Diffuse interface models for incompressible two-phase flows with different densities

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Abstract Diffuse interface models have become an important analytical and numerical method to model two-phase flows. In this contribution we review the subject and discuss in detail a thermodynamically consistent model with a divergence free velocity field for two-phase flows with different densities. The model is derived using basic thermodynamical principles, its sharp interface limits are stated, existence results are given, different numerical approaches are discussed and computations showing features of the model are presented.

1 Introduction

A fundamental problem in fluid dynamics involves changes in topology of interfaces between immiscible or partially miscible fluids. Topological transitions such as pinch off and reconnection of fluid interfaces are important features of many systems and strongly affect the flow. Classical models based on sharp interface approaches typically fail to describe these phenomena. Although sometimes so called reconnection conditions can be formulated it is often not possible to justify them based on physical principles. An approach allowing for topological transitions is based on the level set method [45] which also allows for several computationally efficient discretizations. But also for the level set approach it is not clear whether topological transitions are described in a way which is based on physical principles. For example results often depend on discretization parameters and on the kind of "smoothing" applied.

Another so called implicit formulation is the volume of fluid method (VOF-method), see, e.g., [35]. Here, a so called color function is passively advected by

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the flow. This color function typically has no physical significance and dissipation inequalities are usually not known.

In recent years diffuse interface models turned out to be a promising approach to describe phenomena like droplet coalescence or droplet break-up. In diffuse interface (or phase field) methods an order parameter is introduced which allows for a mixing in an interfacial zone such that the sharp interface is replaced by a thin interfacial layer in which the order parameter, which can be a concentration, rapidly changes its value, see [42], [37],[19],[39], [24], [3], [26], [38]. The diffuse interface approach turns out to be an attractive approach to model and to numerically simulate fluid interfaces.

In the literature, diffuse interface models are well established for two-phase flows of liquids with identical ("matched") densities. A first diffuse-interface model for two-phase flows of liquids with identical ("matched") densities was introduced by Hohenberg and Halperin [36]. In the general case, when the densities are different, several approaches have been discussed in the literature. Lowengrub and Truskinovsky [42] derived quasi-incompressible models, where the corresponding velocity field is not divergence free. On the other hand, Ding et al. [24] proposed a model with solenoidal fluid velocities which is not known to be thermodynamically consistent. Finally, we also mention the work of Aki et al. [14], who derived a diffuse-interface model for a two-phase flow with non-matched densities and a velocity field which is not divergence free.

The first three authors of this contribution proposed a thermodynamically consistent diffuse interface model which is based on a divergence free velocity, see [9]. The new model over the last years has been analyzed with respect to existence of weak and strong solutions, see [6, 7, 5, 46]. In order to show existence of weak solutions it is important that the model introduced in [9] is thermodynamically consistent and hence allows for a global energy inequality which can be used to obtain a priori estimates. The energy inequality is also important for the development of stable numerical schemes. In [30] fully discrete finite-element schemes for the model introduced in [9] have been developed and due to a priori estimates relying on the energy estimate Grün [29] was able to show convergence of discrete solutions. Later Garcke, Hinze, Kahle [28] and Grün, Guillén-González, Metzger [32] were able to derive simpler to solve stable and linear, and respectively, fully decoupled time discretizations for the model in [9].

In general, the evolution of fluid interfaces is influenced by many effects. Species or heat transport at the interfaces strongly affects the interface, e.g., because the surface tension depends on a surfactant concentration or on the temperature at the interfaces. The latter will lead to Marangoni effects at the interface. If in addition a surface active species diffuses on the interfaces, one has to consider convection and diffusion on the interface itself. All these additional effects can in principle be incorporated within a diffuse interface model for fluid interfaces. But so far in the literature only few results with respect to the modelling, analysis and numerics of these phenomena using a diffuse interface approach are known. We will discuss a simple case of transport at the interface in this contribution and refer to the companion contributions [10] and [31] for surfactant transport and micro-macro-models for

transport across fluidic interfaces. Moreover, in [22] the model has been extended to ion transport – this way modeling dynamic electrowetting and other electrokinetic phenomena.

The outline of this paper is as follows. In the following section we derive the thermodynamically consistent phase field model for two-phase flows. Section 3 gives an overview about known analytic results for the model. In Section 4 stable and convergent fully discrete schemes are introduced, convergence results are stated, and a numerical computation is presented.

2 Diffuse interface models for two-phase flows

2.1 Earlier models

Before we discuss the diffuse interface models, let us recall the governing equations for the two-phase incompressible fluid flow in a classical sharp interface model. In the bulk, i.e., in open sets $\Omega_\pm$ which are separated by an interface Γ, one requires

$$\begin{aligned} \operatorname{div} \mathbf{v} &= 0\,, \\ \partial_t(\rho\mathbf{v}) + \operatorname{div}(\rho\mathbf{v}\otimes\mathbf{v}) + \nabla p &= \operatorname{div}\mathbf{S} + \rho\mathbf{g}\,, \end{aligned}$$

where $\mathbf{v}$ is the fluid velocity, ρ is the mass density, p is the pressure, $\mathbf{g}$ describes volume forces and $\mathbf{S}$ is the viscous stress tensor given as

$$\mathbf{S} = 2\eta\mathbf{D}\mathbf{v}, \quad \mathbf{D}\mathbf{v} = \frac{1}{2}(\nabla\mathbf{v} + (\nabla\mathbf{v})^T)\,.$$

At the interface Γ the jump conditions

$$[\mathbf{v}]_-^+ = 0,\ [-\mathbf{S}]_-^+\nu + [p]_-^+\nu = \sigma\kappa\nu + \nabla_\Gamma\sigma$$

have to hold. Here $[.]_-^+$ is the jump across the interface, σ is the surface energy density, κ is the mean curvature (i.e., the sum of the principal curvatures) of the interface Γ, ν is a unit normal to the interface Γ and ∇_Γ is the surface gradient. The term $\nabla_\Gamma\sigma$ takes effects due to a variable surface energy density into account and a non-zero $\nabla_\Gamma\sigma$ leads to Marangoni effects.

In a diffuse interface model, one allows for a partial mixing of the fluids on a small length scale. For systems where the two fluids have densities of a similar size such models are referred to as *model H* in the literature, see [36]. In the case of equal density, a derivation of the diffuse interface model was given by Gurtin, Polignone and Vinals [34] in the context of rational continuum mechanics.

In two-fluid flow, often the situation appears that both fluids are incompressible with a large density difference. This was the motivation of Lowengrub and Truskinovsky [42] to introduce so called quasi-incompressible diffuse interface models for two-fluid flow. The assumptions made are that both fluids are incompressible

but in zones where the fluids mix a variable density is allowed and the velocity field is no longer divergence free. Lowengrub and Truskinovsky [42] introduce a mass concentration field c. The mass ρ is assumed to be independent of the pressure p (and vice versa), which is the assumption of *quasi-incompressibility*. The mass ρ is then postulated to be a function of c and in the case of a simple mixture the mixture relation is

$$\frac{1}{\rho(c)} = \frac{c}{\rho_-} + \frac{1-c}{\rho_+}$$

where ρ_- and ρ_+ are the mass densities of the two fluids involved. Then Lowengrub and Truskinovsky derived the system

$$\begin{aligned} D_t\rho + \rho \operatorname{div} \mathbf{v} = 0, \quad \rho D_t c + \nabla \cdot j = 0\,, \\ \rho D_t \mathbf{v} = \operatorname{div} \mathbf{T} \end{aligned}$$

where D_t is the material derivative and

$$\begin{aligned} j &= -m(c)\nabla\mu \quad \text{is a diffusive flux}\,, \\ \mu &= \frac{\sigma}{\varepsilon}\psi'(c) - \frac{\sigma\varepsilon}{\rho(c)}\nabla\cdot(\rho(c)\nabla c) - \rho'(c)\frac{p}{\rho^2} \quad \text{is the chemical potential}\,, \\ \mathbf{T} &= -pId - \varepsilon\sigma\rho(c)\nabla c\otimes\nabla c + \eta(c)(\nabla\mathbf{v} + \nabla\mathbf{v}^T) \quad \text{is the stress tensor} \end{aligned}$$

with ψ being a double well potential (e.g., of the form $\psi(c) = \frac{1}{2}(1-c^2)^2$), p being the pressure and ε being a small length scale parameter related to the thickness of the interface.

Specific features of the above system are that the pressure explicitly enters the chemical potential μ and that a dissipation inequality for the total energy

$$\rho\left(\frac{\mathbf{u}^2}{2} + \frac{\sigma\varepsilon}{2}|\nabla c|^2 + \frac{\sigma}{\varepsilon}\psi(c)\right) \tag{1}$$

holds, see [42] for details. We also remark that the model of Lowengrub and Truskinovsky reduces to the model H if the densities are equal. An alternative derivation based on the concept of microforces and similar to Gurtin et al. [34] is given in [1].

Some authors tried to modify the model H for the case of fluids with different densities keeping in particular a divergence free velocity field, see, e.g., Jacqmin [37] and Ding et al. [24]. We refer in particular to the paper of Ding et al. [24] who used a volume averaged velocity field to guarantee solenoidality of the velocity field. The first diffuse interface model which is based on a divergence free velocity field *and* at the same time strictly dissipates a physically sound energy has been introduced in [9] and we will now derive this model. The requirement that a dissipation inequality holds is not only necessary for thermodynamical consistency, it would also lead to a priori estimates which are essential for the analysis. They also allow, as we will see, for stable numerical discretizations.

