text{div}_x W\|_{\mathfrak{R}} = \sup_{\substack{\varphi\in C_0^1(Q) \\ \|\varphi\|_{C(Q)}=1}} |(W, \nabla_x \varphi)_Q|,$$

and for the application of the functional $\text{div}_x W$ to $\varphi \in C_0(Q)$ we write

$$\int_Q \varphi\, d(\text{div}_x W).$$

We also need the dual space $\mathfrak{R}^\alpha(Q)$ of the space $C_0^\alpha(Q)$ with $1 > \alpha > 0$. For the weak divergence $\operatorname{div}_x W \in \mathfrak{R}^\alpha(Q)$ we have the same relations as above with $\|\varphi\|_{C(Q)}$ replaced by

$$\|\varphi\|_{C^\alpha(Q)} = \|\varphi\|_{C(Q)} + \sup_{\substack{(t,x),(s,y)\in Q\\ (t,x)\neq(s,y)}} \frac{|\varphi(t,x)-\varphi(s,y)|}{|(t,x)-(s,y)|^\alpha}\,.$$

Theorem 1.3 *Let the hypotheses for $\tilde\psi$ in Theorem 1.1 be satisfied. Assume that $b \in C^5(Q)$ and that the sharp interface problem (1.3) – (1.7) has a solution $(\hat u, \hat T, \Gamma)$ in the domain Q satisfying Assumption A. For $\nu > 0$ let $S^{(\nu)}$ be defined in the transitional region $\Gamma[\nu]$ by the equation (1.23) with the functions S_0, S_1, S_2 given in Theorems 1.1 and 1.2. In the other parts of Q define $S^{(\nu)}$ by*

$$S^{(\nu)}(t,x) = \begin{cases} 1, & (t,x) \in \gamma'\backslash\Gamma[\nu],\\ 0, & (t,x)\in\gamma\backslash\Gamma[\nu]. \end{cases}$$

Define $u^{(\nu)}$ by (1.24) and set

$$T^{(\nu)} = D(\varepsilon(\nabla_x u^{(\nu)}) - \bar\varepsilon S^{(\nu)}). \tag{1.48}$$

Then the expressions $\operatorname{div}_x T^{(\nu)} + b$ and $S_t^{(\nu)} - c\operatorname{div}_x\big((\nabla_x(\psi_S - \nu\Delta_x S^{(\nu)})|\nabla_x S^{(\nu)}|\big)$ are Radon measures on Q. Furthermore, the function $(u^{(\nu)}, T^{(\nu)}, S^{(\nu)})$ satisfies (1.10) and (1.12) asymptotically with a remainder term tending to zero in $\mathfrak{R}$ and in $\mathfrak{R}^\alpha$, respectively: There are constants K_1, K_2 such that for $0 < \alpha \le 1$

$$\|\operatorname{div}_x T^{(\nu)} + b\|_{\mathfrak{R}} \le K_1 \nu^{1/2}, \tag{1.49}$$

$$\Big\|S_t^{(\nu)} - c\operatorname{div}_x\Big((\nabla_x(\psi_S - \nu\Delta_x S^{(\nu)})|\nabla_x S^{(\nu)}|\Big)\Big\|_{\mathfrak{R}^\alpha} \le K_2\,\nu^{\min(\frac{\alpha}{2},\frac14)}. \tag{1.50}$$

In the space $\mathfrak{R}$ the remainder term converges to zero in the weak topology: For all $\varphi \in C_0(Q)$

$$\int_Q \varphi\, d\Big(S_t^{(\nu)} - c\operatorname{div}_x\big(\nabla_x(\psi_S - \nu\Delta_x S^{(\nu)})|\nabla_x S^{(\nu)}|\big)\Big) \to 0, \quad \text{if } \nu \to 0. \tag{1.51}$$

2 Conditions for the double well potential, physical interpretation

The assumptions 1. – 3. in Theorem 1.1 impose conditions on the form of the double well potential $\hat\psi$. In this section we study these conditions and give a physical interpretation.

Note first that $\tilde\psi$ is seven times continuously differentiable with respect to S if the double well potential satisfies $\hat\psi \in C^7(\mathbb{R})$. With the second order polynomial

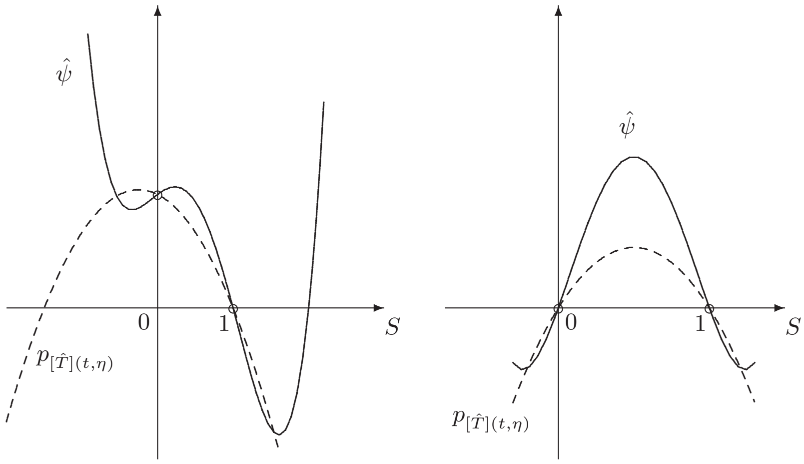
$$p_{[\hat T](t,\eta)}(S) = \hat\psi(0)(1-S) + \hat\psi(1)S - \frac12 \bar\varepsilon\cdot[\hat T](t,\eta)S(1-S)$$

assumptions 2. and 3. are equivalent to

$$\hat\psi(S) > p_{[\hat T](t,\eta)}(S), \qquad 0 < S < 1,\ (t,\eta)\in\Gamma, \tag{2.1}$$

$$\hat\psi'(0) > \max_{(t,\eta)\in\Gamma} p'_{[\hat T](t,\eta)}(0), \tag{2.2}$$

$$\hat\psi'(1) < \min_{(t,\eta)\in\Gamma} p'_{[\hat T](t,\eta)}(1). \tag{2.3}$$



Two examples of admissible potentials $\hat\psi$

The polynomial $p_{[\hat T](t,\eta)}$ passes through the points $(0, \hat\psi(t,\eta,0))$ and $(1, \hat\psi(t,\eta,1))$, and it is concave. This is shown by the following

Lemma 2.1 *The jump of the stress tensor $\hat T$ in solutions of the sharp interface problem* (1.3) – (1.7) *satisfies*

$$\bar\varepsilon \cdot [\hat T](t,\eta) \le 0, \qquad \textit{for all } (t,\eta) \in \Gamma.$$

This lemma is proved below.

Inequality (2.1) thus places a lower bound on the "hump" of the double well potential between the points $S = 0$ and $S = 1$. Actually, if the values $\hat\psi(0)$ and $\hat\psi(1)$ differ strongly, then there need not be a hump at all, it is only required that the values $\hat\psi(S)$ lie high enough above the straight line segment connecting the points $(0, \hat\psi(0))$ and $(1, \hat\psi(1))$. In this case $\hat\psi$ does not need to have two "wells".

For the construction of the asymptotic solution we only need that $\hat\psi$ is defined for $-\delta < S < 1 + \delta$ with small $\delta > 0$. If $\hat\psi$ is defined on all of $\mathbb{R}$ and satisfies $\hat\psi(0) = \hat\psi(1)$, then in order to satisfy (2.2) and (2.3) it must have one minima at a point $S = m_0 < 0$ and another minima at $S = m_1 > 1$.

A physical interpretation could be as follows: The jump in the stress field at the interface caused by a misfit strain generates forces on the atoms in the crystal lattice close to the interface, which tend to reduce the misfit. The double well potential counteracts these elastic forces. The action of the elastic forces is shown by the presence of the polynomial $p_{[\hat T](t,\eta)}(S)$ in the "effective" free energy $\tilde\psi$. This term reduces the potential barrier. If the hump of the double well potential $\hat\psi$ is not large enough, then the elastic forces win and the misfit vanishes, which means that the crystal structure on both sides of the interface assumes the same form, one of the material phases vanish and the solid is built up of one phase only. Mathematically this is shown by the fact, that if $\tilde\psi(t,\eta,S)$ is not positive for $0 < S < 1$, then (1.30) does not have a transition profile S_0 as solution connecting the state $S = 0$ with the state $S = 1$.

To prove Lemma 2.1 we need several definitions and a second lemma. For $\alpha, \beta \in \mathcal{S}^3$ set

$$\alpha :_D \beta = \alpha \cdot (D\beta).$$

This defines a scalar product on $\mathcal{S}^3$, since the elasticity tensor $D : \mathcal{S}^3 \to \mathcal{S}^3$ is symmetric and positive definite. With the unit normal vector $n(t,\eta) \in \mathbb{R}^3$ to $\Gamma(t)$ at $\eta \in \Gamma(t)$ define the linear subspace $\hat{\mathcal{S}}^3_{t,\eta}$ of $\mathcal{S}^3$ by

$$\hat{\mathcal{S}}^3_{t,\eta} = \Big\{ \frac{1}{2}\Big(\omega \otimes n(t,\eta) + n(t,\eta) \otimes \omega \Big) \;\Big|\; \omega \in \mathcal{S}^3 \Big\}.$$

Let $P_{t,\eta} : \mathcal{S}^3 \to \mathcal{S}^3$ be the projector to $\hat{\mathcal{S}}^3_{t,\eta}$, which is orthogonal with respect to the scalar product $\alpha :_D \beta$. We fix (t,η) and for simplicity write $\hat{\mathcal{S}}^3 = \hat{\mathcal{S}}^3_{t,\eta}$, $P = P_{t,\eta}$ and $n = n(t,\eta)$.

Lemma 2.2 *The equations* (1.4)*,* (1.6) *and* (1.7) *imply that*

$$[\varepsilon(\nabla_x \hat{u})] = P\overline{\varepsilon}. \tag{2.4}$$

Proof: Observe first that the equation (1.7) holds if and only if

$$\alpha \cdot [\hat{T}] = 0, \qquad \text{for all } \alpha \in \hat{\mathcal{S}}^3. \tag{2.5}$$

To see this, let $\alpha = \frac{1}{2}(\omega \otimes n + n \otimes \omega)$ with $\omega \in \mathbb{R}^3$. The symmetry of the matrix $[\hat{T}]$ implies

$$\alpha \cdot [\hat{T}] = (\omega \otimes n) \cdot [\hat{T}] = \omega \cdot ([\hat{T}]n),$$

from which the equivalence of (1.7) and (2.5) follows. Observe next that the equation (1.19), which is a consequence of (1.6), yields $[\varepsilon(\nabla_x \hat{u})] \in \hat{\mathcal{S}}^3$. Hence, $P[\varepsilon(\nabla_x \hat{u})] = [\varepsilon(\nabla_x \hat{u})]$. We combine this with (2.5), which must be satisfied since by assumption (1.7) holds, and obtain together with (1.4) that

$$\begin{aligned} \big([\varepsilon(\nabla_x \hat{u})] - P\overline{\varepsilon}\big) :_D \big([\varepsilon(\nabla_x \hat{u})] - P\overline{\varepsilon}\big) &= \big([\varepsilon(\nabla_x \hat{u})] - P\overline{\varepsilon}\big) :_D \big([\varepsilon(\nabla_x \hat{u})] - \overline{\varepsilon}\big) \\ = ([\varepsilon(\nabla_x \hat{u})] - P\overline{\varepsilon}) \cdot D([\varepsilon(\nabla_x \hat{u})] - \overline{\varepsilon}) &= ([\varepsilon(\nabla_x \hat{u})] - P\overline{\varepsilon}) \cdot [\hat{T}] = 0. \end{aligned}$$

This equation implies (2.4).

Proof of Lemma 2.1. Lemma 2.2 yields

$$\begin{aligned} \overline{\varepsilon} \cdot [\hat{T}] &= \overline{\varepsilon} \cdot D\big([\varepsilon(\nabla_x \hat{u})] - \overline{\varepsilon}\big) = \overline{\varepsilon} \cdot D(P\overline{\varepsilon} - \overline{\varepsilon}) \\ &= -\overline{\varepsilon} :_D (I-P)\overline{\varepsilon} = -(I-P)\overline{\varepsilon} :_D (I-P)\overline{\varepsilon} \le 0. \end{aligned}$$

We used that $(I-P) : \mathcal{S}^3 \to \mathcal{S}^3$ is a projector orthogonal with respect to the scalar product $\alpha :_D \beta$, which yields $\alpha :_D (I-P)\beta = (I-P)\alpha :_D (I-P)\beta$ for all $\alpha, \beta \in \mathcal{S}^3$. This proves the lemma.

For completeness we remark that $[\hat{T}]$ defined by $[\hat{T}] = D(P\overline{\varepsilon} - \overline{\varepsilon})$ solves (1.7). To see this, let $\alpha \in \hat{\mathcal{S}}^3$. Then

$$\alpha \cdot [\hat{T}] = \alpha \cdot D(P\overline{\varepsilon} - \overline{\varepsilon}) = -\alpha :_D (I-P)\overline{\varepsilon} = (I-P)\alpha :_D \overline{\varepsilon} = 0,$$

since $P\alpha = \alpha$. By (2.5), this implies (1.7).

3 Derivation of the differential equations for S_0, S_1 and S_2

In this section we start with the proof of Theorem 1.3. To verify (1.50) we first compute an asymptotic expansion of $\partial_S\psi(\varepsilon(\nabla_x u^{(\nu)}), S^{(\nu)}) - \nu\Delta_x S^{(\nu)}$ in terms of ν, where $S^{(\nu)}$ and $u^{(\nu)}$ are given by the ansatz (1.23), (1.24). Setting all the terms in this asymptotic expansion equal to zero yields the equations (1.30), (1.31) and (1.32). Our first goal is to compute the expansion of the function $\partial_S\psi\big(\varepsilon(u^{(\nu)}), S^{(\nu)}\big)$, which depends nonlinearly on $S^{(\nu)}$.

Lemma 3.1 *Let u^*, $u^{(\nu)}$ be defined by* (1.18) *and* (1.24)*, respectively. Then $T^{(\nu)}$ given in* (1.48) *satisfies*

$$\begin{aligned} T^{(\nu)} &= D\big(\varepsilon(\nabla_x u^{(\nu)}) - \bar\varepsilon S^{(\nu)}\big) \\ &= [\hat T]\, S^{(\nu)}\,\phi + D\varepsilon(\nabla_x v) - D\bar\varepsilon\,(1-\phi)S^{(\nu)} \\ &\quad + D\varepsilon\big(\hat\nabla_{\Gamma_\xi}(u^* S^{(\nu)(-1)})\big)\,\phi + S^{(\nu)(-1)} D\varepsilon(u^*\otimes\nabla_x\phi), \end{aligned} \tag{3.1}$$

where $[\hat T] = [\hat T](t,\eta)$, $u^* = u^*(t,\eta)$. All other functions have the argument (t,x) with $x = \eta + n(t,\eta)\xi$.

Proof. By (1.24) we have

$$u^{(\nu)}(t,x) = u^*(t,\eta)S^{(\nu)(-1)}(t,x)\,\phi(t,x) + v(t,x).$$

Thus

$$\begin{aligned} \nabla_x u^{(\nu)} &= \nabla_x v + \partial_\xi(S^{(\nu)(-1)}\phi u^*)\otimes n + \hat\nabla_{\Gamma_\xi}(u^* S^{(\nu)(-1)}\,\phi) \\ &= \nabla_x v + S^{(\nu)}\phi\,(u^*\otimes n) + S^{(\nu)(-1)}(\partial_\xi\phi)(u^*\times n) \\ &\qquad + \phi\,\hat\nabla_{\Gamma_\xi}(u^* S^{(\nu)(-1)}) + S^{(\nu)(-1)}(u^*\otimes\nabla_{\Gamma_\xi}\phi) \\ &= \nabla_x v + S^{(\nu)}\phi\,(u^*\otimes n) + \phi\,\hat\nabla_{\Gamma_\xi}(u^* S^{(\nu)(-1)}) + S^{(\nu)(-1)}(u^*\otimes\nabla_x\phi). \end{aligned}$$

By (1.19) we have $u^*\otimes n = [\nabla_x\hat u]$. If we note that $[\hat T] = D(\varepsilon([\nabla_x\hat u]) - \bar\varepsilon)$ we obtain (3.1).

With this lemma we can compute ψ_S in a neighborhood of $\Gamma(t)$. Since $\phi = 1$ in a neighborhood of $\Gamma(t)$, it follows from from (1.13) and (3.1) that

$$\begin{aligned} \psi_S(\varepsilon(u^{(\nu)}), S^{(\nu)}) &= \hat\psi'(S^{(\nu)}) - \bar\varepsilon\cdot T^{(\nu)} \\ &= \hat\psi'(S^{(\nu)}) - \bar\varepsilon\cdot[\hat T]S^{(\nu)} - \sigma - \bar\varepsilon\cdot D\varepsilon\big(\hat\nabla_{\Gamma_\xi}(u^* S^{(\nu)(-1)})\big) \\ &= \tilde\psi_S(t,\eta,S^{(\nu)}) - \frac{1}{2}\bar\varepsilon\cdot[\hat T] + [\hat\psi] - \sigma - \bar\varepsilon\cdot D\varepsilon\big(\hat\nabla_{\Gamma_\xi}(u^* S^{(\nu)(-1)})\big)\,, \end{aligned} \tag{3.2}$$

with the effective free energy $\tilde\psi$ defined in (1.37) and with σ defined in (1.38). For $(t,\eta)\in\Gamma$ set

$$\hat T^{\pm}(t,\eta) = \lim_{\xi\to 0\pm}\hat T(t,\eta + n(t,\eta)\xi).$$

Since $\hat S = 0$ and $u^*\langle\xi\rangle\phi = 0$ in the domain γ, it follows by combination of (1.4) and (1.20) that in this domain the stress satisfies $\hat T = D(\varepsilon(\nabla_x\hat u) - \bar\varepsilon\hat S) = D\varepsilon(\nabla_x v)$. We have

$x = \eta + n(t,\eta)\xi \in \gamma$ for $\xi < 0$. From (1.38) we thus infer that $\sigma(t,\eta,0) = \overline{\varepsilon} \cdot \hat{T}^-(t,\eta)$. Using the notation $\overline{\sigma}(t,\eta,\xi) = \sigma(t,\eta,\xi) - \sigma(t,\eta,0)$ we consequently get

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

with $\langle \hat{T} \rangle = \frac{1}{2}\big(\hat{T}^+ + \hat{T}^-\big)$ and with the jump $[\hat{C}]$ of the Eshelby tensor $\hat{C}$ across $\Gamma(t)$. The last equality sign is shown to hold in [3, equation (2.4)]. We insert this equation into (3.2) and obtain

$$\psi_S(\varepsilon(u^{(\nu)}), S^{(\nu)}) = \tilde{\psi}_S(t,\eta,S^{(\nu)}) + n \cdot [\hat{C}]n - \overline{\sigma} - \overline{\varepsilon} \cdot D\varepsilon\big(\hat{\nabla}_{\Gamma_\xi}\big(u^* S^{(\nu)(-1)}\big)\big)\,. \tag{3.3}$$

To compute the expansion of ψ_S we consider now every term on the right hand side of this formula separately. To simplify the notation we drop the arguments t and η in the following equations. Taylor's formula and (1.23) yield for the first term

$$\tilde{\psi}_S(S^{(\nu)}) = \tilde{\psi}_S(S_0) + \tilde{\psi}_{SS}(S_0)(\nu^{1/2}S_1 + \nu S_2) + \frac{1}{2}\tilde{\psi}_{SSS}(S_0)\nu S_0^2 + \nu^{3/2}R_{\tilde{\psi}}(\nu, S_0, S_1, S_2). \tag{3.4}$$

The term $n \cdot [\hat{C}]n$ does only depend on (t,η). To treat the third term we use Taylor's formula and (1.39) to obtain

$$\begin{aligned} \overline{\sigma}(\xi) &= \dot{\sigma}(\xi)\xi + \frac{1}{2}\ddot{\sigma}(\xi)\xi^2 + \sigma^*(\xi)\xi^3 \\ &= \nu^{1/2}\dot{\sigma}\Big(\frac{\xi}{\nu^{1/2}}\Big)\frac{\xi}{\nu^{1/2}} + \frac{\nu}{2}\ddot{\sigma}\Big(\frac{\xi}{\nu^{1/2}}\Big)\left(\frac{\xi}{\nu^{1/2}}\right)^2 + \nu^{3/2}R_\sigma(\xi)\left(\frac{\xi}{\nu^{1/2}}\right)^3. \end{aligned} \tag{3.5}$$

To deal with the term $\overline{\varepsilon} \cdot D\varepsilon\big(\hat{\nabla}_{\Gamma_\xi}\big(u^* S^{(\nu)(-1)}\big)\big)$ in (3.3) we apply (1.42) with $\eta \mapsto W(\eta) = u^*(t,\eta)S^{(\nu)(-1)}(t,\eta,\xi) : \Gamma \to \mathbb{R}^3$ to write it in the form

$$\begin{aligned} &\overline{\varepsilon} \cdot D\varepsilon\Big(\hat{\nabla}_{\Gamma_\xi}\big(u^*(t,\eta)S^{(\nu)(-1)}(t,\eta,\xi)\big)\Big) \\ &\qquad = \overline{\varepsilon} \cdot D\varepsilon\Big(\hat{\nabla}_{\Gamma}\big(u^*(t,\eta)S^{(\nu)(-1)}(t,\eta,\xi)\big)A(t,\eta,\xi)\Big). \end{aligned}$$

Since $A(t,\eta,0) = I$, we obtain with the definition of A_1 in (1.43) that

$$A(t,\eta,\xi) = I + \nu^{1/2}\frac{\xi}{\nu^{1/2}}A_1(t,\eta) + \nu\Big(\frac{\xi}{\nu^{1/2}}\Big)^2 R_A(t,\eta,\xi).$$

Together with (1.26) we thus have, again dropping most of the arguments,

$$\begin{aligned} &\overline{\varepsilon} \cdot D\varepsilon\big(\hat{\nabla}_{\Gamma_\xi}\big(u^* S^{(\nu)(-1)}\big)\big) \\ &\quad = \nu^{1/2}\,\overline{\varepsilon} \cdot D\varepsilon\Big(\hat{\nabla}_\Gamma\big(u^* S_0^{(-1)}\big)\Big) + \nu\,\overline{\varepsilon} \cdot D\varepsilon\left(\frac{\xi}{\nu^{1/2}}\hat{\nabla}_\Gamma\big(u^* S_0^{(-1)}\big)A_1 + \hat{\nabla}_\Gamma\big(u^* S_1^{(-1)}\big)\right) \\ &\qquad\qquad + \nu^{3/2}\Big(\frac{\xi}{\nu^{1/2}}\Big)^2 R_{\text{term4}}\Big(\nu, \xi, S_i^{(-1)}\Big), \end{aligned} \tag{3.6}$$

with the remainder term R_{term4} depending linearly on the functions $S_0^{(-1)}, \ldots, S_2^{(-1)}$.

We compute next an expansion of $\Delta_x S^{(\nu)}$ in terms of ν. For $x = (\eta, \xi)$ we have

$$\Delta_x S^{(\nu)}(t,x) = \partial_\xi^2 S^{(\nu)}(t,\eta,\xi) + \kappa(t,\eta,\xi)\partial_\xi S^{(\nu)}(t,\eta,\xi) + \Delta_{\Gamma_\xi} S^{(\nu)}(t,\eta,\xi), \tag{3.7}$$

with twice the mean curvature $\kappa(t,\eta,\xi)$ of the surface $\Gamma_\xi(t)$ and with the surface Laplacian $\Delta_{\Gamma_\xi} = \sum_{1\le|\alpha|\le 2} c_\alpha(t,\eta,\xi)\partial_\eta^\alpha$. Taylor's formula yields

$$\begin{aligned}
\kappa(t,\eta,\xi) &= \kappa_0 + \kappa_1\xi + R_\kappa(\xi)\xi^2 = \kappa_0 + \nu^{1/2}\kappa_1\frac{\xi}{\nu^{1/2}} + \nu R_\kappa(\xi)\Big(\frac{\xi}{\nu^{1/2}}\Big)^2, \\
\Delta_{\Gamma_\xi} &= \sum_{1\le|\alpha|\le 2}\Big(c_\alpha(t,\eta,0) + \xi R_{c_\alpha}(t,\eta,\xi)\Big)\partial_\eta^\alpha = \Delta_\Gamma + \nu^{1/2}\Big(\frac{\xi}{\nu^{1/2}}\Big)R_{\Delta_{\Gamma_\xi}}(\xi,\partial_\eta,\partial_\eta^2)\,,
\end{aligned} \tag{3.8}$$

where we used the notation $\kappa_i(t,\eta) = \partial_\xi^i\kappa(t,\eta,0)$ for $i = 0,1$ introduced in (1.40). We insert these equations and (1.23) into (3.7). With the notation $S_i' = \partial_\zeta S_i$, $S_i'' = \partial_\zeta^2 S_i$ we obtain

$$\begin{aligned}
\nu\Delta_x S^{(\nu)} &= S_0''(\frac{\xi}{\nu^{1/2}}) \\
&\quad + \nu^{1/2}\Big(S_1''(\frac{\xi}{\nu^{1/2}}) + \kappa_0 S_0'(\frac{\xi}{\nu^{1/2}})\Big) \\
&\quad + \nu\Big(S_2''(\frac{\xi}{\nu^{1/2}}) + \kappa_0 S_1'(\frac{\xi}{\nu^{1/2}}) + \kappa_1\frac{\xi}{\nu^{1/2}}S_0'(\frac{\xi}{\nu^{1/2}}) + \Delta_\Gamma S_0(\frac{\xi}{\nu^{1/2}})\Big) \\
&\quad + \nu^{3/2}R_\Delta(\nu,\xi,\frac{\xi}{\nu^{1/2}}).
\end{aligned} \tag{3.9}$$

We insert (3.4) – (3.6) into (3.3) and combine the result with (3.9). If we set $\xi = \nu^{1/2}\zeta$, the resulting equation is

$$\begin{aligned}
&\psi_S(\varepsilon(u^{(\nu)}), S^{(\nu)}) - \nu\Delta_x S^{(\nu)} \\
&= \Big(\tilde\psi_S(S_0) - S_0'' + n\cdot[\hat C]n\Big) \\
&\quad + \nu^{1/2}\Big(\tilde\psi_{SS}(S_0)\,S_1 - S_1'' - \kappa_0 S_0' - \dot\sigma(\zeta)\zeta - \overline{\varepsilon}\cdot D\varepsilon\big(\hat\nabla_\Gamma(u^* S_0^{(-1)})\big)\Big) \\
&\quad + \nu\quad\Big\{\tilde\psi_{SS}(S_0)\,S_2 - S_2'' - \kappa_0 S_1' - \kappa_1\zeta S_0' - \Delta_\Gamma S_0 + \frac12\tilde\psi_{SSS}(S_0)\,S_0^2 \\
&\qquad\quad - \frac12\ddot\sigma(\zeta)\zeta^2 - \overline{\varepsilon}\cdot D\varepsilon\Big(\zeta\,\hat\nabla_\Gamma\big(u^* S_0^{(-1)}\big)A_1 + \hat\nabla_\Gamma\big(u^* S_1^{(-1)}\big)\Big)\Big\} \\
&\quad + \nu^{3/2}R_{\psi_S-\nu\Delta}(\nu,\nu^{1/2}\zeta,\zeta)\,.
\end{aligned} \tag{3.10}$$

Note that the argument of the functions S_i and $S_i^{(-1)}$ in equations (3.4), (3.6) and (3.9) is $(t,\eta,\xi/\nu^{1/2})$. Therefore the argument of these functions on the right hand side of (3.10) and of the functions $\dot\sigma$, $\ddot\sigma$ is (t,η,ζ). The argument of $\kappa_0,\ \kappa_1,\ A_1$ is (t,η), and $\tilde\psi$ depends on (t,η,S_0). From (3.10) we thus obtain

Corollary 3.2 *If the functions S_0, S_1, S_2 satisfy the differential equations* (1.30), (1.31) *and* (1.32) *with the functions f_1, f_2 defined in* (1.33), (1.34), *then*

$$\begin{aligned}
&\psi_S(\varepsilon(u^{(\nu)}), S^{(\nu)}) - \nu\Delta_x S^{(\nu)} \\
&= (n\cdot[\hat C]n)(t,\eta) + \nu^{1/2}C_1(t,\eta) + \nu C_2(t,\eta) + \nu^{3/2}R_{\psi_S-\nu\Delta}(\nu,t,\eta,\xi,\xi/\nu^{1/2})\,.
\end{aligned} \tag{3.11}$$

The estimates in Section 5 are based on this equation. At some point in Section 5 we use (3.11) written in the compact form

$$\psi_S(\varepsilon(u^{(\nu)}), S^{(\nu)}) - \nu\Delta_x S^{(\nu)} = (n\cdot[\hat{C}]n)(t,\eta) + \nu^{1/2}\hat{R}_{\psi_S-\nu\Delta}(\nu,t,\eta,\xi,\xi/\nu^{1/2})\,, \quad (3.12)$$

with

$$\hat{R}_{\psi_S-\nu\Delta} = C_1 + \nu^{1/2}C_2 + \nu R_{\psi_S-\nu\Delta}\,.$$

4 The transition profile functions S_0, S_1, S_2

This section is devoted to the proofs of Theorems 1.1 and 1.2. At the end we derive some estimates for $S^{(\nu)}$ needed in the following sections.

Proof of Theorem 1.1. From $\tilde{\psi}(t,\eta,S) > 0$ for $0 < S < 1$ it follows that the function $(t,\eta,S) \mapsto \sqrt{2\tilde{\psi}(t,\eta,S)}$ is six times continuously differentiable on $\Gamma\times(0,1)$ and Lipschitz continuous with respect to S on every compact subset of this set. The theorem of Picard-Lindelöf thus yields that there is a maximal interval (a,d) with $-\infty \le a = a(t,\eta) < 0$ and $0 < d = d(t,\eta) \le \infty$ and a solution $\zeta \mapsto S_0(t,\eta,\zeta) : (a,d) \to (0,1)$ of (1.44), such that $\liminf_{\zeta\to a} S_0(t,\eta,\zeta) = 0$ and $\liminf_{\zeta\to d} S_0(t,\eta,\zeta) = 1$. The solution satisfies $S_0' > 0$ for $a < \zeta < d$. Moreover, it follows in the standard way that the solution S_0 is six times continuously differentiable with respect to all variables on the set

$$\Gamma(a,b) = \{(t,\eta,\zeta) \mid (t,\eta)\in\Gamma,\ a(t,\eta) < \zeta < d(t,\eta)\}.$$

To study the behavior of the solution at the boundary of this set we square both sides of the differential equation (1.44) and differentiate with respect to ζ to obtain

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

where we dropped the arguments t and η of $\tilde{\psi}$. Since S_0' is positive, it follows that S_0 satisfies

$$\tilde{\psi}_S(S_0) - S_0'' = 0. \quad (4.1)$$

This is (1.30). Since S_0 has values between 0 and 1, this equation shows that S_0'' is bounded. This equation and (1.45) also show that there is $\delta > 0$ such that for all (t,η,ζ) with $S_0(t,\eta,\zeta) < \delta$ the estimate $|S_0''(t,\eta,\zeta)| > c_0/2$ holds; by some considerations it follows from this estimate that the limit values $a(t,\eta)$ and $d(t,\eta)$ are finite.

For every (t,η) (4.1) has a solution $\zeta \mapsto S_0^*(t,\eta,\zeta)$ which exists on an open neighborhood of $[a,d] = [a(t,\eta), d(t,\eta)]$ and coincides with S_0 on (a,d). In this way we extend S_0 from $\Gamma(a,b)$ to a function $(t,\eta,\zeta) \mapsto S_0^*(t,\eta,\zeta)$ defined on a set, which for every $T_1 < t_1 < t_2 < T_2$ is an open neighborhood of $\Gamma[a,d] \cap \big([t_1,t_2]\times\mathbb{R}^3\big)$. As a solution of (4.1), S_0^* is six times continuously differentiable on this set with respect to all variables.

The restriction of S_0^* to the set $\Gamma[a,b]$ is another extension of S_0. For this extension we again use the notation S_0. From $\liminf_{\zeta\searrow a} S_0(t,\eta,\zeta) = 0$ and $\liminf_{\zeta\nearrow d} S_0(t,\eta,\zeta) = 1$ we see that $S_0(t,\eta,a(t,\eta)) = S_0^*(t,\eta,a(t,\eta)) = 0$, $S_0(t,\eta,d(t,\eta)) = S_0^*(t,\eta,d(t,\eta)) = 1$.

By definition, the extended function S_0 has one sided derivatives at $\zeta = a$ and $\zeta = d$ up to sixth order with respect to all variables, which coincide with the derivatives of S_0^*. Since $\tilde{\psi}(t,\eta,0) = \tilde{\psi}(t,\eta,1) = 0$, it follows from (1.44) that $S_0'(t,\eta,a(t,\eta)) = S_0'(t,\eta,d(t,\eta)) = 0$.

By differentiation of the equation $S_0(t,\eta,a(t,\eta)) = 0$ with respect to η_i, $i = 1,2$, we therefore obtain

$$0 = \nabla_\eta S_0(t,\eta,a) + S_0'(t,\eta,a)\nabla_\eta a = \nabla_\eta S_0(t,\eta,a),$$

and similarly $\nabla_\eta S_0(t,\eta,d) = 0$. This proves (i).