There are several other generalizations of the model H for fluids with non-matched densities, cf. [17, 19, 41]. These models look simpler but they miss a phys-

ical sound derivation. Again, the validity of the second law of thermodynamics (in an appropriate mechanical version) is unclear and a global energy estimate is not known to hold. Under the assumption of small density variations, Boyer [19] was able to prove existence of strong solutions for the model derived therein.

2.2 A new thermodynamically consistent model

In order to derive the model introduced by Abels, Garcke and Grün [9] we start with the basic balance equations. The two fluids, which are allowed to mix in a thin interfacial region are assumed to have mass densities ρ_- and ρ_+. The local mass balance equation for the two fluids is given by

$$\partial_t \rho_\pm + \operatorname{div} \widehat{\mathbf{J}}_\pm = 0 \tag{2}$$

with mass fluxes $\widehat{\mathbf{J}}_\pm$. With the help of the velocities

$$\mathbf{v}_\pm = \widehat{\mathbf{J}}_\pm / \rho_\pm$$

and the volume fractions

$$u_\pm = \rho_\pm / \tilde{\rho}_\pm \,,$$

where $\tilde{\rho}_\pm$ are the constant specific densities of the unmixed states, we define the volume averaged velocity

$$\mathbf{v} = u_- \mathbf{v}_- + u_+ \mathbf{v}_+ = \frac{\rho_-}{\tilde{\rho}_-} \mathbf{v}_- + \frac{\rho_+}{\tilde{\rho}_+} \mathbf{v}_+ \,.$$

Assuming volume conservation during the mixing process we require

$$u_- + u_+ = 1$$

which is equivalent to the fact that the excess volume is zero. Weighting (2) with $1/\tilde{\rho}_\pm$ and adding leads to

$$0 = \partial_t (u_- + u_+) + \operatorname{div} \left(u_- \frac{\widehat{\mathbf{J}}_-}{\rho_-} + u_+ \frac{\widehat{\mathbf{J}}_+}{\rho_+} \right) = \partial_t (u_- + u_+) + \operatorname{div} \mathbf{v} = \operatorname{div} \mathbf{v} \,.$$

Introducing $\widetilde{\mathbf{J}}_\pm = \frac{1}{\tilde{\rho}_\pm} \widehat{\mathbf{J}}_\pm - u_\pm \mathbf{v}$ we obtain

$$\partial_t u_\pm + \operatorname{div}(u_\pm \mathbf{v}) + \operatorname{div} \widetilde{\mathbf{J}}_\pm = 0 \,.$$

It is now convenient to rephrase the governing equations with the help of the difference of the volume fractions and therefore we define

$$\varphi := u_+ - u_- \,.$$

It hence holds

$$\partial_t \varphi + \operatorname{div}(\varphi \mathbf{v}) + \operatorname{div} \mathbf{J}_\varphi = 0$$

where

$$\mathbf{J}_\varphi = \widetilde{\mathbf{J}}_+ - \widetilde{\mathbf{J}}_- .$$

The definitions of u_-, u_+, φ and the fact $u_- + u_+ = 1$ now imply that the total mass $\rho = \rho_+ + \rho_+$ is given as

$$\rho = \rho(\varphi) = \tilde{\rho}_+ \frac{1+\varphi}{2} + \tilde{\rho}_- \frac{1-\varphi}{2}$$

and hence due to $\partial_t \rho = \frac{\tilde{\rho}_+ - \tilde{\rho}_-}{2} \partial_t \varphi$ we obtain

$$\partial_t \rho + \operatorname{div}(\rho \mathbf{v}) + \operatorname{div} \tilde{\mathbf{J}} = 0, \tag{3}$$

where we define

$$\widetilde{\mathbf{J}} = \frac{\tilde{\rho}_+ - \tilde{\rho}_-}{2} \mathbf{J}_\varphi .$$

The classical conservation law for linear momentum in its pointwise formulation is given by

$$\partial_t (\rho \mathbf{v}) + \operatorname{div}(\rho \mathbf{v} \otimes \mathbf{v}) = \operatorname{div} \widetilde{\mathbf{T}}$$

with a stress tensor $\widetilde{\mathbf{T}}$. Rewriting this identity with the help of mass conservation (3) leads to

$$\rho(\partial_t \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v}) = \operatorname{div}(\widetilde{\mathbf{T}} + \mathbf{v} \otimes \widetilde{\mathbf{J}}) - \widetilde{\mathbf{J}} \cdot \nabla \mathbf{v} .$$

It was discussed in [9], see also [15], that $\widetilde{\mathbf{T}}$ is not invariant under a change of observer. However, the tensor

$$\mathbf{T} = \widetilde{\mathbf{T}} + \mathbf{v} \otimes \widetilde{\mathbf{J}}$$

is an objective tensor and we obtain

$$\rho \partial_t \mathbf{v} + (\rho \mathbf{v} + \widetilde{\mathbf{J}}) \cdot \nabla \mathbf{v} = \operatorname{div} \mathbf{T} ,$$

see [15] and [9] for details.

To proceed further we need to introduce a total energy density which is given as the sum of kinetic energy and interfacial energy as follows

$$e(\mathbf{v}, \varphi, \nabla \varphi) = \frac{\rho}{2} |\mathbf{v}|^2 + \hat{\sigma} \left(\frac{\varepsilon}{2} |\nabla \varphi|^2 + \frac{1}{\varepsilon} \psi(\varphi) \right) .$$

We now require the following energy inequality

$$\frac{d}{dt} \int_{V(t)} e(\mathbf{v}, \varphi, \nabla \varphi) dx + \int_{\partial V(t)} \mathbf{J}_e \cdot \nu d\mathscr{H}^{d-1} \leq 0 \tag{4}$$

where $\mathbf{J}_e$ is the energy flux, $\mathscr{H}^{d-1}$ is the $(d-1)$-dimensional surface measure and $V(t)$ is a time dependent volume transported with the velocity $\mathbf{v}$. The inequality (4) is the relevant formulation of the second law of thermodynamics in an isothermal situation, cf. [34]. With the help of a transport theorem and using the fact that $V(t)$ is arbitrary we obtain the pointwise inequality

$$-\mathscr{D} := \partial_t e + \operatorname{div}(\mathbf{v}e) + \operatorname{div}\mathbf{J}_e \leq 0\,. \tag{5}$$

Now every solution which fulfills the basic conservation laws and the energy inequality also fulfills

$$-\mathscr{D} = \partial_t e + \mathbf{v}\cdot\nabla\varphi + \operatorname{div}\mathbf{J}_e - \mu(\partial_t\varphi + \mathbf{v}\cdot\nabla\varphi + \operatorname{div}\mathbf{J}_\varphi) \leq 0$$

where μ is a Lagrange multiplier.

With the help of the mass balance and the balance of linear momentum we obtain

$$\begin{aligned}\partial_t\left(\frac{\rho}{2}|\mathbf{v}|^2\right) + \operatorname{div}\left(\frac{\rho}{2}|\mathbf{v}|^2\mathbf{v}\right) &= -\frac{|\mathbf{v}|^2}{2}\operatorname{div}\widetilde{\mathbf{J}} + (\operatorname{div}\mathbf{T} - \widetilde{\mathbf{J}}\cdot\nabla\mathbf{v})\cdot\mathbf{v}\\ &= \operatorname{div}\left(-\frac{1}{2}|\mathbf{v}|^2\widetilde{\mathbf{J}} + \mathbf{T}^T\mathbf{v}\right) - \mathbf{T}:\nabla\mathbf{v}\,.\end{aligned}$$

Using the material derivative $D_t u = \partial_t u + \mathbf{v}\cdot\nabla u$ we obtain

$$D_t\nabla\varphi = \partial_t\nabla\varphi + \mathbf{v}\cdot\nabla(\nabla\varphi) = \nabla D_t\varphi - (\nabla\mathbf{v})^T\nabla\varphi\,.$$

The dissipation term $\mathscr{D}$ can hence be rewritten as

$$\begin{aligned}-\mathscr{D} = \operatorname{div}&\left(\mathbf{J}_e - \widetilde{\mathbf{J}}\frac{|\mathbf{v}|^2}{2} + \mathbf{T}^T\mathbf{v} - \mu\mathbf{J}_\varphi + \hat{\sigma}\varepsilon\nabla\varphi D_t\varphi\right)\\ &+\left(\frac{\hat{\sigma}}{\varepsilon}\psi'(\varphi) - \mu - \hat{\sigma}\varepsilon\Delta\varphi\right)D_t\varphi\\ &-(\mathbf{T} + \hat{\sigma}\varepsilon\nabla\varphi\otimes\nabla\varphi):\nabla\mathbf{v} + \nabla\mu\cdot\mathbf{J}_\varphi = 0\,,\end{aligned}$$

where the :-product for matrices $\mathbf{A},\mathbf{B}$ is given as $\mathbf{A}:\mathbf{B} = tr(\mathbf{A}^T\mathbf{B})$. Defining the energy flux $\mathbf{J}_e$ as

$$\mathbf{J}_e = \widetilde{\mathbf{J}}\frac{|\mathbf{v}|^2}{2} - \mathbf{T}^T\mathbf{v} + \mu\mathbf{J}_\varphi - \hat{\sigma}\varepsilon\nabla\varphi D_t\varphi$$

and the chemical potential

$$\mu = -\hat{\sigma}\varepsilon\Delta\varphi + \frac{\hat{\sigma}}{\varepsilon}\psi'(\varphi)$$

the dissipation inequality is given as

$$\mathscr{D} = (\mathbf{T} + \hat{\sigma}\varepsilon\nabla\varphi\otimes\nabla\varphi):\nabla\mathbf{v} - \nabla\mu\cdot\mathbf{J}_\varphi \geq 0\,. \tag{6}$$