To prove (ii) we again use (1.45), which together with (4.1) implies

$$S_0^{*\prime\prime}(t,\eta,a) = \tilde{\psi}_S(t,\eta,0) \geq c_0 > 0, \quad S_0^{*\prime\prime}(t,\eta,d) = \tilde{\psi}_S(t,\eta,1) \leq -c_0 < 0.$$

Thus, since $S_0^{*\prime}(t,\eta,a(t,\eta)) = 0$ and since $S_0^{*\prime}$ is five times continuously differentiable, the implicit function theorem implies that a is five times continuously differentiable with first derivatives given by

$$\partial_\eta a(t,\eta) = -\frac{\partial_\eta S_0^{*\prime}(t,\eta,a(t,\eta))}{\tilde{\psi}_S(t,\eta,0)}, \quad \partial_t a(t,\eta) = -\frac{\partial_t S_0^{*\prime}(t,\eta,a(t,\eta))}{\tilde{\psi}_S(t,\eta,0)}.$$

The right hand sides are bounded. Similar formulas hold for the higher derivatives, which show that these derivatives are also bounded. Using the equation $S_0^{*\prime}(t,\eta,d(t,\eta)) = 0$ we conclude in the same way that the derivatives $\partial_{(t,\eta)}^m d$ exist and are bounded for $m \leq 5$. The proof of the lemma is complete.

To prove Theorem 1.2 we study the differential equations (1.31), (1.32). These differential equations differ only by the right hand sides. Since the coefficient function $\tilde{\psi}_{SS}(S_0)$ and the right hand side of (1.31) can be computed from the solution S_0 of (1.30), and since the right hand side of (1.32) can be computed from the solutions S_0 and S_1 of (1.30), (1.31), we can consider (1.31), (1.32) to be a recursively solvable system of linear differential equations for S_1 and S_2. Therefore it suffices to study the linear second order differential equation

$$\tilde{\psi}_{SS}(t,\eta,S_0(t,\eta,\zeta))\, w(t,\eta,\zeta) - w''(t,\eta,\zeta) = f(t,\eta,\zeta) + C(t,\eta) \tag{4.2}$$

for w, where S_0 is the function given by Theorem 1.1 and where the right hand side is known. We want to find a solution $\zeta \mapsto w(t,\eta,\zeta) : [a(t,\eta), d(t,\eta)] \to \mathbb{R}$ satisfying the boundary conditions

$$w(t,\eta,a(t,\eta)) = w(t,\eta,d(t,\eta)) = 0. \tag{4.3}$$

We first note that 0 is an eigenvalue and S_0' is an eigenfunction of the boundary value problem (4.2), (4.3). This is seen by differentiation of (4.1) with respect to ζ, which yields

$$\tilde{\psi}_{SS}(S_0)\, S_0' - S_0''' = 0.$$

By (1.46) we have $S_0'(a) = S_0'(d) = 0$. Thus, the homogeneous differential equation and the boundary conditions are satisfied. Since $\tilde{\psi}_{SS}(S_0) - \partial_\zeta^2$ is a symmetric differential operator and since for all nondegenerate ordinary differential operators of second order eigenspaces are necessarily of dimension one, it follows from classical spectral theory for symmetric operators that the boundary value problem (4.2), (4.3) has solutions if and only if the right hand side is orthogonal to the eigenfunction S_0'.

Lemma 4.1 *Assume that $f \in C^m(\Gamma[a,b])$ with $m = 4$ or $m = 5$. Let*

$$C(t,\eta) = -\int_{a(t,\eta)}^{d(t,\eta)} f(t,\eta,\zeta) S_0'(t,\eta,\zeta)\, d\zeta \tag{4.4}$$

for all $(t,\eta)\in\Gamma$. *Then there is a unique solution* $\zeta\mapsto w(t,\eta,\zeta):[a(t,\eta),d(t,\eta)]\to\mathbb{R}$ *of the boundary value problem* (4.2), (4.3), *which is orthogonal to* S_0'. *This means that*

$$\int_{a(t,\eta)}^{d(t,\eta)} w(t,\eta,\zeta)S_0'(t,\eta,\zeta)d\zeta=0.$$

Moreover, w *belongs to the space* $C^m(\Gamma[a,d])$.

Proof. Equation (4.4) implies that the right hand side of (4.2) is orthogonal to S_0'. To see this, note that

$$\int_{a(t,\eta)}^{d(t,\eta)} S_0'(t,\eta,\zeta)d\zeta=S_0(t,\eta,d(t,\eta))-S_0(t,\eta,a(t,\eta))=1, \tag{4.5}$$

which implies $\int_a^d(f+C)S_0'\,d\zeta=\int_a^d fS_0'\,d\zeta+C\int_a^d S_0'\,d\zeta=0$. By the remarks above it thus follows that there is a solution of the boundary value problem (4.2), (4.3). By adding a suitable multiple of the eigenfunction S_0' we obtain the unique solution w of this boundary value problem, which is orthogonal to this eigenfunction.

It remains to show that $w\in C^m(\Gamma[a,d])$. This follows from the perturbation theory for eigenspaces of linear operators. For completeness we sketch here an elementary proof. In this proof we derive a representation formula for the solution, from which the regularity properties of the solution can be read off. To simplify the notation we drop the arguments t and η in most of the following formulas.

A solution of (4.2), (4.3) is given by the integral

$$\tilde{w}(t,\eta,\zeta)=\int_{a(t,\eta)}^{d(t,\eta)} G(t,\eta;\zeta,\vartheta)(f(t,\eta,\vartheta)+C(t,\eta))\,d\vartheta\,, \tag{4.6}$$

with G defined as follows: For fixed $a<\vartheta<d$ the function G is a solution of the differential equation

$$(\tilde{\psi}_{SS}(S_0)-\partial_\zeta^2)G(\zeta,\vartheta)=C_\vartheta\,,\quad a<\zeta<d,\ \zeta\neq\vartheta, \tag{4.7}$$

with the constant $C_\vartheta=-S_0'(\vartheta)$, and of the initial and jump conditions

$$G(a,\vartheta)\;=\;\partial_\zeta G(a,\vartheta)\;=\;0, \tag{4.8}$$

$$G(\vartheta+,\vartheta)\;=\;G(\vartheta-,\vartheta), \tag{4.9}$$

$$\partial_\zeta G(\vartheta+,\vartheta)\;=\;\partial_\zeta G(\vartheta-,\vartheta)-1\,. \tag{4.10}$$

By partial integration we see that G is a solution of

$$(\tilde{\psi}_{SS}(S_0)-\partial_\zeta^2)G(\cdot,\vartheta)=\delta_\vartheta+C_\vartheta\,, \tag{4.11}$$

with the Dirac distribution δ_ϑ supported at ϑ. Noting (4.5) and the definition of C_ϑ, we compute

$$(\delta_\vartheta+C_\vartheta,S_0')_{(a,d)}=S_0'(\vartheta)+C_\vartheta\int_a^d S_0'(\zeta)d\zeta=S_0'(\vartheta)-S_0'(\vartheta)=0.$$

Because S_0' is a solution of the homogeneous boundary value problem (4.2), (4.3) we therefore obtain by another partial integration that

$$\begin{aligned} 0 &= (\delta_\vartheta + C_\vartheta, S_0')_{(a,d)} = \big((\tilde\psi_{SS}(S_0) - \partial_\zeta^2)G(\cdot,\vartheta), S_0'\big)_{(a,d)} \\ &= \big(G(\cdot,\vartheta), (\tilde\psi_{SS}(S_0) - \partial_\zeta^2)S_0'\big)_{(a,d)} \\ &\quad + \partial_\zeta G(a,\vartheta)S_0'(a) - G(a,\vartheta)S_0''(a) - \partial_\zeta G(d,\vartheta)S_0'(d) + G(d,\vartheta)S_0''(d) \\ &= -G(a,\vartheta)S_0''(a) + G(d,\vartheta)S_0''(d) = G(d,\vartheta)S_0''(d)\,. \end{aligned}$$

Since $S_0''(d) \neq 0$, we conclude that

$$G(d,\vartheta) = 0.$$

This equation and (4.8) show that the function $\tilde w$ defined in (4.6) satisfies the boundary conditions (4.3). From (4.11) and (4.4), (4.5) we obtain

$$\begin{aligned} (\tilde\psi_{SS}(S_0) - \partial_\zeta^2)\,\tilde w &= f + C + \int_a^d C_\vartheta\,(f(\vartheta) + C)\,d\vartheta \\ &= f + C - \int_a^d S_0'(\vartheta)f(\vartheta)\,d\vartheta - C\int_a^d S_0'(\vartheta)\,d\zeta = f + C. \end{aligned}$$

We thus see that $\tilde w$ also satisfies the differential equation (4.2). The unique solution w of (4.2), (4.3), which is orthogonal to S_0', is obtained from $\tilde w$ by

$$w = \tilde w - \frac{(\tilde w, S_0')_{(a,d)}}{\|S_0'\|^2_{(a,d)}}\,S_0'\,. \tag{4.12}$$

To study the regularity of w note that since $(t,\eta,\zeta) \mapsto \tilde\psi_{SS}(t,\eta,S_0(t,\eta,\zeta))$ is five times continuously differentiable and since $(t,\eta) \mapsto C_\vartheta(t,\eta) = -S_0'(t,\eta,\vartheta)$, $(t,\eta) \mapsto a(t,\eta)$, $(t,\eta) \mapsto d(t,\eta)$ are five times continuously differentiable, it follows by the standard theory for initial value problems to ordinary differential equations that the function $(t,\eta,\zeta) \mapsto G(t,\eta;\zeta,\vartheta)$ defined by (4.7) – (4.10) is at least five times continuously differentiable with respect to (t,η,ζ) for $\zeta \neq \vartheta$. Using the jump relations (4.9), (4.10) and jump relations for derivatives of G of higher order, which follow from these lower order jump relations and from the differential equation (4.7), we obtain with the distributional derivative ∂ and the classical derivative $\tilde\partial$ that

$$\partial_t^i\partial_\eta^j\partial_\zeta^k G = \tilde\partial_t^i\tilde\partial_\eta^j\tilde\partial_\zeta^k G + \sum_{\ell=0}^{k-2}\partial_\zeta^\ell\big(r_{i,j,k-\ell}(t,\eta,\theta)\,\delta_\vartheta\big), \quad i+j+k \le 5, \tag{4.13}$$

where the coefficient functions $r_{i,j,k}$ have at least $6 - i - j - \min(0, k-4)$ derivatives. For $f \in C^m(\Gamma[a,d])$ the function $C(t,\eta)$ defined in (4.4) belongs to $C^m(\Gamma)$, since $S_0' \in C^5(\Gamma[a,d])$ and $m \le 5$. Using this and (4.13) we conclude that the integral on the right hand side of (4.6) is m–times continuously differentiable with respect to all variables, whence $\tilde w \in C^m(\Gamma[a,d])$. From (4.12) we infer that also $w \in C^m(\Gamma[a,b])$. This concludes the proof of the lemma.

Proof of Theorem 1.2. This Theorem follows immediately from Lemma 4.1, since the differentiability properties of S_0 given in Theorem 1.1 imply $f_1 \in C^5(\Gamma([a,d])$ and

$f_2 \in C^4(\Gamma[a,d])$.

We conclude this section by stating and proving several estimates for the derivatives of the function $S^{(\nu)}$ defined in (1.23) with the functions S_0, S_1, S_2 now constructed. We remind the reader that $(t,x) \in \Gamma[\nu]$ is identified with (t,η,ξ) via the transformation $(t,x) = (t, \eta + n(t,\eta)\xi)$ if not otherwise noted.

Lemma 4.2 *(i) There is a constant K such that for all $0 < \nu \le 1$ the derivatives of $S^{(\nu)}$ satisfy uniformly in $\Gamma[\nu]$ the inequalities*

$$
\begin{aligned}
|\nabla_{\Gamma_\xi} S^{(\nu)}| &\le K, \qquad \big|\hat{\nabla}_{\Gamma_\xi} \nabla_{\Gamma_\xi} S^{(\nu)}\big| \le K, &(4.14)\\
|\nabla_x S^{(\nu)}| &\le K\nu^{-1/2}, &(4.15)\\
\Big|\nabla_{\Gamma_\xi} |\nabla_x S^{(\nu)}|\Big| &\le K\nu^{-1/2}, &(4.16)\\
\Big|\partial_\xi |\nabla_x S^{(\nu)}|\Big| &\le K\nu^{-1}, &(4.17)\\
|\nabla_x S^{(\nu)}(t,\eta,\xi)| &= \partial_\xi S^{(\nu)}(t,\eta,\xi) + R_{\nabla S}(t,\eta,\xi), &(4.18)
\end{aligned}
$$

where the remainder term satisfies $|R_{\nabla S}(t,\eta,\xi)| \le K$. The same estimates hold when ∇_{Γ_ξ} in (4.14), (4.16) *is replaced by ∇_Γ, possibly with a different constant K.*

(ii) There is a constant K such that for all $0 < \nu \le 1$

$$
\sup_{(t,\eta)\in\Gamma} \Big(|\nabla_x S^{(\nu)}|_{\xi=\nu^{1/2} d(t,\eta)} + |\nabla_x S^{(\nu)}|_{\xi=\nu^{1/2} a(t,\eta)} \Big) \le K. \tag{4.19}
$$

Proof. Note first that for functions $w : \Gamma(t) \to \mathbb{R}$ the transformation formula

$$
\nabla_{\Gamma_\xi} (w \circ \mathcal{T}_{t,\xi}^{-1}) \circ \mathcal{T}_{t,\xi}^{-1} = A^T (\nabla_\Gamma w), \tag{4.20}
$$

holds, where A^T is the transpose of the transformation matrix $A(t,\eta,\xi) \in \mathbb{R}^{3\times 3}$ from (1.42). Since by definition of the surface gradient $\nabla_\Gamma W$ in (1.15) we have $\nabla_\Gamma w = (\partial_{\eta_1} w) r_1 + (\partial_{\eta_2} w) r_2$ with suitable coefficient functions $r_i(t,\eta) \in \mathbb{R}^3$ and with the derivatives ∂_{η_i} in directions of coordinates on Γ, we conclude that

$$
|\nabla_{\Gamma_\xi} S^{(\nu)}| = \left| \sum_{i=1}^{2} (A^T r_i) \partial_{\eta_i} S^{(\nu)} \right| = \left| \sum_{i=1}^{2} (A^T r_i) \partial_{\eta_i} (S_0 + \nu^{\frac12} S_1 + \nu S_2) \right| \le K, \tag{4.21}
$$

where the constant K is independent of ν and of $(t,x) \in \Gamma[\nu]$. This proves the first estimate in (4.14). To prove the second we proceed in a similar way to obtain

$$
\big|\hat{\nabla}_{\Gamma_\xi} \nabla_{\Gamma_\xi} S^{(\nu)}\big| = \big|\hat{\nabla}_\Gamma (\nabla_\Gamma S^{(\nu)} A) A\big| \le K_1 . \tag{4.22}
$$

We next use that for $\alpha, \beta \ge 0$ the estimate

$$
0 \le \sqrt{\alpha^2 + \beta^2} - \beta = \frac{\alpha^2}{\sqrt{\alpha^2+\beta^2} + \beta} \le \alpha
$$

holds, which together with (4.14) yields

$$
|R_{\nabla S}| = |\nabla_x S^{(\nu)}| - \partial_\xi S^{(\nu)} = \sqrt{|\nabla_{\Gamma_\xi} S^{(\nu)}|^2 + (\partial_\xi S^{(\nu)})^2} - \partial_\xi S^{(\nu)} \le |\nabla_{\Gamma_\xi} S^{(\nu)}| \le K.
$$

This shows that the decomposition (4.18) holds with a uniformly bounded remainder term. (4.15) is an immediate consequence of (4.18), since

$$|\nabla_x S^{(\nu)}| = |\nu^{-\frac{1}{2}}(S_0' + \nu^{\frac{1}{2}} S_1' + \nu S_2') + R_{\nabla S}| \leq \nu^{-\frac{1}{2}} K. \tag{4.23}$$

We next use the decomposition $\nabla_x S^{(\nu)}(t,\eta,\xi) = n(t,\eta)\partial_\xi S^{(\nu)}(t,\eta,\xi) + \nabla_{\Gamma_\xi} S^{(\nu)}(t,\eta,\xi)$ to obtain

$$|\nabla_x S^{(\nu)}| = \sqrt{(\partial_\xi S^{(\nu)})^2 + |\nabla_{\Gamma_\xi} S^{(\nu)}|^2}. \tag{4.24}$$

Hence,

$$\nabla_{\Gamma_\xi} |\nabla_x S^{(\nu)}| = \frac{\partial_\xi S^{(\nu)}}{|\nabla_x S^{(\nu)}|} \nabla_{\Gamma_\xi} \partial_\xi S^{(\nu)} + \big(\hat{\nabla}_{\Gamma_\xi} \nabla_{\Gamma_\xi} S^{(\nu)}\big) \frac{\nabla_{\Gamma_\xi} S^{(\nu)}}{|\nabla_x S^{(\nu)}|}. \tag{4.25}$$

Again arguing similarly as in (4.21) we obtain

$$\left|\nabla_{\Gamma_\xi} \partial_\xi S^{(\nu)}\right| = \left|A^T \nabla_\Gamma \partial_\xi S^{(\nu)}\right| \;=\; \left|\nu^{-\frac{1}{2}} A^T \nabla_\Gamma (S_0' + \nu^{\frac{1}{2}} S_1' + \nu S_2')\right| \leq \nu^{-\frac{1}{2}} K_2, \tag{4.26}$$

with K_2 independent of ν and of $(t,x) \in \Gamma[\nu]$. Since $\frac{|\partial_\xi S^{(\nu)}|}{|\nabla_x S^{(\nu)}|} \leq 1$ and $\frac{|\nabla_{\Gamma_\xi} S^{(\nu)}|}{|\nabla_x S^{(\nu)}|} \leq 1$, which follows from (4.24), inequality (4.16) is obtained by combination of (4.25), (4.22) and (4.26). The inequality (4.17) is obtained by an obvious modification of the proof of (4.16).

If ∇_{Γ_ξ} in (4.14) and (4.16) is replaced by ∇_Γ, then the matrix $A(t,\eta,\xi)$ in (4.21), (4.22), (4.26) must be replaced by the identity matrix. The resulting estimates do not change by this simplification.

To prove (ii), we note that $S_0'(t,\eta,a(t,\eta)) = S_0'(t,\eta,d(t,\eta)) = 0$, by (1.46). By definition of $S^{(\nu)}$ in (1.23) it therefore follows that at $(x,t) = (t,\eta,\nu^{1/2}a(t,\eta))$ or $(x,t) = (t,\eta,\nu^{1/2}d(t,\eta))$ the inequality (4.23) takes the form

$$|\nabla_x S^{(\nu)}| = |\nu^{-\frac{1}{2}}(\nu^{\frac{1}{2}} S_1' + \nu S_2') + R_{\nabla S}| \leq K.$$

This proves (4.19). The proof of the lemma is complete.

5 Proof of Theorem 1.3, part I

Theorem 1.3 is proved in this section and in Section 6. In the present section we verify the convergence relations (1.50) and (1.51) for the evolution equation (1.12). Estimate (1.49) for the stress field is proved in Section 6. For technical reasons we write in this section S_t for the derivative of the function $t \mapsto S^{(\nu)}(t,\eta,\xi)$ and $\partial_t S^{(\nu)}$ for the derivative of $t \mapsto S^{(\nu)}(t,x) = S^{(\nu)}(t,\eta(t,x),\xi(t,\eta))$.

We must investigate the convergence behavior of the term

$$\left(\partial_t S^{(\nu)}, \varphi\right)_Q + c\left(\nabla_x(\psi_S - \nu \Delta S^{(\nu)}) |\nabla_x S^{(\nu)}|, \nabla_x \varphi\right)_Q \tag{5.1}$$

for $\nu \to 0$ and $\varphi \in C_0^1(Q)$. In these investigations we denote by K various positive constants, which are independent of t, x, η, ξ and ν. Since by definition the function $S^{(\nu)}$ is constant equal to zero in the domain $\gamma \backslash \Gamma[\nu]$ and equal to one in $\gamma' \backslash \Gamma[\nu]$, both terms in (5.1) vanish in these regions. It therefore suffices to estimate these terms in the transitional region $\Gamma[\nu]$. Without mentioning we thus restrict all the estimates in this section to $(t,x) \in \Gamma[\nu]$. If not mentioned otherwise we identify $(t,\eta,\xi) \in \Gamma \times (-\delta,\delta)$ with $(t,x) \in Q$ via the coordinate transformation (1.14).

The surface gradient operator ∇_{Γ_ξ} defined in (1.15) satisfies $\nabla_x = \nabla_{\Gamma_\xi} + n(t,\eta)\partial_\xi$. We replace ∇_x everywhere in (5.1) by this decomposition and note the orthogonality relation $n(t,\eta) \cdot \nabla_{\Gamma_\xi} w(t,\eta,\xi) = 0$ to obtain

$$\begin{aligned}\Big(\partial_t S^{(\nu)}, \varphi\Big)_Q &+ c\Big(\nabla_x(\psi_S - \nu\Delta_x S^{(\nu)})|\nabla_x S^{(\nu)}|, \nabla_x\varphi\Big)_Q \\ &= c\Big(\partial_\xi(\psi_S - \nu\Delta_x S^{(\nu)})|\nabla_x S^{(\nu)}|, \partial_\xi\varphi\Big)_Q \\ &\quad + c\Big(\partial_t S^{(\nu)}, \varphi\Big)_Q + \Big(\nabla_{\Gamma_\xi}(\psi_S - \nu\Delta_x S^{(\nu)})|\nabla_x S^{(\nu)}|, \nabla_{\Gamma_\xi}\varphi\Big)_Q. \qquad (5.2)\end{aligned}$$

Our first goal is to show that the first term on the right hand side tends to zero for $\nu \to 0$. For this term to become small it is necessary that $S^{(\nu)}$ has the asymptotic expansion derived in Section 4. Thus, this term determines the shape of the transition profile. The second and third term do not converge to zero separately, only their sum tends to zero. For this to happen it is necessary that the transition profile moves with the normal speed $-c\Delta_\Gamma(n \cdot [\hat{C}]n)$ of the sharp interface. Therefore these two terms together determine the propagation speed of the profile. We start with the estimates for the first term.

Lemma 5.1 *There is a positive number K such that for all $\varphi \in C_0^1(Q)$ and all $0 < \nu \le 1$*

$$\left|\Big(\partial_\xi(\psi_S - \nu\Delta_x S^{(\nu)})|\nabla_x S^{(\nu)}|, \partial_\xi\varphi\Big)_Q\right| \le K\nu^{\frac{1}{2}}\|\varphi\|_{L^\infty(Q)}. \qquad (5.3)$$

Proof. Equation (3.11) implies

$$\partial_\xi(\psi_S - \nu\Delta S^{(\nu)}) = \nu^{\frac{3}{2}}\partial_\xi R_{\psi_S-\nu\Delta}(\nu,t,\eta,\xi,\frac{\xi}{\nu^{1/2}}) = \nu R^*_{\psi_S-\nu\Delta}(\nu,t,\eta,\xi,\frac{\xi}{\nu^{1/2}}), \qquad (5.4)$$

with

$$\begin{aligned}\left|R^*_{\psi_S-\nu\Delta}(\nu,t,\eta,\xi,\frac{\xi}{\nu^{1/2}})\right| &= \left|\nu^{\frac{1}{2}}\partial_\xi R_{\psi_S-\nu\Delta}(\nu,t,\eta,\xi,\frac{\xi}{\nu^{1/2}})\right| \\ &= \left|\nu^{\frac{1}{2}}\partial_\xi R_{\psi_S-\nu\Delta}(\nu,t,\eta,\xi,\zeta)_{|\zeta=\xi\nu^{-1/2}} + \partial_\zeta R_{\psi_S-\nu\Delta}(\nu,t,\eta,\xi,\zeta)_{|\zeta=\xi\nu^{-1/2}}\right| \le K, \qquad (5.5)\end{aligned}$$

and similarly with

$$\left|\partial_\xi R^*_{\psi_S-\nu\Delta}(\nu,t,\eta,\xi,\frac{\xi}{\nu^{1/2}})\right| \le K\nu^{-\frac{1}{2}}. \qquad (5.6)$$

In the following computation we note that $\nabla_x S^{(\nu)}$ vanishes outside the set $\Gamma[\nu]$, employ (5.4) and, in order to integrate by parts with respect to ξ, transform the integral from (t,x)–coordinates to (t,η,ξ)–coordinates. With the Jacobi determinant

$\omega(t,\eta,\xi) = |\det(\frac{\partial(t,x)}{\partial(t,\eta,\xi)})|$ we obtain

$$
\begin{aligned}
\Big(\partial_\xi(\psi_S - \nu\Delta_x S^{(\nu)})|\nabla_x S^{(\nu)}|, \partial_\xi\varphi\Big)_Q &= \nu \left(R^*_{\psi_S-\nu\Delta}|\nabla_x S^{(\nu)}|, \partial_\xi\varphi\right)_{\Gamma[\nu]} \\
&= \nu \int_\Gamma \int_{\nu^{1/2}a(t,\eta)}^{\nu^{1/2}d(t,\eta)} \omega R^*_{\psi_S-\nu\Delta}|\nabla_x S^{(\nu)}|\, \partial_\xi\varphi \, d\xi d\sigma \\
&= \nu \int_\Gamma \left[\omega R^*_{\psi_S-\nu\Delta}|\nabla_x S^{(\nu)}|\varphi\right]_{\xi=\nu^{1/2}a(t,\eta)}^{\xi=\nu^{1/2}d(t,\eta)} d\sigma \\
&\quad - \nu \int_\Gamma \int_{\nu^{1/2}a(t,\eta)}^{\nu^{1/2}d(t,\eta)} (\partial_\xi\omega) R^*_{\psi_S-\nu\Delta}|\nabla_x S^{(\nu)}|\, \varphi \, d\xi d\sigma \\
&\quad - \nu \int_\Gamma \int_{\nu^{1/2}a(t,\eta)}^{\nu^{1/2}d(t,\eta)} \omega\, \partial_\xi\Big(R^*_{\psi_S-\nu\Delta}|\nabla_x S^{(\nu)}|\Big)\, \varphi \, d\xi d\sigma \\
&= \hat{I}_1 + \hat{I}_2 + \hat{I}_3 \,. \qquad (5.7)
\end{aligned}
$$

From $\sup_{\Gamma[\nu]} |\omega| \le K$ and from (5.5), (4.19) we conclude that

$$
\begin{aligned}
|\hat{I}_1| &\le \nu K \sup_{\Gamma[\nu]} |\omega| \sup_{\Gamma[\nu]} |R^*_{\psi_S-\nu\Delta}| \Big(\sup_{\xi=\nu^{1/2}a} |\nabla_x S^{(\nu)}| + \sup_{\xi=\nu^{1/2}d} |\nabla_x S^{(\nu)}| \Big) \sup_{\Gamma[\nu]} |\varphi| \\
&\le \nu K \|\varphi\|_{L^\infty(Q)} \,. \qquad (5.8)
\end{aligned}
$$

The estimates $\sup_{\Gamma[\nu]} |\partial_\xi\omega| \le K$ and $\operatorname{meas}(\Gamma[\nu]) \le K\nu^{\frac{1}{2}}$ yield together with (5.5), (4.15) that

$$
|\hat{I}_2| = \nu K \nu^{-\frac{1}{2}} \operatorname{meas}(\Gamma[\nu]) \sup_{\Gamma[\nu]} |\varphi| \le \nu K \|\varphi\|_{L^\infty(Q)} \,. \qquad (5.9)
$$

Finally, (5.5), (5.6) and (4.17) together imply

$$
|\hat{I}_3| \le \nu K \nu^{-1} \operatorname{meas}(\Gamma[\nu]) \sup_{\Gamma[\nu]} |\varphi| \le \nu^{\frac{1}{2}} K \|\varphi\|_{L^\infty(Q)} \,. \qquad (5.10)
$$

The statement of the lemma follows by insertion of (5.8) – (5.10) into (5.7).

The coordinate transformation $(t,x) \mapsto (t,\eta(t,x),\xi(t,\eta))$ is determined by the following conditions: $\eta \in \Gamma(t)$ is the unique point such that

$$
|x-\eta| = \operatorname{dist}(x,\Gamma(t)). \qquad (5.11)
$$

If η is known, then $\xi \in \mathbb{R}$ is obtained from the equation

$$
x = \eta + \xi\, n(t,\eta). \qquad (5.12)
$$

To compute $\partial_t\xi(t,x)$, note first that (5.12) yields

$$
0 = \partial_t x = n\partial_t\xi + \xi\partial_t n + \partial_t\eta.
$$

Since $0 = \partial_t 1 = \partial_t|n|^2 = 2n\cdot\partial_t n$, we obtain by scalar multiplication of this equation with n that

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

By definition of the normal speed s we obtain from this equation and from (5.11) that

$$\begin{aligned} s &= -\operatorname{sign}(\xi)\frac{\partial}{\partial t}\operatorname{dist}(x,\Gamma(t)) \\ &= -\operatorname{sign}(\xi)\frac{\partial}{\partial t}|x-\eta| = \operatorname{sign}(\xi)\frac{(x-\eta)\cdot\partial_t\eta}{|x-\eta|} = n\cdot\partial_t\eta = -\partial_t\xi. \end{aligned} \tag{5.13}$$

Lemma 5.2 *We have*

$$\partial_t S^{(\nu)}(t,\eta,\xi) = S_t^{(\nu)}(t,\eta,\xi) + \nabla_\eta S^{(\nu)}(t,\eta,\xi)\,\partial_t\eta + c\Delta_\Gamma\Big(n\cdot[\hat{C}]n\Big)(t,\eta)\,\partial_\xi S^{(\nu)}(t,\eta,\xi).$$

This lemma follows immediately by combination of (5.13) with (1.5).

The surface divergence $\operatorname{div}_{\Gamma_\xi}$ is defined as follows: Let $\tau_1=\tau_1(\eta)$, $\tau_2=\tau_2(\eta)\in\mathbb{R}^3$ be two orthogonal unit tangent vectors to $\Gamma(t)$ at $\eta\in\Gamma(t)$. For vector fields $W:\Gamma_\xi(t)\to\mathbb{R}^3$, which are tangential to $\Gamma_\xi(t)$, we set

$$\operatorname{div}_{\Gamma_\xi}W = \tau_1\cdot\partial_{\tau_1}W + \tau_2\cdot\partial_{\tau_2}W.$$

Because $\nabla_{\Gamma_\xi}(\psi_S-\nu\Delta_x S^{(\nu)})|\nabla_x S^{(\nu)}|\,\varphi$ is a tangential vector field to Γ_ξ, we can apply Stoke's theorem on the surfaces Γ_ξ and obtain with the surface divergence

$$\begin{aligned} &\Big(\nabla_{\Gamma_\xi}(\psi_S-\nu\Delta_x S^{(\nu)})|\nabla_x S^{(\nu)}|,\nabla_{\Gamma_\xi}\varphi\Big)_Q \\ &= \Big(\nabla_{\Gamma_\xi}(\psi_S-\nu\Delta_x S^{(\nu)})|\nabla_x S^{(\nu)}|,\nabla_{\Gamma_\xi}\varphi\Big)_{\Gamma[\nu]} \\ &= -\Big(\operatorname{div}_{\Gamma_\xi}\Big(\nabla_{\Gamma_\xi}(\psi_S-\nu\Delta_x S^{(\nu)})|\nabla_x S^{(\nu)}|\Big),\varphi\Big)_{\Gamma[\nu]} \\ &\quad + \int_{\partial\Gamma[\nu]} n_{\Gamma_\xi}\cdot\nabla_{\Gamma_\xi}(\psi_S-\nu\Delta_x S^{(\nu)})|\nabla_x S^{(\nu)}|\varphi\,d\sigma_x\,. \\ &= -\Big(\Delta_{\Gamma_\xi}(\psi_S-\nu\Delta_x S^{(\nu)})|\nabla_x S^{(\nu)}|,\varphi\Big)_{\Gamma[\nu]} \\ &\quad -\Big(\nabla_{\Gamma_\xi}(\psi_S-\nu\Delta_x S^{(\nu)})\cdot\nabla_{\Gamma_\xi}|\nabla_x S^{(\nu)}|,\varphi\Big)_{\Gamma[\nu]} \\ &\quad + \int_{\partial\Gamma[\nu]} n_{\Gamma_\xi}\cdot\nabla_{\Gamma_\xi}(\psi_S-\nu\Delta_x S^{(\nu)})|\nabla_x S^{(\nu)}|\varphi\,d\sigma_x\,. \end{aligned} \tag{5.14}$$

Here we used that $\Delta_{\Gamma_\xi}=\operatorname{div}_{\Gamma_\xi}\nabla_{\Gamma_\xi}$. The vector $n_{\Gamma_\xi}=n_{\Gamma_\xi}(t,\eta,\xi)\in\mathbb{R}^3$ lies in the tangent plane to $\Gamma_\xi(t)$ and is obtained as projection to this tangent plane of a unit vector $\tilde{n}(t,\eta,\xi)\in\mathbb{R}^4$, which is normal to the boundary $\partial\Gamma[\nu]$. In the (t,η,ξ)–coordinate system the parts of the boundary, where this projection is different from zero, are determined by the equations $\xi-\nu^{1/2}a(t,\eta)=0$ or $\xi-\nu^{1/2}d(t,\eta)=0$. In the (t,x)–coordinates the first equation takes the form $\xi(t,x)-\nu^{1/2}a(t,\eta(t,x))=0$. A normal vector is thus given by $-\big(\partial_t\xi-\nu^{1/2}a_t(t,\eta)-\nu^{1/2}\nabla_\eta\,a(t,\eta)\partial_t\eta\,,\ \nabla_x\,\xi-\nu^{1/2}\nabla_\eta\,a(t,\eta)\frac{\partial\eta}{\partial x}\big)\in\mathbb{R}^4$, where $\frac{\partial\eta}{\partial x}=\frac{\partial(\eta_1,\eta_2)}{\partial(x_1,x_2,x_3)}$ is the Jacobi matrix.