As in [34] we introduce the pressure p and rewrite the above inequality as

$$\mathbf{S} : \nabla \mathbf{v} - \nabla \mu \cdot \mathbf{J}_\varphi \leq 0$$

with the viscous stress tensor

$$\mathbf{S} = \mathbf{T} + pId + \hat{\sigma}\varepsilon \nabla\varphi \otimes \nabla\varphi \,.$$

The dissipation inequality is fulfilled by assuming viscous friction in the definition for $\mathbf{S}$ and Fick's law in the definition of $\mathbf{J}_\varphi$. We hence choose

$$\mathbf{S} = 2\eta(\varphi) D\mathbf{v} \,, \quad \mathbf{J}_\varphi = -m(\varphi)\nabla\mu$$

with $\eta(\varphi), m(\varphi) \geq 0$.

The final diffuse interface model is given as follows

$$\rho \partial_t \mathbf{v} + (\rho \mathbf{v} + \widetilde{\mathbf{J}}) \cdot \nabla \mathbf{v} - \operatorname{div}(2\eta(\varphi) D\mathbf{v}) + \nabla p = -\hat{\sigma}\varepsilon \operatorname{div}(\nabla\varphi \otimes \nabla\varphi) \,, \tag{7}$$

$$\operatorname{div} \mathbf{v} = 0 \,, \tag{8}$$

$$\partial_t \varphi + \mathbf{v} \cdot \nabla\varphi = \operatorname{div}(m(\varphi)\nabla\mu) \,, \tag{9}$$

$$\frac{\hat{\sigma}}{\varepsilon}\psi'(\varphi) - \hat{\sigma}\varepsilon\Delta\varphi = \mu \,, \tag{10}$$

where

$$\widetilde{\mathbf{J}} = \frac{\tilde{\rho}_+ - \tilde{\rho}_-}{2}\mathbf{J}_\varphi = -\frac{\tilde{\rho}_+ - \tilde{\rho}_-}{2} m(\varphi)\nabla\mu.$$

We notice that the term involving $\widetilde{\mathbf{J}}$ in the momentum equation vanishes for equal densities, i.e., if $\tilde{\rho}_+ = \tilde{\rho}_-$.

It is also possible to redefine the pressure as

$$\hat{p} = p - \hat{\sigma}\left(\frac{\varepsilon}{2}|\nabla\varphi|^2 + \frac{1}{\varepsilon}\psi(\varphi)\right) \tag{11}$$

and in this case the momentum equation becomes

$$\rho \partial_t \mathbf{v} + (\rho \mathbf{v} + \widetilde{\mathbf{J}}) \cdot \nabla \mathbf{v} - \operatorname{div}(2\eta(\varphi) D\mathbf{v}) + \nabla \hat{p} = \mu \nabla\varphi \,. \tag{12}$$

With even another pressure the momentum equation becomes

$$\rho \partial_t \mathbf{v} + (\rho \mathbf{v} + \widetilde{\mathbf{J}}) \cdot \nabla \mathbf{v} - \operatorname{div}(\eta(\varphi) D\mathbf{v}) + \nabla \tilde{p} \tag{13}$$

$$= \operatorname{div}\left(\hat{\sigma}\left(\frac{\varepsilon}{2}|\nabla\varphi|^2 + \frac{1}{\varepsilon}\psi(\varphi)\right) Id - \hat{\sigma}\varepsilon \nabla\varphi \otimes \nabla\varphi\right) \tag{14}$$

where $\hat{\sigma}(\frac{\varepsilon}{2}|\nabla\varphi|^2 + \frac{1}{\varepsilon}\psi(\varphi))Id - \hat{\sigma}\varepsilon\nabla\varphi\otimes\nabla\varphi$ can be interpreted as an approximation of the surface stress tensor in a sharp interface model, see [15]. It is also sometimes convenient to write the acceleration part in a conservative form, see [28],

$$\partial_t(\rho\mathbf{v}) + \operatorname{div}(\mathbf{v} \otimes (\rho\mathbf{v} + \tilde{\mathbf{J}})) - \operatorname{div}(2\eta(\varphi) D\mathbf{v}) + \nabla p = \mu\nabla\varphi \,. \tag{15}$$

2.3 Including transport effects of a soluble species

We now want to include the transport of a soluble species as an additional effect. We focus on a species that does not influence the surface tension at the interface and refer to [10] for the case of surface active agents (surfactants). Denoting the concentration of the soluble species by w we add to the conservation law

$$\partial_t w + \mathbf{v} \cdot \nabla w + \operatorname{div} \mathbf{J}_w = 0 \tag{16}$$

where $\mathbf{J}_w$ is the corresponding mass flux to the governing balance equations from the previous subsection. We also add the term

$$\int_\Omega \{g(w) + \beta(\varphi) w\} dx$$

to the total energy where g is an entropic term and β attains for $\varphi \leq -1$ or $\varphi \geq 1$ the values β_1 or β_2 respectively. These values will reappear in the Henry condition of the sharp interface limit in the following section. In [9] the authors derived a thermodynamically consistent model coupling (16) to the model of the previous subsection. In the model the momentum equation (7), the divergence equation (8) and the equation for the phase field (9) remain unchanged and the equation for the chemical potential now becomes

$$\mu = -\hat{\sigma}\varepsilon\Delta\varphi + \frac{\hat{\sigma}}{\varepsilon}\psi'(\varphi) + \beta'(\varphi) w\,.$$

All these equations are coupled to

$$\partial_t w + \mathbf{v} \cdot \nabla w - \operatorname{div}(K(\varphi) w \nabla(g'(w) + \beta(\varphi))) = 0\,,$$

where $K(\varphi)$ is related to the diffusion parameter in the phases. Under appropriate boundary condition the overall system decreases the total energy

$$\int_\Omega \frac{\rho}{2}|\mathbf{v}|^2 dx + \int_\Omega \hat{\sigma}\left(\frac{\varepsilon}{2}|\nabla\varphi|^2 + \frac{1}{\varepsilon}\psi(\varphi)\right) dx + \int_\Omega \{g(w) + \beta(\varphi) w\} dx.$$

3 Sharp interface limit

The parameter ε in the above models is related to the interfacial thickness of the diffuse interfacial layer. As ε tends to zero classical and new sharp interface models are attained. So far this has been shown by formally matched asymptotic expansions, see [9] and in certain situations a rigorous convergence result in a very weak varifold setting, see [11] or [12]. Which sharp interface limit we obtain depends on the mobility and we consider four cases

$$m_\varepsilon(\varphi) = \begin{cases} m_0 & \text{case I}, \\ \varepsilon m_0 & \text{case II}, \\ \frac{m_1}{\varepsilon}(1-\varphi^2)_+ & \text{case III}, \\ m_1(1-\varphi^2)_+ & \text{case IV}. \end{cases}$$

Here m_0 and m_1 are positive constants and $(1-\varphi^2)_+ = \max(1-\varphi^2, 0)$. We assume for simplicity that $g(w) = w(\log w - 1)$ and set $K_\pm = K(\pm 1)$, $\eta_\pm = \eta(\pm 1)$. In the cases II-IV we obtain in the bulk regions Ω_- and Ω_+ for $i \in \{-,+\}$

$$\begin{aligned} \rho_i(\partial_t \mathbf{v} + \operatorname{div}(\mathbf{v}\otimes\mathbf{v})) - \eta_i \Delta \mathbf{v} + \nabla p &= 0, \\ \operatorname{div}\mathbf{v} &= 0, \\ \partial_t w + \mathbf{v}\cdot\nabla w &= K_i \Delta w \end{aligned}$$

and in case I the momentum balance has to be replaced by

$$\rho_i \partial_t \mathbf{v} + \operatorname{div}\left(\mathbf{v} \otimes \left(\rho_i \mathbf{v} + \tfrac{\rho_- - \rho_+}{2} m_0 \nabla \mu\right)\right) - \eta_i \Delta \mathbf{v} + \nabla p = 0, \tag{17}$$

i.e., a non-classical term $\frac{\rho_- - \rho_+}{2} m_0 \nabla \mu$ appears for non-matched densities where μ solves the quasi-static diffusion equation

$$\Delta \mu = 0 \qquad \text{in} \qquad \Omega_\pm.$$

On the interface Γ we have in all four cases

$$\begin{aligned} [\mathbf{v}]_-^+ &= 0, \\ \frac{w_+}{w_-} &= \exp(\beta_- - \beta_+), \\ (\mathscr{V} - \mathbf{v}\cdot\nu)[w]_-^+ &= -[K\nabla w]_-^+ \cdot \nu, \end{aligned}$$

where $\mathscr{V}$ is the normal velocity of Γ. The remaining conditions depend on which of the cases we consider. In the cases II and IV we obtain

$$\begin{aligned} -[2\eta D\mathbf{v}]_-^+ \cdot \nu + [p]_-^+ \nu &= \sigma \kappa \nu, \\ \mathscr{V} &= \mathbf{v}\cdot\nu \end{aligned}$$

where the surface tension σ can be computed from $\hat{\sigma}$ and ψ, see [9] for details. We hence note that if one wants to approximate classical sharp interface models with the help of a diffuse interface model one hence has to choose

$$m_\varepsilon(\varphi) = \varepsilon m_0 \quad \text{or} \quad m_\varepsilon(\varphi) = m_1(1-\varphi^2)_+.$$

In case I on the other hand we obtain

$$-[2\eta D\mathbf{v}]_-^+\nu + [p]_-^+\nu = \sigma\kappa\nu, \tag{18}$$
$$2(\mathbf{v}\cdot\nu - \mathscr{V}) = m_0[\nabla\mu]_-^+\cdot\nu, \tag{19}$$
$$2\mu = \sigma\kappa - [w]_-^+ \tag{20}$$

which is remarkable as the interface is not transported by the fluid velocity.

In case III we obtain

$$-\tfrac{1}{2}[\rho]_-^+\hat{m}((\nabla_\Gamma\mu)\cdot\nabla_\Gamma)\mathbf{v} - 2[\eta D\mathbf{v}]_-^+\nu + [p]_-^+\nu = \sigma\kappa\nu\,, \tag{21}$$
$$2(\mathbf{v}\cdot\nu - \mathscr{V}) = \hat{m}\Delta_\Gamma\mu\,, \tag{22}$$
$$2\mu = \sigma\kappa - [w]_-^+ \tag{23}$$

where Δ_Γ is the Laplace-Beltrami operator on the interface and $\hat{m}$ is a constant related to ψ. We hence obtain surface diffusion, cf. [25], in the equation for the normal velocity and we obtain the non-classical term $-\frac{1}{2}[\rho]_-^+\hat{m}((\nabla_\Gamma\mu)\cdot\nabla_\Gamma)\mathbf{v}$ in the interfacial stress balance.

In [9] the following theorem has been shown in which in particular the different dissipation mechanisms can be read off.

Theorem 1. *(Free energy inequality).*

We assume $\eta,\rho,K,w,m_0,\hat{m} > 0$. Then a sufficiently smooth solution of the sharp interface problem defined in a spatial domain Ω with $\Gamma(t)\subset\Omega$, for all $t\geq 0$, fulfills

$$\frac{d}{dt}\left[\int_\Omega\left(\frac{\rho}{2}|\mathbf{v}|^2 + (g(w)+\beta w)\right)dx + \int_{\Gamma(t)}\sigma d\mathscr{H}^{d-1}\right] = -\mathscr{D}\leq 0\,,$$

provided the integrals are finite. Here $\rho=\rho_-,\rho_+$ and $\beta=\beta_-,\beta_+$ holds in the two phases. The quantity $\mathscr{D}$ is given as

$$\text{Case I} \quad : \quad \mathscr{D} = \int_\Omega 2\eta|D\mathbf{v}|^2\,dx + \int_\Omega K\frac{1}{w}|\nabla w|^2\,dx + \int_\Omega m_0|\nabla\mu|^2\,dx\,,$$
$$\text{Cases II and IV} \quad : \quad \mathscr{D} = \int_\Omega 2\eta|D\mathbf{v}|^2\,dx + \int_\Omega K\frac{1}{w}|\nabla w|^2\,dx\,,$$
$$\text{Case III} \quad : \quad \mathscr{D} = \int_\Omega 2\eta|D\mathbf{v}|^2\,dx + \int_\Omega K\frac{1}{w}|\nabla w|^2\,dx + \int_{\Gamma(t)}\hat{m}|\nabla_\Gamma\mu|^2 d\mathscr{H}^{d-1}\,.$$

4 Existence results

In this subsection analytic results for the system (7)-(10) are discussed, i.e.,

$$\rho\partial_t \mathbf{v} + (\rho\mathbf{v} + \widetilde{\mathbf{J}}) \cdot \nabla \mathbf{v} - \operatorname{div}(2\eta(\varphi)D\mathbf{v}) + \nabla p = -\hat{\sigma}\varepsilon \operatorname{div}(\nabla\varphi \otimes \nabla\varphi), \tag{24}$$

$$\operatorname{div} \mathbf{v} = 0, \tag{25}$$

$$\partial_t \varphi + \mathbf{v} \cdot \nabla\varphi = \operatorname{div}(m(\varphi)\nabla\mu), \tag{26}$$

$$\mu = -\hat{\sigma}\varepsilon\Delta\varphi + \frac{\hat{\sigma}}{\varepsilon}\psi'(\varphi) \tag{27}$$

in $\Omega \times (0,T)$, where $\Omega \subseteq \mathbb{R}^d$, $d = 2,3$, is a bounded domain with smooth boundary and

$$\rho = \rho(\varphi) = \tilde{\rho}_+ \frac{1+\varphi}{2} + \tilde{\rho}_- \frac{1-\varphi}{2}, \tag{28}$$

$$\widetilde{\mathbf{J}} = \frac{\tilde{\rho}_+ - \tilde{\rho}_-}{2}\mathbf{J}_\varphi = -\frac{\tilde{\rho}_+ - \tilde{\rho}_-}{2} m(\varphi)\nabla\mu.$$

In order to obtain a well-posed problem we have to close the system with initial conditions

$$(\mathbf{v}, \varphi)|_{t=0} = (\mathbf{v}_0, \varphi_0) \tag{29}$$

and suitable boundary conditions. A standard choice, which is made for the following analytic results, is

$$\mathbf{v}|_{\partial\Omega} = \mathbf{0}, \nu \cdot \nabla\varphi|_{\partial\Omega} = \nu \cdot \nabla\mu|_{\partial\Omega} = 0. \tag{30}$$

For the following we set $\hat{\sigma} = 1$ for simplicity.

First of all smooth solutions of (24)-(27) together with (30) satisfy the energy dissipation identity

$$\frac{d}{dt}\int_\Omega \left(\tfrac{\rho|\mathbf{v}|^2}{2} + \tfrac{\varepsilon|\nabla\varphi|^2}{2} + \tfrac{\psi(\varphi)}{\varepsilon}\right) dx = -\int_\Omega 2\eta(\varphi)|D\mathbf{v}|^2\,dx - \int_\Omega m(\varphi)|\nabla\mu|^2\,dx \tag{31}$$

for all $t \in (0,T)$. This follows from integration of the dissipation relation (5) and (6). This identity yields a priori bounds for

$$\mathbf{v} \in L^\infty((0,\infty); L^2_\sigma(\Omega)) \cap L^2((0,\infty); H^1_0(\Omega)^d), \varphi \in L^\infty((0,\infty); H^1(\Omega)),$$
$$\nabla\mu \in L^2(\Omega \times (0,T))^d \text{ if } m(\varphi) \geq m_0 > 0$$

as long as $\rho(\varphi)$ is bounded below, which is the case if φ only attains values in the physical reasonable interval $[-1,1]$. Here $L^p(\Omega)$, $1 \leq p \leq \infty$, is the standard Lebesgue space (with respect to the Lebesgue measure) consisting of measurable functions $f\colon \Omega \to \mathbb{R}$ such that $|f|^p$ is integrable if $p < \infty$, $|f|$ is essentially bounded if $p = \infty$, respectively. Moreover, $L^p(\Omega;X)$ is its X-valued analogue, $H^k(\Omega)$ is the L^2-Sobolev space of k-the order and $H^1_0(\Omega)$ is the closure of smooth, compactly supported functions in $H^1(\Omega)$. Furthermore, $L^2_\sigma(\Omega)$ denotes the closure of divergence-free, smooth, and compactly supported vector-fields.

For the mathematical analysis it is essential that ρ stays positive, which is true as long as $\varphi \in [-1,1]$. In order to guarantee this property mathematically we worked with so-called singular free energy densities as e.g. given by

$$\psi(\varphi) = \frac{\theta}{2}\left((1+\varphi)\ln(1+\varphi) + (1-\varphi)\ln(1-\varphi)\right) - \frac{\theta_c}{2}\varphi^2 \quad \text{for } \varphi \in [-1,1], \quad (32)$$

where $0 < \theta < \theta_c$. This was used by Cahn and Hilliard [23] to describe physical relevant so-called regular solution models. Mathematically, the singularity in ψ' ensures that the order parameter φ stays in the physically reasonable interval $[-1,1]$. But it leads to additional difficulties due to singular terms in the equation for the chemical potential. For non-singular ψ (and non-degenerate $m(\varphi)$) this property is unknown.