Since $\nabla_x\,\xi$ is orthogonal to the surface Γ_ξ, it follows that the projection of this vector to the tangent plane of Γ_ξ is $\nu^{1/2}\nabla_\eta\,a(t,\eta)\frac{\partial\eta}{\partial x}$. Hence, at the part of the boundary $\partial\Gamma[\nu]$ determined by the equation $\xi-\nu^{1/2}a(t,\eta)=0$ we have

$$n_{\Gamma_\xi} = \frac{\nu^{1/2}\,\nabla_\eta a\,\frac{\partial\eta}{\partial x}}{|(\partial_t\xi-\nu^{1/2}a_t-\nu^{1/2}\nabla_\eta a\,\partial_t\eta\,,\ \nabla_x\xi-\nu^{1/2}\nabla_\eta a\,\frac{\partial\eta}{\partial x})|}\,. \tag{5.15}$$

For the part of the boundary determined by the equation $\xi - \nu^{1/2} d(t,\eta) = 0$ we obtain in the same way

$$n_{\Gamma_\xi} = \frac{-\nu^{1/2}\, \nabla_\eta d\, \frac{\partial\eta}{\partial x}}{|(\partial_t \xi - \nu^{1/2} d_t - \nu^{1/2}\nabla_\eta d\, \partial_t \eta\,,\ \nabla_x \xi - \nu^{1/2}\nabla_\eta d\, \frac{\partial \eta}{\partial x})|}\,. \tag{5.16}$$

In the next step we replace the term $\psi_S - \nu\Delta_x S^{(\nu)}$ in (5.14) by the decomposition $n\cdot[\hat{C}]n + \nu^{1/2}\hat{R}_{\psi_S-\Delta S}$ given in (3.12). We combine the resulting equation with Lemma 5.2 and obtain

Lemma 5.3 *(i) Let $\varphi \in C_0^1(Q)$. Then*

$$\begin{aligned}
&\Big(\partial_t S^{(\nu)}, \varphi\Big)_Q + c\Big(\nabla_{\Gamma_\xi}(\psi_S - \nu\Delta_x S^{(\nu)})|\nabla_x S^{(\nu)}|, \nabla_{\Gamma_\xi}\varphi\Big)_Q \\
=\ & \Big(S_t^{(\nu)} + \nabla_\eta S^{(\nu)}\partial_t\eta, \varphi\Big)_{\Gamma[\nu]} \\
&+ c\Big(\Delta_\Gamma\big(n\cdot[\hat{C}]n\big)\partial_\xi S^{(\nu)}, \varphi\Big)_{\Gamma[\nu]} - c\Big(\Delta_{\Gamma_\xi}(n\cdot[\hat{C}]n)\,|\nabla_x S^{(\nu)}|, \varphi\Big)_{\Gamma[\nu]} \\
&- \nu^{1/2} c\Big(\Delta_{\Gamma_\xi}\hat{R}_{\psi_S-\nu\Delta}\,|\nabla_x S^{(\nu)}|, \varphi\Big)_{\Gamma[\nu]} \\
&- c\Big(\nabla_{\Gamma_\xi}(n\cdot[\hat{C}]n)\cdot\nabla_{\Gamma_\xi}|\nabla_x S^{(\nu)}|, \varphi\Big)_{\Gamma[\nu]} \\
&- \nu^{1/2} c\Big(\nabla_{\Gamma_\xi}\hat{R}_{\psi_S-\nu\Delta}\cdot\nabla_{\Gamma_\xi}|\nabla_x S^{(\nu)}|, \varphi\Big)_{\Gamma[\nu]} \\
&+ c\int_{\partial\Gamma[\nu]} n_{\Gamma_\xi}\cdot\nabla_{\Gamma_\xi}\Big(n\cdot[\hat{C}]n + \nu^{1/2}\hat{R}_{\psi_S-\Delta S}\Big)\,|\nabla_x S^{(\nu)}|\varphi\, d\sigma_x\,. \\
=\ & I_1 + I_2 + I_3 + I_4 + I_5 + I_6\,.
\end{aligned} \tag{5.17}$$

(ii) There is a constant K such that for $i = 1,2,3,5,6$, for all $\varphi \in C_0(Q)$ and for all $\nu > 0$

$$|I_i| \le \nu^{1/2} K\|\varphi\|_{L^\infty(Q)}. \tag{5.18}$$

(iii) There is a constant K such that for all $\varphi \in C_0(Q)$ and all $\nu > 0$

$$|I_4| \le K\|\varphi\|_{L^\infty(Q)}\,. \tag{5.19}$$

The convergence of the term I_4 for $\nu \to 0$ will be studied in the next lemma.

Proof. Equation (5.17) has been derived above. To verify (ii) note that by definition of $\Gamma[\nu]$ we have $\text{meas}(\Gamma[\nu]) \le K\nu^{1/2}$ for all $0 < \nu \le 1$. We thus have

$$|I_1| = \left|\Big(S_t^{(\nu)} + \nabla_\eta S^{(\nu)}\partial_t\eta, \varphi\Big)_{\Gamma[\nu]}\right| \le K\sup_{\Gamma[\nu]}|\varphi|\,\text{meas}(\Gamma[\nu]) \le \nu^{1/2}K\|\varphi\|_{L^\infty(Q)}\,.$$

Using that $\sup_{\Gamma[\nu]}|\Delta_{\Gamma_\xi}\hat{R}_{\psi_S-\nu\Delta}| \le K$ and $\sup_{\Gamma[\nu]}|\nabla_{\Gamma_\xi}\hat{R}_{\psi_S-\nu\Delta}| \le K$, we obtain together with (4.15) and with (4.16) that

$$\begin{aligned}
|I_3| + |I_5| \ &= \ \left|\nu^{1/2}c\Big(\Delta_{\Gamma_\xi}\hat{R}_{\psi_S-\nu\Delta}\,|\nabla_x S^{(\nu)}|, \varphi\Big)_{\Gamma[\nu]}\right| \\
&\qquad + \left|\nu^{1/2}c\Big(\nabla_{\Gamma_\xi}\hat{R}_{\psi_S-\nu\Delta}\cdot\nabla_{\Gamma_\xi}|\nabla_x S^{(\nu)}|, \varphi\Big)_{\Gamma[\nu]}\right| \\
&\le \ \nu^{1/2}K\nu^{-1/2}\sup_{\Gamma[\nu]}|\varphi|\,\text{meas}(\Gamma[\nu]) \ \le \ \nu^{1/2}K\|\varphi\|_{L^\infty(Q)}\,.
\end{aligned}$$

To estimate I_6 we note that $\sup_{\Gamma[\nu]} |\nabla_{\Gamma_\xi}(n\cdot[\hat{C}]n + \nu^{1/2}\hat{R}_{\psi_S-\Delta S})| \le K$. From (5.15), (5.16) and from (4.19) we thus infer

$$\begin{aligned} |I_6| &= \left| c\int_{\partial\Gamma[\nu]} n_{\Gamma_\xi}\cdot\nabla_{\Gamma_\xi}\Big(n\cdot[\hat{C}]n + \nu^{1/2}\hat{R}_{\psi_S-\Delta S}\Big)\,|\nabla_x S^{(\nu)}|\varphi\, d\sigma_x \right| \\ &\le \nu^{1/2} K \sup_{\partial\Gamma[\nu]} |\varphi|\ \mathrm{meas}(\partial\Gamma[\nu]) \le \nu^{1/2}K\|\varphi\|_{L^\infty(Q)}\,. \end{aligned}$$

To deal with I_2 we use (4.18) and the decomposition of the surface Laplacian $\Delta_{\Gamma_\xi} = \Delta_\Gamma + \xi R_{\Delta_{\Gamma_\xi}}$ given in (3.8) to conclude that

$$\begin{aligned} \Delta_{\Gamma_\xi}(n\cdot[\tilde{C}]n)\,|\nabla_x S^{(\nu)}| &= \Delta_\Gamma(n\cdot[\hat{C}]n)\,\partial_\xi S^{(\nu)} + \Delta_\Gamma(n\cdot[\hat{C}]n)\,R_{\nabla S} \\ &\quad + \xi\, R_{\Delta_{\Gamma_\xi}}(\xi,\partial\eta,\partial^2\eta)(n\cdot[\hat{C}]n)\,|\nabla_x S^{(\nu)}|. \end{aligned}$$

Since the estimates $|R_{\nabla S}(t,\eta,\xi)| \le K$, $|R_{\Delta_{\Gamma_\xi}}(\xi,\partial\eta,\partial^2\eta)(n\cdot[\hat{C}]n)| \le K$ and $|\xi| \le K\nu^{1/2}$ hold on the set $\Gamma[\nu]$, we obtain together with (4.15)

$$\begin{aligned} |I_2| &= \left| c\Big(\Delta_\Gamma(n\cdot[\hat{C}]n)\partial_\xi S^{(\nu)} - \Delta_{\Gamma_\xi}(n\cdot[\hat{C}]n)\,|\nabla_x S^{(\nu)}|,\,\varphi\Big)_{\Gamma[\nu]}\right| \\ &= \left| c\Big(\Delta_\Gamma(n\cdot[\hat{C}]n)\,R_{\nabla S} + \xi\,R_{\Delta_{\Gamma_\xi}}(\xi,\partial\eta,\partial^2\eta)(n\cdot[\hat{C}]n)\,|\nabla_x S^{(\nu)}|,\,\varphi\Big)_{\Gamma[\nu]}\right| \\ &\le K\sup_{\Gamma[\nu]}|\varphi|\,\mathrm{meas}(\Gamma[\nu]) \le \nu^{1/2}K\|\varphi\|_{L^\infty(Q)}\,. \end{aligned}$$

To prove (5.19) we use (4.16) to conclude

$$\begin{aligned} |I_4| &= \left| c\Big(\nabla_{\Gamma_\xi}(n\cdot[\hat{C}]n)\cdot\nabla_{\Gamma_\xi}|\nabla_x S^{(\nu)}|,\varphi\Big)_{\Gamma[\nu]}\right| \\ &\le \nu^{-1/2}K\sup_{\Gamma[\nu]}|\varphi|\,\mathrm{meas}(\Gamma[\nu]) \le K\|\varphi\|_{L^\infty(Q)}\,. \end{aligned}$$

The proof is complete.

Lemma 5.4 *(i) The term I_4 from Lemma 5.3 satisfies for all $\varphi \in C_0(Q)$*

$$\lim_{\nu\to 0} I_4 = \lim_{\nu\to 0} c\Big(\nabla_{\Gamma_\xi}(n\cdot[\hat{C}]n)\cdot\nabla_{\Gamma_\xi}|\nabla_x S^{(\nu)}|,\varphi\Big)_Q = 0\,. \tag{5.20}$$

(ii) There is a constant K such that for all $\varphi\in C_0^\alpha(Q)$ with $0<\alpha\le 1$

$$|I_4| = \left|\Big(\nabla_{\Gamma_\xi}(n\cdot[\hat{C}]n)\cdot\nabla_{\Gamma_\xi}|\nabla_x S^{(\nu)}|,\varphi\Big)_Q\right| \le K\nu^{\min(\frac{\alpha}{2},\frac14)}\|\varphi\|_{C^\alpha(Q)}\,. \tag{5.21}$$

Proof. Before (1.42) we remarked that the matrix function A satisfies $A(t,\eta,0)=I$. From the transformation formula (4.20) and from Taylor's formula we thus have for functions $w:\Gamma\to\mathbb{R}$ that

$$\nabla_{\Gamma_\xi}(w\circ\mathcal{T}_{t,\xi}^{-1})\big(\mathcal{T}_{t,\xi}(\eta)\big) = A(t,\eta,\xi)^T\nabla_\Gamma w(\eta) = \nabla_\Gamma w(\eta) + \xi\,R_\nabla(t,\eta,\xi,\partial_\eta)w(\eta).$$

With this decomposition of ∇_{Γ_ξ} and with $w(\eta) = |\nabla_x S^{(\nu)}(t,\eta,\xi)|$ we write I_4 as a sum of three terms:

$$\begin{aligned}
I_4 &= c\Big(\nabla_{\Gamma_\xi}(n\cdot[\hat{C}]n)\cdot\nabla_{\Gamma_\xi}|\nabla_x S^{(\nu)}|,\varphi\Big)_{\Gamma[\nu]} \\
&= c\Big(\nabla_{\Gamma_\xi}(n\cdot[\hat{C}]n)\cdot\nabla_{\Gamma}|\nabla_x S^{(\nu)}|,\varphi\Big)_{\Gamma[\nu]} \\
&\quad + c\Big(\nabla_{\Gamma_\xi}(n\cdot[\hat{C}]n)\cdot\xi\, R_\nabla(t,\eta,\xi,\partial_\eta)|\nabla_x S^{(\nu)}|,\varphi\Big)_{\Gamma[\nu]} \\
&= c\Big(\nabla_{\Gamma_\xi}(n\cdot[\hat{C}]n)\cdot\nabla_{\Gamma}|\nabla_x S^{(\nu)}|,\varphi|_{\xi=0}\Big)_{\Gamma[\nu]} \\
&\quad + c\Big(\nabla_{\Gamma_\xi}(n\cdot[\hat{C}]n)\cdot\nabla_{\Gamma}|\nabla_x S^{(\nu)}|,\varphi-\varphi|_{\xi=0}\Big)_{\Gamma[\nu]} \\
&\quad + c\Big(\nabla_{\Gamma_\xi}(n\cdot[\hat{C}]n)\cdot\xi\, R_\nabla(t,\eta,\xi,\partial_\eta)\,|\nabla_x S^{(\nu)}|,\varphi\Big)_{\Gamma[\nu]} \\
&= J_1 + J_2 + J_3\,. \qquad (5.22)
\end{aligned}$$

The term J_3 can be treated most easily. Since the differential operator $R_\nabla(t,\eta,\xi,\partial_\eta)$ contains only derivatives with respect to η, it follows from (4.16) that the estimate $\big|R_\nabla(t,\eta,\xi,\partial_\eta)\,|\nabla_x S^{(\nu)}|\,\big| \le K\nu^{-1/2}$ holds. On the other hand, we have $|\xi| \le K\nu^{1/2}$ on $\Gamma[\nu]$. If we combine both estimates and use that $|\nabla_{\Gamma_\xi}(n\cdot[\hat{C}]n)| \le K$, we obtain

$$|J_3| \le K\sup_{\Gamma[\nu]}|\varphi|\,\mathrm{meas}(\Gamma[\nu]) \le \nu^{1/2}K\|\varphi\|_{L^\infty(Q)}\,. \qquad (5.23)$$

To estimate J_1 we must first study the term $\nabla_\Gamma|\nabla_x S^{(\nu)}|$ carefully. From (4.24) it follows that

$$\begin{aligned}
\nabla_\Gamma|\nabla_x S^{(\nu)}| &= \frac{\partial_\xi S^{(\nu)}}{|\nabla_x S^{(\nu)}|}\nabla_\Gamma\partial_\xi S^{(\nu)} + \hat{\nabla}_\Gamma\nabla_{\Gamma_\xi}S^{(\nu)}\frac{\nabla_{\Gamma_\xi}S^{(\nu)}}{|\nabla_x S^{(\nu)}|} \\
&= \partial_\xi\nabla_\Gamma S^{(\nu)} - \frac{\sqrt{1+\frac{|\nabla_{\Gamma_\xi}S^{(\nu)}|^2}{(\partial_\xi S^{(\nu)})^2}}-1}{\sqrt{1+\frac{|\nabla_{\Gamma_\xi}S^{(\nu)}|^2}{(\partial_\xi S^{(\nu)})^2}}}\partial_\xi\nabla_\Gamma S^{(\nu)} + \hat{\nabla}_\Gamma\nabla_{\Gamma_\xi}S^{(\nu)}\frac{\nabla_{\Gamma_\xi}S^{(\nu)}}{|\nabla_x S^{(\nu)}|} \\
&= \partial_\xi\nabla_\Gamma S^{(\nu)} + F_1^{(\nu)}(t,\eta,\xi) + F_2^{(\nu)}(t,\eta,\xi). \qquad (5.24)
\end{aligned}$$

Since $\frac{|\nabla_{\Gamma_\xi}S^{(\nu)}|}{|\nabla_x S^{(\nu)}|} \le 1$ and since $\hat{\nabla}_\Gamma\nabla_{\Gamma_\xi}S^{(\nu)}$ only contains derivatives with respect to η and therefore satisfies $|\hat{\nabla}_\Gamma\nabla_{\Gamma_\xi}S^{(\nu)}| \le K$, cf. (4.14), it follows that

$$|F_2^{(\nu)}(t,\eta,\xi)| \le K. \qquad (5.25)$$

To estimate $F_1^{(\nu)}$ note that for $\alpha \ge 0$ we have $\frac{\sqrt{1+\alpha}-1}{\sqrt{1+\alpha}} \le \frac{\alpha}{\sqrt{1+\alpha}} \le \alpha$, which together with (4.14) and $|\partial_\xi\nabla_\Gamma S^{(\nu)}| \le \nu^{-1/2}K$, cf. (4.26), yields that

$$|F_1^{(\nu)}(t,\eta,\xi)| \le \nu^{-1/2}K|\partial_\xi S^{(\nu)}|^{-2}. \qquad (5.26)$$

With the functions a, d introduced in Theorem 1.1 define

$$a_\nu(t,\eta) = \nu^{1/2}a(t,\eta) + \nu^{3/4}, \quad d_\nu(t,\eta) = \nu^{1/2}d(t,\eta) - \nu^{3/4}, \quad (t,\eta)\in\Gamma$$

and

$$\Gamma[a_\nu, d_\nu] = \{(t,\eta,\xi) \mid (t,\eta) \in \Gamma,\ a_\nu(t,\eta) \le \xi \le d_\nu(t,\eta)\}.$$

Note that $a_\nu(t,\eta) < d_\nu(t,\eta)$ for all sufficiently small ν.

Claim 1. There is a constant $M_1 > 0$ such that for all sufficiently small $\nu > 0$ and for all $(t,\eta,\xi) \in \Gamma[a_\nu, d_\nu]$

$$|F_1^{(\nu)}(t,\eta,\xi)| \le \frac{K}{M_1^2}\,.$$

This claim follows immediately if we can show that there is $M_1 > 0$ such that

$$\partial_\xi S^{(\nu)}(t,\eta,\xi) \ge M_1 \nu^{-1/4} \tag{5.27}$$

holds for all $(t,\eta,\xi) \in \Gamma[a_\nu, d_\nu]$. To verify this inequality remember that we showed in the proof of Theorem 1.1 that there are $\delta > 0, c_0 > 0$, which can be chosen uniformly with respect to $(t,\eta) \in \Gamma$, such that

$$\begin{aligned} \partial_\zeta^2 S_0(t,\eta,\zeta) &> c_0, \quad \text{for } a(t,\eta) \le \zeta \le a(t,\eta) + \delta,\\ \partial_\zeta^2 S_0(t,\eta,\zeta) &< -c_0, \quad \text{for } d(t,\eta) - \delta \le \zeta \le d(t,\eta). \end{aligned}$$

From $S_0(t,\eta,a) = \partial_\zeta S_0(t,\eta,a) = 0$ and from $S_0(t,\eta,d) = 1$, $\partial_\zeta S_0(t,\eta,d) = 0$ we thus infer

$$\begin{aligned} &\partial_\zeta S_0(t,\eta,\zeta) \ge c_0(\zeta - a(t,\eta)), \qquad S_0(t,\eta,\zeta) \ge \frac{c_0}{2}(\zeta - a(t,\eta))^2, \quad \text{for } |\zeta - a(t,\eta)| \le \delta,\\ &\partial_\zeta S_0(t,\eta,\zeta) \ge c_0(d(t,\eta) - \zeta), \qquad S_0(t,\eta,\zeta) \le 1 - \frac{c_0}{2}(d(t,\eta) - \zeta)^2, \quad \text{for } |\zeta - d(t,\eta)| \le \delta. \end{aligned}$$

Since $\zeta \mapsto S_0(t,\eta,\zeta)$ is monotonically increasing, this implies in particular that $\frac{c_0}{2}\delta^2 \le S_0(t,\eta,\zeta) \le 1 - \frac{c_0}{2}\delta^2$ for $a(t,\eta) + \delta \le \zeta \le d(t,\eta) - \delta$. Since by definition S_0 satisfies (1.44) and since by assumption we have $\tilde\psi(t,\eta,S) \ge \frac{c_1^2}{2}$ for $\frac{c_0}{2}\delta^2 \le S \le 1 - \frac{c_0}{2}\delta^2$ with a suitable constant $c_1 > 0$, we finally conclude that

$$\partial_\zeta S_0(t,\eta,\zeta) \ge \begin{cases} \partial_\zeta S_0(t,\eta,\zeta) \ge c_0(\zeta - a(t,\eta)), & a(t,\eta) \le \zeta \le a(t,\eta) + \delta,\\ c_1, & a(t,\eta) + \delta < \zeta < d(t,\eta) - \delta,\\ \partial_\zeta S_0(t,\eta,\zeta) \ge c_0(d(t,\eta) - \zeta), & d(t,\eta) - \delta \le \zeta \le d(t,\eta). \end{cases}$$

This, in turn, implies for $0 < \nu \le \nu_0 = \min(\delta, c_1/c_0)^4$ that

$$\partial_\zeta S_0(t,\eta,\zeta) \ge c_0 \nu^{1/4}, \quad a(t,\eta) + \nu^{1/4} \le \zeta \le d(t,\eta) - \nu^{1/4},$$

whence

$$\partial_\xi S_0(t,\eta,\frac{\xi}{\nu^{1/2}}) \ge c_0 \nu^{-1/4}, \qquad \text{for } (t,\eta,\xi) \in \Gamma[a_\nu, d_\nu].$$

Since $|\nu^{1/2}\partial_\xi S_1(t,\eta,\frac{\xi}{\nu^{1/2}}) + \nu \partial_\xi S_2(t,\eta,\frac{\xi}{\nu^{1/2}})| \le K$ for all ν, it follows from (1.23) and from the last estimate that

$$\partial_\xi S^{(\nu)}(t,\eta,\xi) \ge c_0 \nu^{-1/4} - K \ge M \nu^{1/4}, \qquad \text{for } (t,\eta,\xi) \in \Gamma[a_\nu, d_\nu],$$

with $M_1 = \frac{c_0}{2}$ and $\nu \le \min(\nu_0, \big(\frac{c_0}{2K}\big)^4)$. This shows that (5.27) holds and finishes the proof of Claim 1.

Claim 2. There is a constant $M_2 > 0$ such that

$$\sup_{(t,\eta)\in\Gamma} \Big(|\nabla_\Gamma S^{(\nu)}|_{\xi=d_\nu(t,\eta)} + |\nabla_\Gamma S^{(\nu)}|_{\xi=a_\nu(t,\eta)} \Big) \le M_2\, \nu^{1/4}.$$

To prove this claim we note that by Theorem 1.1 the function S_0 has continuous derivatives up to fourth order up to the boundary of $\Gamma[a,d]$, and that $\nabla_\eta S_0(t,\eta,\zeta)\big|_{\zeta=a(t,\eta)} = 0$. By the mean value theorem we thus find that there is a constant M, which can be chosen uniformly with respect to $(t,\eta)\in\Gamma$, such that

$$|\nabla_\eta S_0(t,\eta,\zeta)| \le M\,|\zeta - a(t,\eta)|.$$

Since $a_\nu(t,\eta) - \nu^{1/2}a(t,\eta) = \nu^{3/4}$, this yields

$$\nabla_\eta S_0(t,\eta,\frac{\xi}{\nu^{1/2}})|_{\xi=a_\nu(t,\eta)} \le M\,\nu^{1/4}. \tag{5.28}$$

If we now remember the estimate $|\nu^{1/2}\nabla_\eta S_1(t,\eta,\frac{\xi}{\nu^{1/2}}) + \nu\nabla_\eta S_2(t,\eta,\frac{\xi}{\nu^{1/2}})| \le K\nu^{1/2}$ and observe that ∇_Γ is a linear combination of the derivatives ∂_{η_1} and ∂_{η_2}, we see that the estimate for $|\nabla_\Gamma S^{(\nu)}|_{\xi=a_\nu(t,\eta)}$ in Claim 2 follows immediately from (1.23) and from (5.28) with a suitable constant M_2. The estimate for $|\nabla_\Gamma S^{(\nu)}|_{\xi=d_\nu(t,\eta)}$ is obtained in the same way. This proves the claim.

Now we have collected all the necessary information about the term $\nabla_\Gamma|\nabla_x S^{(\nu)}|$ and are in a position to estimate the term J_1 in (5.22). Let

$$G[\nu] = \{(t, x(t,\eta,\xi)) \mid (t,\eta,\xi)\in\Gamma[a_\nu,d_\nu]\}$$

be the image of $\Gamma[a_\nu,d_\nu]$ under the coordinate transformation $(t,\eta,\xi)\mapsto(t,x(t,\eta,\xi))$. Using (5.24) we write

$$\begin{aligned}
J_1 &= \Big(\nabla_{\Gamma_\xi}(n\cdot[\hat C]n)\cdot\nabla_\Gamma|\nabla_x S^{(\nu)}|, \varphi|_{\xi=0}\Big)_{\Gamma[\nu]} \\
&= \Big(\nabla_{\Gamma_\xi}(n\cdot[\hat C]n)\cdot\nabla_\Gamma|\nabla_x S^{(\nu)}|, \varphi|_{\xi=0}\Big)_{\Gamma[\nu]\backslash G[\nu]} \\
&\quad + \Big(\nabla_{\Gamma_\xi}(n\cdot[\hat C]n)\cdot\partial_\xi\nabla_\Gamma S^{(\nu)}, \varphi|_{\xi=0}\Big)_{G[\nu]} \\
&\quad + \Big(\nabla_{\Gamma_\xi}(n\cdot[\hat C]n)\cdot(F_1^{(\nu)} + F_2^{(\nu)}), \varphi|_{\xi=0}\Big)_{G[\nu]} \\
&= J_{11} + J_{12} + J_{13}\,.
\end{aligned} \tag{5.29}$$

Since $\text{meas}\,(\Gamma[\nu]\backslash G[\nu]) \le K\nu^{3/4}$ we obtain from (4.16) that

$$|J_{11}| \le K\nu^{-1/2}\,\text{meas}\,(\Gamma[\nu]\backslash G[\nu]) \sup_{\Gamma[\nu]\backslash G[\nu]} |\varphi| \le \nu^{1/4}\,K\|\varphi\|_{L^\infty(Q)}\,. \tag{5.30}$$

From (5.25) and Claim 1 we conclude

$$|J_{13}| \le K\big(\frac{1}{M_1^2} + 1\big)\,\text{meas}\big(G[\nu]\big) \sup_{G[\nu]} |\varphi| \le \nu^{1/2} K\|\varphi\|_{L^\infty(Q)}\,. \tag{5.31}$$

To estimate J_{12} we transform the integral to (t,η,ξ)–coordinates and obtain with the Jacobi determinant $\omega(t,\eta,\xi) = |\det(\frac{\partial(t,x)}{\partial(t,\eta,\xi)})|$ that

$$\begin{aligned}
|J_{12}| &= \left|\Big(\nabla_{\Gamma_\xi}(n\cdot[\hat{C}]n)\cdot\partial_\xi\nabla_\Gamma S^{(\nu)}, \varphi|_{\xi=0}\Big)_{G[\nu]}\right| \\
&= \left|\int_\Gamma\int_{a_\nu(t,\eta)}^{d_\nu(t,\eta)} \omega(t,\eta,\xi)\nabla_{\Gamma_\xi}(n\cdot[\hat{C}]n)\cdot\partial_\xi\nabla_\Gamma S^{(\nu)}\varphi(t,\eta,0)\,d\xi\,d\sigma\right| \\
&= \Bigg|-\int_\Gamma\int_{a_\nu(t,\eta)}^{d_\nu(t,\eta)} \partial_\xi\Big(\omega(t,\eta,\xi)\nabla_{\Gamma_\xi}(n\cdot[\hat{C}]n)\Big)\cdot\nabla_\Gamma S^{(\nu)}\varphi(t,\eta,0)\,d\xi\,d\sigma \\
&\qquad + \int_\Gamma\Big[\omega(t,\eta,\xi)\nabla_{\Gamma_\xi}(n\cdot[\hat{C}]n)\cdot\nabla_\Gamma S^{(\nu)}\Big]_{\xi=a_\nu(t,\eta)}^{\xi=d_\nu(t,\eta)}\varphi(t,\eta,0)\,d\sigma\Bigg| \\
&\le K\sup_{(t,\eta)\in\Gamma}|\varphi(t,\eta,0)|\,\mathrm{meas}(\Gamma)\sup_{(t,\eta)\in\Gamma}\big(d_\nu(t,\eta)-a_\nu(t,\eta)\big) \\
&\qquad + K\sup_{(t,\eta)\in\Gamma}|\varphi(t,\eta,0)|\,\mathrm{meas}(\Gamma)\sup_{(t,\eta)\in\Gamma}\Big(|\nabla_\Gamma S^{(\nu)}|_{\xi=d_\nu(t,\eta)} + |\nabla_\Gamma S^{(\nu)}|_{\xi=a_\nu(t,\eta)}\Big) \\
&\le \nu^{1/2}K\|\varphi\|_{L^\infty(Q)} + \nu^{1/4}M_2K\|\varphi\|_{L^\infty(Q)}\,,
\end{aligned}$$

where in the last step we used Claim 2 and noted that $d_\nu(t,\eta) - a_\nu(t,\eta) \le \nu^{1/2}K$. Combination of (5.29) with the last inequality and with (5.30), (5.31) yields

$$|J_1| \le \nu^{1/4}K\|\varphi\|_{L^\infty(Q)}\,. \tag{5.32}$$

Noting again the estimate $\nabla_{\Gamma_\xi}(n\cdot[\hat{C}]n) \le K$ and employing (4.16) we obtain for the term J_2 in (5.22) and for all $\varphi \in C_0(Q)$ that

$$\begin{aligned}
\lim_{\nu\to 0}|J_2| &= \lim_{\nu\to 0}\left|c\Big(\nabla_{\Gamma_\xi}(n\cdot[\hat{C}]n)\cdot\nabla_\Gamma|\nabla_x S^{(\nu)}|, \varphi - \varphi|_{\xi=0}\Big)_{\Gamma[\nu]}\right| \\
&\le \lim_{\nu\to 0}\left(K\nu^{-1/2}\,\mathrm{meas}(\Gamma[\nu])\sup_{(t,\eta,\xi)\in\Gamma[\nu]}\big|\varphi(t,\eta,\xi)-\varphi(t,\eta,0)\big|\right) \\
&\le K\lim_{\nu\to 0}\sup_{\substack{(t,\eta)\in\Gamma\\ |\xi|\le C\nu^{1/2}}}\big|\varphi(t,\eta,\xi)-\varphi(t,\eta,0)\big| = 0\,,
\end{aligned}$$

where in the last step we used that $\varphi \in C_0(Q)$ is uniformly continuous. This relation and (5.22), (5.23), (5.32) together show that (5.20) is satisfied.

To prove (5.21) we estimate J_2 differently. Namely, since the Hölder continuity of $\varphi \in C_0^\alpha(Q)$ implies for $(t,\eta,\xi) \in \Gamma[\nu]$ that $|\varphi(t,\eta,\xi) - \varphi(t,\eta,0)| \le |\xi - 0|^\alpha\,\|\varphi\|_{C^\alpha(Q)} \le C\nu^{\alpha/2}\|\varphi\|_{C^\alpha(Q)}$, we obtain similarly as above

$$|J_2| \le K\sup_{(t,\eta,\xi)\in\Gamma[\nu]}\big|\varphi(t,\eta,\xi)-\varphi(t,\eta,0)\big| \le K\,\nu^{\alpha/2}\|\varphi\|_{C^\alpha(Q)}\,.$$

This estimate together with (5.22), (5.23), (5.32) yield (5.21). The proof of Lemma 5.4 is complete.

Proof of (1.50) **and** (1.51) **in Theorem 1.3.** We combine Lemma 5.1 and Lemma 5.3

to estimate the right hand side of (5.2). In this estimation we can either use the inequality (5.19) in Lemma 5.3 or the inequality (5.21) in Lemma 5.4 to bound the term I_4 in (5.17). This yields for every $\varphi \in C_0^1(Q)$

$$\big|\big(\partial_t S^{(\nu)}, \varphi\big)_Q + c\big(\nabla_x(\psi_S - \nu\Delta_x S^{(\nu)})|\nabla_x S^{(\nu)}|, \nabla_x\varphi\big)_Q\big| \leq \begin{cases} K\|\varphi\|_{C(Q)}\,, \\ K\nu^{\min(\frac{\alpha}{2},\frac{1}{4})}\|\varphi\|_{C^\alpha(Q)}\,. \end{cases}$$

(1.50) follows immediately from the second of these inequalities and from the definition of the norm $\|\cdot\|_{\mathfrak{R}_\alpha}$. To prove (1.51) we conclude from the first of these inequalities that

$$\|\partial_t S^{(\nu)} - c\,\mathrm{div}_x\big(\nabla_x(\psi_S - \nu\Delta_x S^{(\nu)})|\nabla_x S^{(\nu)}|\big)\|_{\mathfrak{R}} \leq K\,, \tag{5.33}$$

with a constant K independent of ν. We next combine (5.2), Lemma 5.1, Lemma 5.3 and the convergence relation (5.20) in Lemma 5.4 to obtain for every $\varphi \in C_0^1(Q)$ that

$$\big(\partial_t S^{(\nu)}, \varphi\big)_Q + c\big(\nabla_x(\psi_S - \nu\Delta_x S^{(\nu)})|\nabla_x S^{(\nu)}|, \nabla_x\varphi\big)_Q \to 0, \quad \text{if } \nu \to 0.$$

This can be written in the form

$$\int_Q \varphi\, d\left(\partial_t S^{(\nu)} - c\,\mathrm{div}_x\big(\nabla_x(\psi_S - \nu\Delta_x S^{(\nu)})|\nabla_x S^{(\nu)}|\big)\right) \to 0. \tag{5.34}$$

To extend this result to all $\varphi \in C(Q)$, we observe that $C_0^1(Q)$ is a dense subspace of $C(Q)$ and that the family $\{\partial_t S^{(\nu)} - c\,\mathrm{div}_x\big(\nabla_x(\psi_S - \nu\Delta_x S^{(\nu)})|\nabla_x S^{(\nu)}|\big)\}_{\nu>0}$ is uniformly bounded in $\mathfrak{R}$, by (5.33). Standard arguments then yield that (5.34) holds for all $\varphi \in C(Q)$. This proves (1.51).