Existence of weak solutions of (24)-(27) was shown by Abels, Depner, and Garcke in [6] and [7] in the case of singular free energies with non-degenerate and degenerate mobility, respectively. More precisely, in the non-degenerate case the following result was shown:

Theorem 2. (Existence of Weak Solutions, [6, Theorem 3.4])
Let $m\colon \mathbb{R} \to \mathbb{R}$ be continuously differentiable, $\eta\colon \mathbb{R} \to \mathbb{R}$ be continuous and assume that $k \le m(s), \eta(s) \le K$ for all $s \in \mathbb{R}$ and some $k, K > 0$. Moreover, let ψ be as in (32)*. Then for every $v_0 \in L^2_\sigma(\Omega)$ and $\varphi_0 \in H^1(\Omega)$ with $|\varphi_0| \le 1$ almost everywhere and $\frac{1}{|\Omega|}\int_\Omega \varphi_0\,dx \in (-1,1)$ there exists a weak solution (v,φ,μ) of* (24)-(27) *together with* (29)-(30) *such that for any $0 < T < \infty$*

$$\begin{aligned}
&v \in L^\infty((0,\infty);L^2_\sigma(\Omega)) \cap L^2((0,\infty);H^1_0(\Omega)^d),\\
&\varphi \in L^\infty((0,\infty);H^1(\Omega)) \cap L^2((0,T);H^2(\Omega)),\ \psi'(\varphi) \in L^2(\Omega\times(0,T)),\\
&\mu \in L^2((0,T);H^1(\Omega)) \ \text{ with } \ \nabla\mu \in L^2(\Omega\times(0,\infty))^d.
\end{aligned}$$

Actually, the result holds true under more general assumptions. For the precise definition of weak solutions we refer to [6, Definition 3.3]. As usual the pressure p is not part of the weak formulation since (24) is tested with divergence free test functions.

The structure of the proof of Theorem 2 is as follows: System (24)-(27) is first approximated with the aid of a semi-implicit time discretization, which satisfies the same kind of energy identity as the continuous system. Hence one obtains a priori bounds for

$$\begin{aligned}
&\mathbf{v}^N \in L^\infty((0,\infty);L^2_\sigma(\Omega)) \cap L^2((0,\infty);H^1_0(\Omega)^d),\, \varphi^N \in L^\infty((0,\infty);H^1(\Omega)),\\
&\nabla\mu^N \in L^2(\Omega\times(0,\infty)),
\end{aligned}$$

where $(\mathbf{v}^N, \varphi^N, \mu^N)$ are suitable interpolations of solutions of the time discretized system with discretization parameter $h = \frac{1}{N}$. In order pass to the limit $N \to \infty$ it is essential to obtain a bound for

$$\varphi^N \in L^2((0,T),H^2(\Omega)), \quad \psi'(\varphi^N) \in L^2(\Omega\times(0,T))$$

for any $T > 0$. To this end one uses that $\psi'(\varphi) = \psi_0'(\varphi) - \theta_c\varphi$, where ψ_0 is convex together with a priori estimates in $H^2(\Omega)$ for the non-linear elliptic equation

$$-\Delta\varphi + \psi_0'(\varphi) = g := \mu + \theta_c\varphi, \qquad \nu\cdot\nabla\varphi|_{\partial\Omega} = 0$$

due to Abels and Wilke [13, Theorem 4.3]. This theorem is also used to obtain existence of solutions for the time discretized system.

In the case of degenerate mobility it is assumed that

$$m(s) = \begin{cases} 1-s^2 & \text{if } s \in [-1,1], \\ 0 & \text{else} \end{cases}$$

and $\psi\colon \mathbb{R} \to \mathbb{R}$ is continuously differentiable. In this case one does not obtain an a priori bound for $\nabla\mu$ in $L^2((0,\infty)\times\Omega)$. Instead one obtains an a priori bound for $\widehat{\mathbf{J}} := \sqrt{m(\varphi)}\nabla\mu$ and $\mathbf{J} := m(\varphi)\nabla\mu$. Therefore one has to avoid $\nabla\mu$ in the weak formulation and has to formulate the equations in terms of $\mathbf{J}$. More precisely, the triple $(\mathbf{v},\varphi,\mathbf{J})$ should satisfy the weak formulations:

$$\begin{aligned} &-\int_0^T\int_\Omega \rho\mathbf{v}\cdot\partial_t\boldsymbol{\psi}\,dx\,dt + \int_0^T\int_\Omega \operatorname{div}(\rho\mathbf{v}\otimes\mathbf{v})\cdot\boldsymbol{\psi}\,dx\,dt \\ &+\int_0^T\int_\Omega 2\eta(\varphi)D\mathbf{v} : D\boldsymbol{\psi}\,dx\,dt - \int_0^T\int_\Omega (\mathbf{v}\otimes\tfrac{\tilde\rho_+-\tilde\rho_-}{2}\mathbf{J}) : \nabla\boldsymbol{\psi}\,dx\,dt \\ &= -\int_0^T\int_\Omega \varepsilon\Delta\varphi\nabla\varphi\cdot\boldsymbol{\psi}\,dx\,dt \end{aligned} \tag{33}$$

for all $\boldsymbol{\psi} \in C_0^\infty(\Omega\times(0,T))^d$ with $\operatorname{div}\boldsymbol{\psi} = 0$,

$$-\int_0^T\int_\Omega \varphi\,\partial_t\zeta\,dx\,dt + \int_0^T\int_\Omega (\mathbf{v}\cdot\nabla\varphi)\,\zeta\,dx\,dt = \int_0^T\int_\Omega \mathbf{J}\cdot\nabla\zeta\,dx\,dt \tag{34}$$

for all $\zeta \in C_0^\infty((0,T);C^1(\overline{\Omega}))$ and

$$\int_0^T\int_\Omega \mathbf{J}\cdot\boldsymbol{\eta}\,dx\,dt = -\int_0^T\int_\Omega \left(\frac{1}{\varepsilon}\psi'(\varphi)) - \varepsilon\Delta\varphi\right)\operatorname{div}(m(\varphi)\boldsymbol{\eta})\,dx\,dt \tag{35}$$

for all $\boldsymbol{\eta} \in L^2(0,T;H^1(\Omega)^d)\cap L^\infty(\Omega\times(0,T))^d$ which fulfill $\nu\cdot\boldsymbol{\eta}|_{\partial\Omega} = 0$ on $\partial\Omega\times(0,T)$. Here $C_0^\infty(\Omega\times(0,T)), C_0^\infty((0,T);X)$ is the set of all smooth functions $\varphi\colon \Omega\times(0,T)\to\mathbb{R}$, $\varphi\colon (0,T)\to X$ with compact support. We refer to [7, Definition 3.3] for the complete definition of weak solutions.

We remark that (35) is a weak formulation of

$$\mathbf{J} = -m(\varphi)\nabla\left(\frac{1}{\varepsilon}\psi'(\varphi) - \varepsilon\Delta\varphi\right).$$

Theorem 3. (Existence of Weak Solutions, [7, Theorem 3.5])
Let m, ψ be as before and η be as in Theorem 2, $\mathbf{v}_0 \in L^2_\sigma(\Omega)$ and $\varphi_0 \in H^1(\Omega)$ with $|\varphi_0| \le 1$ almost everywhere in Ω. Then there exists a weak solution $(\mathbf{v},\varphi,\boldsymbol{J})$ of (24)-(27) *together with* (29)-(30).

The theorem is proved by approximating m by a sequence of strictly positive mobilities m_δ and ψ by

$$\psi_\delta(s) := \psi(s) + \delta(1+s)\ln(1+s) + \delta(1-s)\ln(1-s), \quad s \in [-1,1],$$

where $\delta > 0$. Then existence of weak solutions $(\mathbf{v}_\delta, \varphi_\delta, \mu_\delta)$ for $\delta > 0$ follows from Theorem 2. In order to pass to the limit one uses the energy identity (31). But this does not give a bound for $\varphi_\delta \in L^2(0,T;H^2(\Omega))$, which is essential to pass to the limit in the weak formulation of (24). In order to obtain this bound one tests the weak formulation of (26) with $G'_\delta(\varphi_\delta)$, where $G''(s) = \frac{1}{m_\delta(s)}$ for $s \in (-1,1)$ and $G'_\delta(0) = G_\delta(0) = 0$, see [7, Proof of Lemma 3.7] for the details.

In the case of non-degenerate mobility existence of a unique strong solution was shown by Weber [46]:

Theorem 4. (Existence of strong solutions [46, Theorem 5.4])
Let Ω, η, m, and ψ be sufficiently smooth, η, m be positive, and $4 < p < 6$. Moreover, let $\mathbf{v}_0 \in H^1_0(\Omega)^d \cap L^2_\sigma(\Omega)$ and $\varphi_0 \in W^4_p(\Omega)$ with $\nu \cdot \nabla \varphi_0|_{\partial\Omega} = 0$ and $|\varphi_0| \leq 1$. Then there exists some $T > 0$ such that (24)-(27) *in $\Omega \times (0,T)$ together with* (29)-(30) *has a unique strong solution*

$$\begin{aligned}
&\mathbf{v} \in W^1_2(0,T;L^2_\sigma(\Omega)) \cap L^2(0,T;H^2(\Omega)^d \cap H^1_0(\Omega)^d),\\
&\varphi \in W^1_p(0,T;L^p(\Omega)) \cap L^p(0,T;W^4_p(\Omega)).
\end{aligned}$$

Finally, we mention that existence of weak solutions of (24)-(27) together with (29)-(30) was proven in the case of power-law type fluids of exponent $p > \frac{2d+2}{d+2}$, $d = 2,3$, by Abels and Breit [5]. In this work the case of constant, positive mobility together with a suitable smooth free energy density ψ is considered. Unfortunately, in this case there is no mechanism, which enables to show that $\varphi \in [-1,1]$. Hence one has to modify ρ, defined as in (28) for $\varphi \in [-1,1]$, outside of $[-1,1]$ suitably such that it stays positive. But then (3) is no longer valid and one obtains instead

$$\partial_t \rho + \operatorname{div}(\rho \mathbf{v} + \tilde{\mathbf{J}}) = R, \quad \text{where } R = -\nabla \rho'(\varphi) \cdot m \nabla \mu, \tilde{\mathbf{J}} = -\rho'(\varphi) m \nabla \mu. \tag{36}$$

Here R is an additional source term, which vanishes in the interior of $\{\varphi \in [-1,1]\}$. In order to obtain a local dissipation inequality and a global energy estimate the equation of linear momentum (24) has to be modified to

$$\rho \partial_t \mathbf{v} + (\rho \mathbf{v} + \tilde{\mathbf{J}})) \cdot \nabla \mathbf{v} + R\frac{\mathbf{v}}{2} - \operatorname{div}\mathbf{S}(\varphi, D\mathbf{v}) + \nabla p = -\varepsilon \operatorname{div}\big(\nabla \varphi \otimes \nabla \varphi\big).$$

Under these assumptions existence of weak solutions is shown with the aid of the so-called L^∞-truncation method, cf. [5] for the details.