6 Proof of Theorem 1.3, part II

To finish the proof of Theorem 1.3 it remains to verify the inequality (1.49). This section is devoted to this verification. We need the following auxiliary result:

Lemma 6.1 *There are constants $K_1, \ldots, K_5$ such that for all (t, η, ξ) and all $\nu > 0$ the estimates*

$$\big|\hat{S}(t,\eta,\xi) - S^{(\nu)}(t,\eta,\xi)\big| \leq \begin{cases} K_1, & \nu^{1/2}a(t,\eta) \leq \xi \leq \nu^{1/2}d(t,\eta), \\ 0, & \text{otherwise}, \end{cases} \tag{6.1}$$

$$\big|\langle\xi\rangle - S^{(\nu)(-1)}(t,\eta,\xi)\big| \leq K_2\nu^{1/2}, \tag{6.2}$$

$$\big|\nabla_{\Gamma_\xi}\big(\langle\xi\rangle - S^{(\nu)(-1)}(t,\eta,\xi)\big)\big| \leq K_3\nu^{1/2}, \tag{6.3}$$

$$\big|\nabla_{\Gamma_\xi}\partial_{\eta_j}\big(\langle\xi\rangle - S^{(\nu)(-1)}(t,\eta,\xi)\big)\big| \leq K_4\nu^{1/2}, \qquad j = 1,2, \tag{6.4}$$

$$\big|\nabla_{\Gamma_\xi}\partial_\xi\big(\langle\xi\rangle - S^{(\nu)(-1)}(t,\eta,\xi)\big)\big| \leq \begin{cases} K_5, & \nu^{1/2}a(t,\eta) \leq \xi \leq \nu^{1/2}d(t,\eta), \\ 0, & \text{otherwise}, \end{cases} \tag{6.5}$$

hold. Here $\langle\xi\rangle$ is defined in (1.21).

Proof: To verify (6.1) we note that by definition the functions $\hat{S}$ and $S^{(\nu)}$ both have the value 0 for $\xi \le \nu^{1/2}a(t,\eta)$ and the value 1 for $\nu^{1/2}d(t,\eta) \le \xi$. This property and (1.23) together imply (6.1). To prove (6.2) – (6.4) we use that $\langle\xi\rangle = \max(0,\xi)$, by definition. From (1.26) we thus conclude for $\nu^{1/2}a(t,\eta) \le \xi \le \nu^{1/2}d(t,\eta)$ that

$$\langle\xi\rangle - S^{(\nu)(-1)}(t,\eta,\xi) = \nu^{\frac{1}{2}}\Big(\frac{\max(0,\xi)}{\nu^{1/2}} - \sum_{i=0}^{2} \nu^{\frac{i}{2}} S_i^{(-1)}\big(t,\eta,\frac{\xi}{\nu^{1/2}}\big)\Big).$$

The inequalities (6.2) – (6.4) follow from this equation for this range of ξ, since $0 \le \max(0,\xi/\nu^{1/2}) \le d(t,\eta) \le C$ and since the surface gradient ∇_{Γ_ξ} and the differential operator $\nabla_{\Gamma_\xi}\partial_{\eta_j}$ contain only derivatives with respect to η. To show the inequalities (6.2) – (6.4) for ξ satisfying $\nu^{1/2}d(t,\eta) \le \xi$ we use that for such ξ we have $S^{(\nu)}(t,\eta,\xi) = 1$. Together with (1.26) we therefore compute

$$\begin{aligned}
&\langle\xi\rangle - S^{(\nu)(-1)}(t,\eta,\xi) \\
&= \xi - \int_0^{\xi} S^{(\nu)}(t,\eta,\zeta)d\zeta \\
&= \xi - \int_0^{\nu^{1/2}d(t,\eta)} S^{(\nu)}(t,\eta,\zeta)d\zeta - \int_{\nu^{1/2}d(t,\eta)}^{\xi} S^{(\nu)}(t,\eta,\zeta)d\zeta \\
&= \nu^{1/2}d(t,\eta) - S^{(\nu)(-1)}\big(t,\eta,\nu^{1/2}d(t,\eta)\big) \\
&= \nu^{1/2}\Big(d(t,\eta) - \sum_{i=0}^{2} \nu^{\frac{i}{2}} S_i^{(-1)}\big(t,\eta,d(t,\eta)\big)\Big).
\end{aligned}$$

The inequalities (6.2) – (6.4) follow from this equation as above. To prove these inequalities for $\xi \le \nu^{1/2}a(t,\eta)$ we use that $\langle\xi\rangle = S^{(\nu)}(t,\eta,\xi) = 0$ in this range of ξ to get in the same way

$$\langle\xi\rangle - S^{(\nu)(-1)}(t,\eta,\xi) = -\nu^{1/2}\sum_{i=0}^{2} \nu^{\frac{i}{2}} S_i^{(-1)}\big(t,\eta,a(t,\eta)\big),$$

from which equation the estimates follow. To prove (6.5) we note that

$$\nabla_{\Gamma_\xi}\partial_\xi\big(\langle\xi\rangle - S^{(\nu)(-1)}(t,\eta,\xi)\big) = -\nabla_{\Gamma_\xi} S^{(\nu)}(t,\eta,\xi). \tag{6.6}$$

(1.23) yields for $\nu^{1/2}a(t,\eta) \le \xi \le \nu^{1/2}d(t,\eta)$ that

$$\Big|\nabla_{\Gamma_\xi} S^{(\nu)}(t,\eta,\xi)\Big| = \Big|\nabla_{\Gamma_\xi} \sum_{i=0}^{2} \nu^{i/2} S_i\big(t,\eta,\frac{\xi}{\nu^{1/2}}\big)\Big| \le K_5. \tag{6.7}$$

Since $S^{(\nu)}(t,\eta,\xi)$ is equal to 0 or 1 for ξ outside of the interval $\big(\nu^{1/2}a(t,\eta),\nu^{1/2}d(t,\eta)\big)$, the estimate (6.5) follows by combination of (6.6) and (6.7). This finishes the proof of the Lemma.

Corollary 6.2 *For all $\nu > 0$ and $i = 1,2,3$ the function $\langle\xi\rangle - S^{(\nu)(-1)}$ satisfies*

$$\Big|\nabla_x\big(\langle\xi\rangle - S^{(\nu)(-1)}(t,\eta,\xi)\big)\Big| \le \begin{cases} K_6, & \nu^{1/2}a(t,\eta) \le \xi \le \nu^{1/2}d(t,\eta), \\ K_7\nu^{1/2}, & \text{otherwise}, \end{cases} \tag{6.8}$$

$$\Big|\partial_{x_i}\nabla_{\Gamma_\xi}\big(\langle\xi\rangle - S^{(\nu)(-1)}(t,\eta,\xi)\big)\Big| \le \begin{cases} K_8, & \nu^{1/2}a(t,\eta) \le \xi \le \nu^{1/2}d(t,\eta), \\ K_9\nu^{1/2}, & \text{otherwise}, \end{cases} \tag{6.9}$$

Proof: Since $\nabla_x = n(t,\eta)\big(n(t,\eta)\cdot\nabla_x\big) + \nabla_{\Gamma_\xi} = n(t,\eta)\partial_\xi + \nabla_{\Gamma_\xi}$, and since

$$\partial_{x_i}\nabla_{\Gamma_\xi} = \sum_{|\alpha|=2} e_{(\alpha,0)}\partial_\eta^\alpha + \sum_{|\alpha|=1} e_{(\alpha,1)}\partial_\eta^\alpha\partial_\xi + e_{(0,1)}\partial_\xi$$

with suitable vectors $e_{(\alpha,j)}(t,\eta,\xi) \in \mathbb{R}^3$, the statement follows immediately from the estimates (6.1), (6.3) – (6.5), if we also note that $\partial_\xi\big(\langle\xi\rangle - S^{(\nu)(-1)}\big) = \hat{S} - S^{(\nu)}$.

Lemma 6.3 *Let $\hat{u}$, $\hat{T}$, $\hat{S}$ satisfy* (1.4) *and let u^*, v be defined in* (1.18) *and in* (1.20)*, respectively. Then*

$$\begin{aligned}\hat{T} &= D\big(\varepsilon(\nabla_x\hat{u}) - \overline{\varepsilon}\hat{S}\big)\\ &= [\hat{T}]\,\hat{S}\,\phi + D\varepsilon(\nabla_x v) - D\overline{\varepsilon}\,(1-\phi)\hat{S}\\ &\quad + D\varepsilon\big(\hat{\nabla}_{\Gamma_\xi}(u^*\langle\xi\rangle)\big)\,\phi + \langle\xi\rangle D\varepsilon(u^*\otimes\nabla_x\phi),\end{aligned} \tag{6.10}$$

where $[\hat{T}] = [\hat{T}](t,\eta)$, $u^* = u^*(t,\eta)$. All other functions have the argument (t,x) with $x = \eta + n(t,\eta)\xi$.

The proof of this lemma is almost the same as the proof of Lemma 3.1.

Lemma 6.4 *There is a constant K such that for all $\nu > 0$ and all $\varphi \in C_0^1(Q)$*

$$\big|(T^{(\nu)},\nabla_x\varphi)_Q - (b,\varphi)_Q\big| \le K\nu^{1/2}\|\varphi\|_{C(Q)}\,. \tag{6.11}$$

Proof. We subtract (3.1) from (6.10) to obtain

$$\begin{aligned}\hat{T} - T^{(\nu)} &= [\hat{T}](\hat{S} - S^{(\nu)})\phi - D\overline{\varepsilon}(1-\phi)(\hat{S} - S^{(\nu)})\\ &\quad + D\varepsilon\Big(\hat{\nabla}_{\Gamma_\xi}\big(u^*(\langle\xi\rangle - S^{(\nu)(-1)})\big)\Big)\phi\\ &\quad + \big(\langle\xi\rangle - S^{(\nu)(-1)}\big)D\varepsilon(u^*\otimes\nabla_x\phi)\\ &= [\hat{T}](\hat{S} - S^{(\nu)})\\ &\quad + \big(\langle\xi\rangle - S^{(\nu)(-1)}\big)\Big(D\varepsilon\big(\hat{\nabla}_{\Gamma_\xi}u^*\big)\phi + D\varepsilon(u^*\otimes\nabla_x\phi)\Big)\\ &\quad + \phi D\varepsilon\Big(u^*\otimes\nabla_{\Gamma_\xi}\big(\langle\xi\rangle - S^{(\nu)(-1)}\big)\Big)\\ &= I_1 + I_2 + I_3.\end{aligned} \tag{6.12}$$

To obtain the second equality sign we used that ϕ is equal to one in a neighborhood of Γ, from which it follows by (6.1) that for all sufficiently small $\nu > 0$ we have $\hat{S} - S^{(\nu)} = 0$ in the region where $\phi \neq 1$. We next use that $\hat{T}$ satisfies $(\hat{T},\nabla_x\varphi)_Q - (b,\varphi)_Q = 0$ for all $\varphi \in C_0^1(Q,\mathbb{R}^3)$. From (6.12) we therefore deduce

$$\begin{aligned}(b,\varphi)_Q - (T^{(\nu)},\nabla_x\varphi)_Q &= (\hat{T} - T^{(\nu)},\nabla_x\varphi)_Q \;=\; (I_1 + I_2 + I_3,\nabla_x\varphi)_Q\\ &= (I_1,\nabla_x\varphi)_Q - (\operatorname{div}_x(I_2 + I_3),\varphi)_Q\,.\end{aligned} \tag{6.13}$$

We estimate both terms on the right hand side separately. Note first that from the definition of I_2 and I_3 in (6.12) we obtain by application of the chain rule and by using the estimates (6.2), (6.3), (6.8) and (6.9) that

$$|\mathrm{div}_x(I_2+I_3)| \leq \begin{cases} K, & (x,t)\in\Gamma[\nu], \\ K\nu^{1/2}, & elsewhere. \end{cases}$$

This implies

$$|(\mathrm{div}_x(I_2+I_3),\varphi)_Q| \leq \Big(K_1\nu^{1/2}+K_2\mathrm{meas}(\Gamma[\nu])\Big)\,\|\varphi\|_{C(Q)} \leq K_3\nu^{1/2}\|\varphi\|_{C(Q)}\,. \tag{6.14}$$

Observe next that $\hat S$ is piecewise constant with the jump $[\hat S]=1$ along Γ and that $[\hat T]=[\hat T](t,\eta)$ with $[\hat T]n=0$. This yields

$$\begin{aligned}(I_1,\nabla_x\varphi)_Q &= \int_Q[\hat T](\hat S-S^{(\nu)})\nabla\varphi\,d(t,x) = \int_0^{T_e}\int_{\Gamma(t)}[\hat T]n\,\varphi\,d\sigma_x dt \\ &\quad -\int_{Q\setminus\Gamma}\mathrm{div}_x\Big([\hat T](t,\eta)\big(\hat S-S^{(\nu)}\big)(t,x)\Big)\,\varphi(t,x)\,d(t,x) \\ &= -\int_{\Gamma[\nu]\setminus\Gamma}\mathrm{div}_x\Big([\hat T](t,\eta)\big(\hat S-S^{(\nu)}\big)(t,x)\Big)\,\varphi(t,x)\,d(t,x).\end{aligned} \tag{6.15}$$

In the last step we used that $\hat S-S^{(\nu)}=0$ outside of $\Gamma[\nu]$, by (6.1). In the next computation we employ that $\nabla_x=n(t,\eta)\partial_\xi+\nabla_{\Gamma_\xi}$. In this computation we omit the arguments (t,η) and (t,x) for simplicity in notation. We obtain

$$\begin{aligned}\mathrm{div}_x\Big([\hat T]\big(\hat S-S^{(\nu)}\big)\Big) &= \big(\mathrm{div}_x[\hat T]\big)\big(\hat S-S^{(\nu)}\big)+[\hat T]\nabla_x\big(\hat S-S^{(\nu)}\big) \\ &= \big(\mathrm{div}_x[\hat T]\big)\big(\hat S-S^{(\nu)}\big)-[\hat T]n\,\partial_\xi S^{(\nu)}-[\hat T]\,\nabla_{\Gamma_\xi}S^{(\nu)} \\ &= \big(\mathrm{div}_x[\hat T]\big)\big(\hat S-S^{(\nu)}\big)-[\hat T]\,\nabla_{\Gamma_\xi}S^{(\nu)}.\end{aligned} \tag{6.16}$$

Here we used again that $[\hat T]n=0$ and that $\hat S$ is piecewise constant. Since ∇_{Γ_ξ} only contains derivatives with respect to η, we have $|\nabla_{\Gamma_\xi}S^{(\nu)}|\leq K$ with a constant K independent of ν. Together with (6.1) it follows that the function on the right hand side of (6.16) is bounded on $\Gamma[\nu]$, uniformly with respect to ν. From (6.15) we thus conclude that

$$|(I_1,\nabla_x\varphi)_Q| \leq K_1\,\mathrm{meas}(\Gamma[\nu])\,\|\varphi\|_{C(Q)} \leq K_2\nu^{1/2}\|\varphi\|_{C(Q)}\,.$$

Combination of this estimate with (6.13) and (6.14) yields the statement of the lemma. The proof is complete.

Proof of (1.49)**.** The inequality (1.49) follows immediately from (6.11) and from the definition of the norm $\|\cdot\|_{\mathfrak{R}}$. This finishes the proof of Theorem 1.3.

7 The sharp interface model for interface diffusion driven by a free energy with bulk terms.

Here we discuss the formulation of a general model for the evolution of a sharp interface in a solid body separating material phases, for which the free energy consists of a sum of the interface energy and the bulk energy. If the interface energy is neglected, the model reduces to the sharp interface model (1.3) – (1.7). We use the notations introduced in Section 1.