5 Numerical approximation

In this subsection, we discuss numerical aspects of the diffusive interface model (8)-(10) and (12). For the ease of presentation, we choose the parameters $\hat{\sigma}$ and ε equal to one.

Having a dissipative model consistent with thermodynamics at hand, it becomes realistic to look for stable numerical schemes and for convergence results - see [26] in the setting of Navier-Stokes-Cahn-Hilliard models with *identical* mass densities. Since system (8)-(10), (12) is formulated with solenoidal vector fields, one expects the classical discretization spaces for Navier-Stokes-Systems and Cahn-Hilliard equations to be applicable, too. For details of the discretization, e.g. the choice of spaces, initial data, discretization of nonlinearities etc., we refer to the Appendix.

To obtain a discrete formulation that permits to establish a discrete energy estimate just by testing with admissible functions, i.e. the momentum equation by the velocity field $\mathbf{v}$, the phase-field equation by the chemical potential μ and the weak formulation relating μ and φ by an appropriate discrete time derivative of φ, it is promising to replace the naive weak formulation of the momentum equation

$$\begin{aligned}\int \rho(\varphi)\partial_t \mathbf{v}\cdot\mathbf{w} + \int \rho\mathbf{v}\cdot(\nabla\mathbf{v})^T\mathbf{w} + \int \rho'(\varphi)\mathbf{J}_\varphi\cdot(\nabla\mathbf{v})^T\mathbf{w} + \int 2\eta(\varphi)\mathbf{D}\mathbf{v}:\mathbf{D}\mathbf{v}\\ = \int \mu\nabla\varphi\cdot\mathbf{w} \qquad \forall \mathbf{w}\in W^{1,2}_{0,\mathrm{div}}(\Omega)\end{aligned}$$

by

$$\begin{aligned}\int \partial_t(\rho(\varphi)\mathbf{v})\mathbf{w} &- \frac{1}{2}\int \partial_t\rho(\varphi)\langle\mathbf{v},\mathbf{w}\rangle\\ &- \frac{1}{2}\int \rho(\varphi)\langle\mathbf{v},(\nabla\mathbf{w})^T\mathbf{v}\rangle + \frac{1}{2}\int \rho(\varphi)\langle\mathbf{v},(\nabla\mathbf{v})^T\mathbf{w}\rangle\\ &+ \frac{1}{2}\int \rho'(\varphi)\langle\mathbf{J}_\varphi,(\nabla\mathbf{v})^T\mathbf{w}\rangle - \frac{1}{2}\int \rho'(\varphi)\langle\mathbf{J}_\varphi,(\nabla\mathbf{w})^T\mathbf{v}\rangle\\ &+ \int 2\eta(\varphi)\mathbf{D}\mathbf{v}:\mathbf{D}\mathbf{v} = -\int \varphi\langle\nabla\mu,\mathbf{w}\rangle \qquad \forall \mathbf{w}\in W^{1,2}_{0,\mathrm{div}}(\Omega)\end{aligned}$$

which follows by adding an appropriate zero (see [30] for details).

Let $(\mathbf{W}_h, S_h)$ be an *admissible pair of discretization spaces for hydrodynamics* as defined in the Appendix, for instance the spaces associated with P_2P_1- or with P_2P_0-elements, and assume the hypotheses (H1)-(H6) and (T) in the Appendix to hold. In [30], the following discrete system has been suggested.

For given functions $(\varphi^0,\mathbf{v}^0)\in U_h\times\mathbf{W}_h$ and $k=0,\dots,N-1$ we have to find functions $(\varphi^{k+1},\mu^{k+1},\mathbf{v}^{k+1},p^{k+1})\in U_h\times U_h\times\mathbf{W}_h\times S_h$ such that

$$\Big(\partial_\tau^-\varphi^{k+1},\theta\Big)_h - \int_\Omega \Big\langle \mathbf{v}^{k+1},\nabla\theta\Big\rangle\varphi^k + \int_\Omega \Big\langle\nabla\mu^{k+1},\nabla\theta\Big\rangle = 0 \quad \forall\theta\in U_h, \tag{37a}$$

$$\Big(\mu^{k+1},\theta\Big)_h = \int_\Omega \Big\langle\nabla\varphi^{k+1},\nabla\theta\Big\rangle + \int_\Omega \mathscr{I}_h\Big(\psi'_{\tau h}(\varphi^{k+1},\varphi^k)\theta\Big) \quad \forall\theta\in U_h. \tag{37b}$$

$$\begin{aligned}\int_\Omega \Big\langle \partial_\tau^-(\rho^{k+1}\mathbf{v}^{k+1}),\mathbf{w}\Big\rangle - \tfrac{1}{2}\int_\Omega \partial_\tau^-\rho^{k+1}\Big\langle \mathbf{v}^{k+1},\mathbf{w}\Big\rangle \\ - \tfrac{1}{2}\int_\Omega \rho^k\Big\langle \mathbf{v}^k,(\nabla\mathbf{w})^T\mathbf{v}^{k+1}\Big\rangle + \tfrac{1}{2}\int_\Omega \rho^k\Big\langle \mathbf{v}^k,(\nabla\mathbf{v}^{k+1})^T\mathbf{w}\Big\rangle \\ + \tfrac{1}{2}\int_\Omega \tfrac{\delta\rho}{\delta\varphi}\Big\langle \mathbf{j}^{k+1},(\nabla\mathbf{v}^{k+1})^T\mathbf{w}\Big\rangle - \tfrac{1}{2}\int_\Omega \tfrac{\delta\rho}{\delta\varphi}\Big\langle \mathbf{j}^{k+1},(\nabla\mathbf{w})^T\mathbf{v}^{k+1}\Big\rangle \\ + \int_\Omega 2\eta(\varphi^k)\mathbf{D}\mathbf{v}^{k+1}:\mathbf{D}\mathbf{w} - \int_\Omega p^{k+1}\operatorname{div}\mathbf{w} \\ = -\int_\Omega \varphi^k\Big\langle \nabla\mu^{k+1},\mathbf{w}\Big\rangle \quad \forall \mathbf{w}\in\mathbf{X}_h, \end{aligned} \tag{37c}$$

$$\int_\Omega \theta\operatorname{div}\mathbf{v}^{k+1} = 0 \quad \forall\theta\in S_h. \tag{37d}$$

Here, we use the abbreviations $\rho^{k+1} := \rho(\varphi^{k+1})$ and $\frac{\delta\rho}{\delta\varphi} := \frac{\tilde\rho_+-\tilde\rho_-}{2}$. Moreover, we define $\mathbf{j}^{k+1} := -\nabla\mu^{k+1}$. Note that $\psi'_{\tau h}(\varphi^{k+1},\varphi^k)$ is an appropriate discretization of ψ'. Famous is the convex-concave splitting $\psi'_{\tau h}(\varphi^{k+1},\varphi^k) = \psi'_+(\varphi^{k+1}) + \psi'_-(\varphi^k)$ where $\psi = \psi_+ + \psi_-$ with ψ_+ and $-\psi_-$ being convex functions.

Using the skew-symmetry of the convective term in (37c), an energy-estimate is readily established - with the free energy given by

$$\mathscr{E}(\mathbf{v}^k,\rho^k,\varphi^k) := \frac{1}{2}\int_\Omega \rho(\varphi^k)|\mathbf{v}^k|^2 + \frac{1}{2}\int_\Omega |\nabla\varphi^k|^2 + \int_\Omega \mathscr{I}_h\psi(\varphi^k).$$

Observe that for

$$\rho(\varphi) = \frac{\tilde\rho_+-\tilde\rho_-}{2}\varphi + \frac{\tilde\rho_++\tilde\rho_-}{2}$$

we have positivity of $\rho(\varphi)$ if $\varphi > -(\mathfrak{At})^{-1}$, where

$$\mathfrak{At} := \frac{\tilde\rho_+-\tilde\rho_-}{\tilde\rho_++\tilde\rho_-}$$

for $\tilde\rho_+ \geq \tilde\rho_-$ is the Atwood number. In the engineering literature, it is used to measure density discrepancies of the two liquids involved - an Atwood number 0.998 corresponds to a ratio $\frac{\tilde\rho_+}{\tilde\rho_-} = 1000$.