The formulation is based on the second law of thermodynamics, which requires that to the mechanical system formed by the solid body a free energy density ψ^* and a flux q must be associated such that during the evolution of the system the Clausius-Duhem inequality

$$\frac{\partial}{\partial t}\psi^* + \operatorname{div}_x q \le b \cdot u_t \tag{7.1}$$

is satisfied. If the free energy and the flux are found, then as usual this inequality places a restriction on the form of the constitutive equation, which in our case is the equation for the normal speed of the interface. To find the free energy we first note the well known fact that the total free energy associated to the system modeled by (1.1) is the interface energy

$$\Psi(t) = c_1 \int_{\Gamma(t)} d\sigma. \tag{7.2}$$

This means that the solid body is considered to be rigid; the always present elasticity of the body, which contributes bulk terms to the total free energy, is neglected. If we add the free energy associated to small elastic deformations we obtain for the total free energy the expression

$$\Psi(t) = \int_\Omega \frac{1}{2}\Big(D\big(\varepsilon(\nabla_x u(t,x)) - \overline{\varepsilon} S(t,x)\big)\Big) \cdot \big(\varepsilon(\nabla_x u(t,x)) - \overline{\varepsilon} S(t,x)\big) dx + c_1 \int_{\Gamma(t)} d\sigma. \tag{7.3}$$

with a constant $c_1 \ge 0$.

To apply (7.1) we need the density $\tilde{\psi}(t)$ of this free energy. Yet, since $\Psi(t)$ contains the integral over the interface $\Gamma(t)$, a two-dimensional manifold in the three-dimensional space of Lebesgue measure zero, $\Psi(t)$ cannot be written as an integral with respect to the three dimensional Lebesgue measure over a density function. Therefore we must generalize (7.1) to densities, which are measures. Below we show that this generalization is naturally possible. For the density of $\Psi(t)$ we thus take the measure

$$\psi^*(t) = \psi_1(t,\cdot)\,\lambda + c_1\,\mathcal{H}_2 \lfloor \Gamma(t),$$

where λ is the three dimensional Lebesgue measure, the density function $\psi_1 : [0,\infty) \times \Omega \to [0,\infty)$ is given by

$$\psi_1(t,x) = \frac{1}{2}\Big(D\big(\varepsilon(\nabla_x u(t,x)) - \overline{\varepsilon} S(t,x)\big)\Big) \cdot \big(\varepsilon(\nabla_x u(t,x)) - \overline{\varepsilon} S(t,x)\big),$$

and $\mathcal{H}_2 \lfloor \Gamma(t)$ denotes the restriction of the two-dimensional Hausdorff measure on $\mathbb{R}^3$ to the surface $\Gamma(t)$. By definition we thus have for measurable subsets $V \subseteq \mathbb{R}^3$ that

$$\big(\mathcal{H}_2 \lfloor \Gamma(t)\big)(V) = \mathcal{H}_2\big(\Gamma(t) \cap V\big) = \int_{\Gamma(t)\cap V} d\sigma(x).$$

Here and in the following we assume that $\Gamma(t)$ is sufficiently smooth such that the Lebesgue surface measure σ is defined on $\Gamma(t)$. Since atoms diffuse along the interface and transport energy, also the flux must have an interface part. For the flux we thus take the measure

$$q(t) = -(Tu_t)\,\lambda + \Big(c_1 sn - c\big(n\cdot[\hat{C}]n + 2c_1\kappa\big)\,\nabla_\Gamma\big(n\cdot[\hat{C}]n + 2c_1\kappa\big)\Big)\,\mathcal{H}_2 \lfloor \Gamma(t), \tag{7.4}$$

with a non-negative constant c and with the normal velocity $s = s(t,x)$ of $\Gamma(t)$ at $x \in \Gamma(t)$ in direction of the unit normal vector $n(t,x)$. Note that $-Tu_t$, which denotes the matrix product, is the ordinary flux of the free energy used in elasticity theory.

To extend (7.1) to measures, we use that the measures ψ^* and q define distributions on $C_0^\infty((0,\infty)\times\Omega,\mathbb{R})$ and on $C_0^\infty((0,\infty)\times\Omega,\mathbb{R}^3)$, respectively, which we again denote by ψ^* and q. The derivatives in (7.1) are then taken in the distributional sense. Precisely, for $\varphi \in C_0^\infty((0,\infty)\times\Omega,\mathbb{R})$ or $\varphi \in C_0^\infty((0,\infty)\times\Omega,\mathbb{R}^3)$ we define

$$(\psi^*,\varphi) = \int_0^\infty \int_\Omega \varphi(t)d\psi^*(t)dt = \int_0^\infty \Big(\int_\Omega \psi_1(t,x)\varphi(t,x)dx + c_1\int_{\Gamma(t)} \varphi(t,x)d\sigma(x)\Big)dt,$$

$$(q,\varphi) = \int_0^\infty \int_\Omega \varphi(t)\cdot dq(t)dt = \int_0^\infty \Big(-\int_\Omega (Tu_t)\cdot\varphi(t)dxdt + \int_{\Gamma(t)} \Big(c_1 s\, n - c(n\cdot[\hat{C}]n + 2c_1\kappa)\,\nabla_\Gamma(n\cdot[\hat{C}]n + 2c_1\kappa)\Big)\cdot\varphi(t,x)d\sigma(x)\Big)dt.$$

Theorem 7.1 *Assume that (u,T,S) is a solution of the sharp interface problem*

$$-\mathrm{div}_x T = b, \tag{7.5}$$
$$T = D(\varepsilon(\nabla_x u) - \bar{\varepsilon}S), \tag{7.6}$$
$$s = -c\,\Delta_\Gamma(n\cdot[\hat{C}]n + 2c_1\kappa), \tag{7.7}$$
$$[u] = 0, \tag{7.8}$$
$$[T]n = 0, \tag{7.9}$$

where $S(t,x)$ only takes the values 0 and 1 with a jump at $\Gamma(t)$, and the unit normal vector $n(t,x) \in \mathbb{R}^3$ points into the region where $S = 1$. Then the Clausius-Duhem inequality (7.1) holds in the distributional sense. This means that for all $\varphi \in C_0^\infty((0,\infty)\times\Omega,[0,\infty))$ we have

$$(\psi_t^* + \mathrm{div}_x q - b\cdot u_t, \varphi) = -(\psi,\varphi_t) - (q,\nabla_x\varphi) - (b\cdot u_t,\varphi) \le 0.$$

For the proof we need two auxiliary results:

Lemma 7.2 *If (u,T,S) satisfies the equations (7.5), (7.6), (7.8), (7.9), then in the sense of distributions*

$$(\partial_t\psi_1 - \mathrm{div}_x(Tu_t) - b\cdot u_t, \varphi) = -\int_0^\infty \int_{\Gamma(t)} (n\cdot[\hat{C}]n)s\varphi\, d\sigma(x)dt. \tag{7.10}$$

This lemma is proved in [1].

Lemma 7.3 *Assume that Γ is a sufficiently smooth three-dimensional surface in $(0,\infty)\times\Omega$ such that the normal velocity $s(t,x)$ is different from zero at every $x \in \Gamma(t)$. Then we have for every $\varphi \in C_0^\infty((0,\infty)\times\Omega)$ that*

$$\int_0^\infty \int_{\Gamma(t)} \varphi_t\, d\sigma(x)dt = \int_0^\infty \int_{\Gamma(t)} s\,\big(2\kappa\varphi - \frac{\partial}{\partial n}\varphi\big)\, d\sigma(x)dt. \tag{7.11}$$

Proof: Let t_0 be a given time. If Γ is sufficiently regular and if s is everywhere different from zero we can choose $\delta > 0$ small enough such that for all times $t_1 \neq t_2$ with $|t_i - t_0| < \delta$ the subsets $\Gamma(t_1)$ and $\Gamma(t_2)$ of $\mathbb{R}^3$ are disjoint. This implies that to every x from the set

$$\Lambda = \Big(\bigcup_{|t-t_0|<\delta} \Gamma(t) \Big) \subseteq \mathbb{R}^3$$

there is a unique $t(x)$ such that $x \in \Gamma(t(x))$. Therefore we can define a vector field $m : \Lambda \to \mathbb{R}^3$ by

$$m(x) = s(t(x), x)\, n(t(x), x).$$

For $x_0 \in \Gamma(t_0)$ let $t \mapsto x(t, x_0)$ be the integral curve of the vector field m such that $x(t_0, x_0) = x_0$. then $x_0 \mapsto x(t, x_0) : \Gamma(t_0) \to \Gamma(t)$ is a parametrization of the surface $\Gamma(t)$ and

$$x_t(t, x_0) = s(t, x(t, x_0))\, n(t, x(t, x_0)) \tag{7.12}$$

is a normal vector to $\Gamma(t)$ at $x(t, x_0)$. Moreover, there is a function ω such that

$$\int_{\Gamma(t)'} d\sigma(x) = \int_{\Gamma(t_0)'} \omega(t, x_0)\, d\sigma(x_0)$$

for every measurable subset $\Gamma(t_0)'$ of $\Gamma(t_0)$ and for the image $\Gamma(t)'$ of $\Gamma(t_0)'$ under the mapping $x_0 \mapsto x(t, x_0)$. Since

$$\int_{\Gamma(t_0)'} \omega_t(t, x_0) d\sigma(x_0) = \frac{d}{dt} \int_{\Gamma(t_0)'} \omega(t, x_0) d\sigma(x_0) = \frac{d}{dt} \int_{\Gamma(t)'} d\sigma(x),$$

and since it is well known that

$$\begin{aligned}\frac{d}{dt} \int_{\Gamma(t)'} d\sigma(x) &= -\int_{\Gamma(t)'} 2s(t, x)\kappa(t, x) d\sigma(x) \\ &= -\int_{\Gamma(t_0)'} 2s(t, x(t, x_0))\kappa(t, x(t, x_0))\omega(t, x_0) d\sigma(x_0),\end{aligned}$$

it follows that $\omega_t = -2s\kappa\omega$. Now let $\varphi \in C_0^\infty((0, \infty) \times \Lambda, \mathbb{R})$. Then

$$\begin{aligned}\int_0^\infty \int_{\Gamma(t)} \varphi_t d\sigma dt &= \int_0^\infty \int_{\Gamma(t_0)} \varphi_t(t, x(t, x_0))\omega(t, x_0) d\sigma(x_0) dt \\ &= \int_0^\infty \int_{\Gamma(t_0)} \Big(\frac{d}{dt} \varphi(t, x(t, x_0)) - \nabla_x \varphi(t, x(t, x_0)) \cdot x_t \Big) \omega(t, x_0) d\sigma(x_0) dt \\ &= \int_0^\infty \int_{\Gamma(t_0)} \Big(-\varphi(t, x(t, x_0))\omega_t(t, x_0) + (sn \cdot \nabla_x \varphi)\omega \Big) d\sigma(x_0) dt \\ &= \int_0^\infty \int_{\Gamma(t_0)} \big(2s\kappa\varphi\omega - s \frac{\partial}{\partial n} \varphi\omega \big)\, d\sigma(x_0) dt \\ &= \int_0^\infty \int_{\Gamma(t)} \big(2s\kappa\varphi - s \frac{\partial}{\partial n} \varphi \big)\, d\sigma(x) dt.\end{aligned}$$

To obtain the third equality we used (7.12). This proves the statement of the lemma.

Proof of Theorem 7.1. For $x \in \Gamma(t)$ we have the decomposition

$$\nabla_x \varphi(t,x) = n(t,x)\,(n(t,x)\cdot\nabla_x\varphi(t,x)) + \nabla_\Gamma\,\varphi(t,x).$$

Since $n(t,x)$ is orthogonal to the vectors $\nabla_\Gamma\varphi$ and $\nabla_\Gamma\kappa$ we therefore obtain

$$\Big(c_1 s\, n - c(n\cdot[\hat{C}]n + 2c_1\kappa)\,\nabla_\Gamma(n\cdot[\hat{C}]n + 2c_1\kappa)\Big)\cdot\nabla_x\varphi$$
$$= c_1 s\,\frac{\partial}{\partial n}\varphi - c(n\cdot[\hat{C}]n + 2c_1\kappa)\,\nabla_\Gamma(n\cdot[\hat{C}]n + 2c_1\kappa)\cdot\nabla_\Gamma\varphi.$$

Stokes' theorem thus yields

$$\int_{\Gamma(t)}\Big(c_1 s\, n - c(n\cdot[\hat{C}]n + 2c_1\kappa)\,\nabla_\Gamma(n\cdot[\hat{C}]n + 2c_1\kappa)\Big)\cdot\nabla_x\varphi\, d\sigma(x)$$
$$= \int_{\Gamma(t)} c_1 s\,\frac{\partial}{\partial n}\varphi + c\,\mathrm{div}_\Gamma\Big((n\cdot[\hat{C}]n + 2c_1\kappa)\,\nabla_\Gamma(n\cdot[\hat{C}]n + 2c_1\kappa)\Big)\varphi\, d\sigma(x).$$

We note the definition of the distributions ψ^* and q and combine the last equation with (7.10) and (7.11) to obtain for $\varphi \in C_0^\infty((0,\infty),[0,\infty))$

$$
\begin{aligned}
&-(\psi^*,\partial_t\varphi) - (q,\nabla_x\varphi) - (b\cdot u_t,\varphi)\\
&= \big(\partial_t\psi_1 - \mathrm{div}_x(Tu_t) - b\cdot u_t,\varphi\big) - \int_0^\infty\int_{\Gamma(t)} c_1\big(\partial_t\varphi + s\,\frac{\partial}{\partial n}\varphi\big)\, d\sigma(x)\, dt\\
&\quad - \int_0^\infty\int_{\Gamma(t)} c\,\mathrm{div}_\Gamma\Big(\big(n\cdot[\hat{C}]n + 2c_1\kappa\big)\,\nabla_\Gamma\big(n\cdot[\hat{C}]n + 2c_1\kappa\big)\Big)\varphi\, d\sigma(x)dt\\
&= -\int_0^\infty\int_{\Gamma(t)} s\big(n\cdot[\hat{C}]n + 2c_1\kappa\big)\varphi\, d\sigma(x)dt\\
&\quad - \int_0^\infty\int_{\Gamma(t)} c\,\Big|\nabla_\Gamma\big(n\cdot[\hat{C}]n + 2c_1\kappa\big)\Big|^2\varphi\, d\sigma(x)dt\\
&\quad - \int_0^\infty\int_{\Gamma(t)} c\,\big(n\cdot[\hat{C}]n + 2c_1\kappa\big)\,\Delta_\Gamma\big(n\cdot[\hat{C}]n + 2c_1\kappa\big)\,\varphi\, d\sigma(x)dt\\
&= -\int_0^\infty\int_{\Gamma(t)} c\,\Big|\nabla_\Gamma\big(n\cdot[\hat{C}]n + 2c_1\kappa\big)\Big|^2\varphi\, d\sigma(x)dt \le 0\,.
\end{aligned}
\tag{7.13}
$$

To get the last equality sign we inserted $s = -c\,\Delta_\Gamma\big(n\cdot[\hat{C}]n + 2c_1\kappa\big)$ from (7.7). This proves Theorem 7.1.

Remarks. Of course, if $c_1 = 0$ in (7.3), then the sharp interface problem (7.5) – (7.9) reduces to (1.3) – (1.7). On the other hand, if the solid body is rigid, then no elastic displacements occur. Hence, the bulk term in (7.3) vanishes and the free energy is reduced to (7.2). The free energy density and the flux take the form

$$\psi^*(t) = c_1\mathcal{H}_2\,\lfloor\,\Gamma(t),\quad q(t) = c_1 s n - c(2c_1\kappa)\,\nabla_\Gamma(2c_1\kappa)\,\mathcal{H}_2\,\lfloor\,\Gamma(t).$$

The above considerations are still valid for this new free energy and flux with obvious simplifications. It turns out that the Clausius-Duhem inequality is satisfied if the normal velocity s satisfies the constitutive equation $s = -cc_1\Delta_\Gamma\kappa$. This is (1.1).

From (7.13) it seems that the constitutive equation for s must necessarily have the form (7.7). This is not the case, however, since the flux $q(t)$ can be chosen in various ways different from (7.4).

In [4] it is shown that also for the diffusive interface model (1.10) – (1.12) the Clausius-Duhem inequality is satisfied if one chooses for the free energy ψ^* and the flux q the expressions

$$\psi^*(\varepsilon, S, \nabla_x S) = \psi(\varepsilon, S) + \frac{\nu}{2}|\nabla_x S|^2,$$

$$q(u_t, S_t, \varepsilon, \nabla_x \varepsilon, S, \dots, \nabla_x^3 S) = -Tu_t - \nu S_t \nabla_x S - c(\psi_S - \nu\Delta_x S)\nabla_x(\psi_S - \nu\Delta_x S)\,|\nabla_x S|,$$

with ψ given by (1.9). For more details we refer to [4].

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