Hence, the discrete energy estimate in its pure form guarantees stability only for values of $\varphi > -(\mathfrak{At})^{-1}$.

In the continuous setting (assuming in particular a mechanism which confines the values of the phase-field function to the interval $[-1,1]$, for instance by choosing a degenerate mobility or a logarithmic potential ψ), ρ depends linearly on φ via (28) and is therefore bounded from below by a positive constant by definition. In the discrete setting, however, it is not possible to mimic singular or degenerate behaviour – regularization is indispensable. Hence, strict inclusions $\varphi\in[-1,1]$ for

discrete solutions φ cannot be expected in general. Bounds on solutions can only be obtained via integral estimates as the phase-field equation is fourth-order parabolic and therefore comparison principles do not hold. However, the energy of the system is not necessarily decreasing in time due to the work done by external forces. As a consequence, bounds on φ always will depend on the special choice of external forces. Therefore, we use the cut-off mechanism of (H6) to guarantee definiteness of ρ and hence definiteness of the density $\rho|\mathbf{v}|^2$ of the kinetic energy as well.

To proceed, observe that the discretizations of the momentum equation and of the Cahn-Hilliard equation in (37a)-(37d) would decouple if $\mathbf{v}^{k+1}$ was replaced on the left-hand-side of (37a) by a velocity-term not depending on the $(k+1)$th time step in the momentum equation.
Following ideas in [18, 43], see [32], we update the velocity $\mathbf{v}^k$ by adding an additional momentum $\tau\varphi^k\nabla\mu^{k+1}$ divided by a mass density term for which we choose $\rho^k_{\min}$. Summing up, equations (37a)-(37b) are replaced by equation

$$\left(\partial_\tau^-\varphi^{k+1},\theta\right)_h-\int_\Omega\varphi^k\left\langle\mathbf{v}^k,\nabla\theta\right\rangle+\tau\int_\Omega\frac{\left|\varphi^k\right|^2}{\rho^k_{\min}}\left\langle\nabla\mu^{k+1},\nabla\theta\right\rangle+\int_\Omega\left\langle\nabla\mu^{k+1},\nabla\theta\right\rangle=0 \tag{38}$$

for all $\theta\in U_h$, and

$$\left(\mu^{k+1},\theta\right)_h=\int_\Omega\left\langle\nabla\varphi^{k+1},\nabla\theta\right\rangle+\left(\psi'_{\tau h}\left(\varphi^{k+1},\varphi^k\right),\theta\right)_h \tag{39}$$

for all $\theta\in U_h$. One readily obtains a discrete version of the energy estimate.

Lemma 1. *For every $1\le l\le N$ we have*

$$\begin{aligned}
&\frac12\int_\Omega\rho^l\left|\mathbf{v}^l\right|^2+\frac12\int_\Omega\left|\nabla\varphi^l\right|^2+\int_\Omega\mathscr{I}_h\left(\psi_{\tau h}\left(\varphi^l\right)\right)\\
&+\frac{\tau^2}{4}\sum_{m=0}^{l-1}\int_\Omega\rho^m\left|\partial_\tau^-\mathbf{v}^{m+1}\right|^2+\frac{\tau^2}{2}\sum_{m=0}^{l-1}\int_\Omega\left|\partial_\tau^-\nabla\varphi^{m+1}\right|^2+\frac{\tau^2}{3}\sum_{m=0}^{l-1}\int_\Omega\frac{|\varphi^m|^2}{\rho^m_{min}}|\mathbf{j}^{m+1}|^2\\
&\qquad+\tau\sum_{m=0}^{l-1}\int_\Omega2\eta\left(\varphi^{m+1}\right)\left|\mathbf{D}\mathbf{v}^{m+1}\right|^2+\tau\sum_{m=0}^{l-1}\int_\Omega\left|\mathbf{j}^{m+1}\right|^2\\
&\qquad\le\frac12\int_\Omega\rho^0\left|\mathbf{v}^0\right|^2+\frac12\int_\Omega\left|\nabla\varphi^0\right|^2+\int_\Omega\mathscr{I}_h\left(\psi_{\tau h}\left(\varphi^0\right)\right).
\end{aligned}\tag{40}$$

For the resulting splitting scheme which consists of successively computing updates for $\varphi^{k+1}_{\tau h}$ and $\mu^{k+1}_{\tau h}$ and then in a second step for $\mathbf{v}^{k+1}_{\tau h}$, the following convergence results hold true.

Theorem 5. *Let $\Omega\subset\mathbb{R}^d$, $d\in\{2,3\}$ be a convex polyhedral domain and let initial data Φ_0 and $\mathbf{V}_0$ be given. Let $I=(0,T)$ and suppose $(\mathbf{W}_h,S_h)$ to be an admissible pair of discretization spaces in hydrodynamics. Assume that hypotheses (T) and (H1)-(H6) are satisfied and that $(\varphi_{\tau h},\mu_{\tau h},\mathbf{v}_{\tau h})$ is a sequence of discrete solutions to the system* (37)*. Then there is a subsequence which converges in $L^2(\Omega_T)\cap$*

$L^\infty_{weak}(I;H^1))\cap H^1_{weak}(I;L^2(\Omega))\times L^2_{weak}(I;H^1)\times L^2(\Omega_T)\cap L^2_{weak}(I;\mathbf{W}^{1,2}_0(\Omega))$ *to functions* $(\mathbf{v},\varphi,\mu)$ *which solve the system* (8)-(10)*,* (12) *in the following generalized sense.*

$$\begin{aligned}-\iint_{\Omega_T}\langle\rho\mathbf{v}-\rho(\Phi_0)\mathbf{V}_0,\partial_t\mathbf{w}\rangle-\frac{1}{2}\iint_{\Omega_T}\partial_t\rho\langle\mathbf{v},\mathbf{w}\rangle-\frac{1}{2}\iint_{\Omega_T}\rho\Big\langle\mathbf{v},(\nabla\mathbf{w})^T\mathbf{v}\Big\rangle\\ +\frac{1}{2}\iint_{\Omega_T}\rho\Big\langle\mathbf{v},(\nabla\mathbf{v})^T\mathbf{w}\Big\rangle+\frac{1}{2}\iint_{\Omega_T}\frac{\delta\rho}{\delta\varphi}\Big\langle\mathbf{j},(\nabla\mathbf{v})^T\mathbf{w}\Big\rangle-\frac{1}{2}\iint_{\Omega_T}\frac{\delta\rho}{\delta\varphi}\Big\langle\mathbf{j},(\nabla\mathbf{w})^T\mathbf{v}\Big\rangle\\ +\iint_{\Omega_T}2\eta(\varphi)\mathrm{d}\mathbf{v}:\mathrm{d}\mathbf{w}=\iint_{\Omega_T}\mu\langle\nabla\varphi,\mathbf{w}\rangle\end{aligned}\tag{41}$$

for all $\mathbf{w}\in C^1\Big(I;\mathbf{W}^{1,2}_{0,\mathrm{div}}(\Omega)\Big)$ *satisfying* $\mathbf{w}(\cdot,T)=0$*,*

$$\iint_{\Omega_T}\partial_t\varphi\theta+\iint_{\Omega_T}\langle\nabla\varphi,\mathbf{v}\rangle\theta+\iint_{\Omega_T}\langle\nabla\mu,\nabla\theta\rangle=0\tag{42}$$

for all $\theta\in L^2(I;H^1(\Omega))$*, and*

$$\mu(\cdot,t)=-\Delta\varphi(\cdot,t)+\psi'(\varphi(\cdot,t))\tag{43}$$

for almost all $t\in I$*.*

Remark 1. If the solution φ only attains values in the linear regime of ρ, then the weak formulation (41) of the momentum equation simplifies to become

$$\begin{aligned}-\iint_{\Omega_T}\langle\rho\mathbf{v}-\rho(\Phi_0)\mathbf{V}_0,\partial_t\mathbf{w}\rangle-\iint_{\Omega_T}\partial_t\rho\langle\mathbf{v},\mathbf{w}\rangle+\iint_{\Omega_T}\rho\Big\langle\mathbf{v},(\nabla\mathbf{v})^T\mathbf{w}\Big\rangle\\ +\iint_{\Omega_T}\rho'(\varphi)\Big\langle\mathbf{j},(\nabla\mathbf{v})^T\mathbf{w}\Big\rangle+\iint_{\Omega_T}2\eta(\varphi)\mathbf{D}\mathbf{v}:\mathbf{D}\mathbf{w}=\iint_{\Omega_T}\mu\langle\nabla\varphi,\mathbf{w}\rangle\end{aligned}\tag{44}$$

for all $\mathbf{w}\in C^1\Big(I;W^{1,2}_{0,\mathrm{div}}(\Omega)\Big)$ satisfying $\mathbf{w}(\cdot,T)=0$.

Remark 2. In [28], a different splitting scheme has been suggested. It is a fully linear and stable, convergence, however, has not been studied, yet.

It is worth mentioning that this result and its predecessor - an analogous result for the scheme using the discrete Cahn-Hilliard equation (37a) - are - to the best of our knowledge - the only convergence results for numerical schemes for two-phase flows with different mass densities obtained so far.

Let us make some comments on the proof of Theorem 5. Naively, one would be tempted first to look for time compactness of the velocity field $\mathbf{v}_{\tau h}$. Obtaining formally only $(H^1)'$-regularity for time-derivatives of φ by the standard estimates of the Cahn-Hilliard equation, it seems necessary to control $\langle\mathbf{v}^{k+1},\mathbf{w}_h\rangle$ in H^1. As $\mathbf{w}_h$ is the projection of an arbitrary element in $W^{1,2}_{0,\mathrm{div}}(\Omega)$ onto the space of discretely solenoidal vector fields, this is not possible. Hence, we look for higher regularity for φ. We have (see [29] and [32])

Lemma 2. *Let* $(\varphi_{\tau h}, \mu_{\tau h}, \mathbf{v}_{\tau h}, p_{\tau h})$ *be a discrete solution of* (37) *on* $[0,T]$. *Then the sum*

$$\|\varphi_{\tau h}\|_{L^4(0,T;L^\infty(\Omega))} + \|\Delta_h \varphi_{\tau h}\|_{L^\infty(0,T;L^2(\Omega))} + \|\partial_\tau^- \varphi_{\tau h}\|_{L^2(\Omega_T)}$$

is uniformly bounded in $(\tau, h) \to (0,0)$.

As a direct consequence, the discrete Laplacian of the chemical potential $\mu_{\tau h}$ can be bounded in $L^2(\Omega_T)$. Combining this result with a discrete Gagliardo-Nirenberg inequality, the fluxes $\mathbf{j}_{\tau h}$ are proven to converge - up to a subsequence - strongly in $L^2(0,T;L^2(\Omega))$. This allows us to pass to the limit in the $\mathbf{j}_{\tau h}(\nabla \mathbf{v}_{\tau h})^T$-term in the momentum equation.
Concerning the passage to the limit in the parabolic term of the momentum equation, it is sufficient to establish strong convergence of the discrete Helmholtz projection of $\rho_{\tau h}\mathbf{v}_{\tau h}$ towards the Helmholtz projection of $\rho\mathbf{v}$ which is achieved in Lemma 4.8 of [29].

Practical computations have been performed using the inhouse finite-element/finite-volume code EconDrop developed by G. Grün, F. Klingbeil, S. Metzger with contributions by H. Grillmeier and P. Weiss (see [30]). The scheme allows for adaptivity in space and time.
Let us discuss some aspects related to simulations of falling droplets. Due to numerical dissipation, the energy estimate (40) differs from its continuous counterpart in particular by showing an inequality sign. A practical consequence is evident: The higher the numerical dissipation, the lower the kinetic energy and the velocity of falling droplets. As a consequence, one is tempted to reduce numerical dissipation caused by the double-well potential ψ as much as possible – see [33]. For the classical double well potential $\psi_{class}(\varphi) := \frac{1}{4}(1-\varphi^2)^2$, a reduction to zero is possible by discretizing ψ'_{class} by

$$\begin{aligned}\psi'_{dis}(\varphi^{k+1}, \varphi^k) &= \frac{\psi_{class}(\varphi^{k+1}) - \psi_{class}(\varphi^k)}{\varphi^{k+1} - \varphi^k} \\ &= \tfrac{1}{4}\left((\varphi^{k+1})^3 + (\varphi^{k+1})^2\varphi^k + \varphi^{k+1}(\varphi^k)^2 + (\varphi^k)^3\right) - \tfrac{1}{2}\left(\varphi^{k+1} - \varphi^k\right).\end{aligned}$$

In [32], this approach has been tested for two-phase flow with an Atwood number $\mathfrak{At} = 0.999$, i.e. corresponding to a density ratio above 1000. It turns out that φ^k does not stay in the admissible interval $(-\mathfrak{At}^{-1}, \mathfrak{At}^{-1})$ where ρ is linear. As a consequence, modified energies have been studied in [32] as well. By adding a penalty term, we get

$$\psi_{pen}(\varphi) := \psi_{class}(\varphi) + \tfrac{1}{\delta}\max\{|\varphi| - 1, 0\}^2$$

to be a natural candidate. This leads to discretizations

$$\psi'_{dis,pen}(a,b) := \psi'_{dis}(a,b) + \tfrac{1}{\delta}\tfrac{d}{d\varphi}|_{\varphi=a}\max\{|\varphi| - 1, 0\}^2$$

and secondly

$$\psi'_{conv,pen}(a,b) := \psi'_{pen}(a) - \tfrac{1}{2}(a+b).$$

Decomposing $\psi_{pen}(\varphi) = \psi_+(\varphi) + \psi_-(\varphi)$ into a sum of a convex and concave function with the concave part given by $\psi_-(\varphi) := -\frac{1}{2}\varphi^2$, we note the discretization $\psi'_{dis,pen}$ to be close to the classical convex-concave splitting $\psi_{pen}(a,b) = \psi_+(a) + \psi_-(b)$. Numerical experiments on falling droplets presented in [32] indicate that already for parameters $\delta = 4 \cdot 10^{-3}$ φ-stability is achieved with φ staying bounded in $(-1.\overline{001}, 1.\overline{001})$ which corresponds to an Atwood number $\mathfrak{At} = 0.999$. Moreover, only negligible differences in falling velocities have been observed when comparing results corresponding to non-dissipative schemes with those corresponding to a discretization using ψ'_{dis}.

Finally, let us indicate that the scheme based on $\psi'_{dis,pen}$ has been implemented in rotational geometry, too. Figure 1 shows a characteristic sequence of a falling droplet entering a bath – an example for topological changes. The computational domain is given by $\Omega := \{\mathbf{x} \in \mathbb{R}^3 : x_1^2 + x_3^2 < 1, 0 < x_2 < 6\}$ with the gravitational acceleration $(0,-10,0)$. As initial data for fluid phase 1, we take a ball around $(0,0,5)$ of radius 0.3 and a bath of depth 2. The adaptive spatial grid attains grid parameters in $(0.0045, 0.0714)$, and the density ratio is 3.

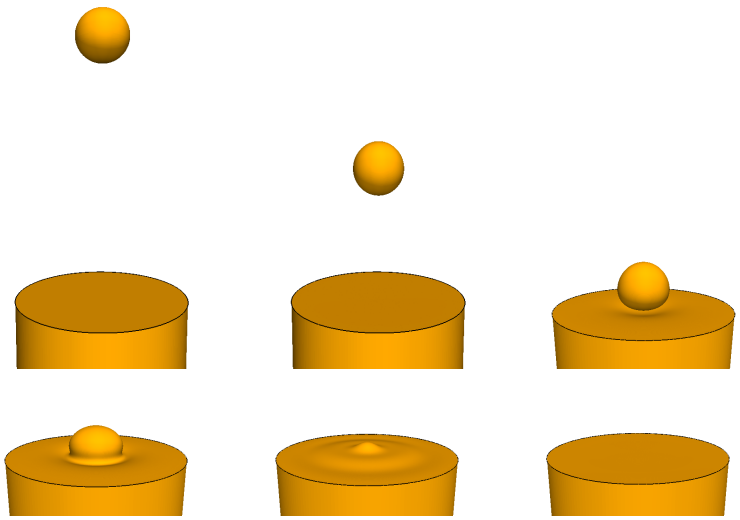

Fig. 1: Falling droplet at times $t = 0.0$, 1.1, 1.75 1.85, 1.95, 3.0. Discretization based on $\psi_{dis,pen}$ with $\delta = 4 \cdot 10^{-3}$.

6 Appendix

6.1 Discretization in space and time

We assume $\mathscr{T}_h$ to be a quasiuniform triangulation of Ω with simplicial elements in the sense of [21].
Concerning discretization with respect to time, we assume that

(T) the time interval $I := [0,T)$ is subdivided in intervals $I_k = [t_k, t_{k+1})$ with $t_{k+1} = t_k + \tau_k$ for time increments $\tau_k > 0$ and $k = 0, \cdots, N-1$. For simplicity, we take $\tau_k \equiv \tau$ for $k = 0, \cdots, N-1$.

We write v^k for $v(\cdot, k\tau)$, $k \in \mathbb{N}$, and we denote step functions in time mapping $I = [0,T]$ onto one of the discrete function spaces X_h, ... by an index τh.
For the approximation of both the phase-field φ and the chemical potential μ, we introduce the space U_h of continuous, piecewise linear finite element functions on $\mathscr{T}_h$. The expression $\mathscr{I}_h$ stands for the nodal interpolation operator from $C^0(\Omega)$ to U_h defined by $\mathscr{I}_h u := \sum_{j=1}^{\dim U_h} u(x_j)\theta_j$, where the functions θ_j form a dual basis to the nodes x_j, i.e. $\theta_i(x_j) = \delta_{ij}$, $i, j = 1, \ldots, \dim U_h$.
Let us furthermore introduce the well–known lumped masses scalar product corresponding to the integration formula

$$(\Theta, \Psi)_h := \int_\Omega \mathscr{I}_h(\Theta\Psi).$$

For the discretization of the velocity field $\mathbf{v}$ and the pressure p, we use function spaces $\mathbf{W}_h \subset \mathbf{X}_h \subset \mathbf{W}_0^{1,2}(\Omega)$ and $S_h \subset L_0^2(\Omega) := \{v \in L^2(\Omega) | \int_\Omega v = 0\}$ which form an *admissible pair of discretization spaces in hydrodynamics*. This means that besides the conditions

(S1) $\mathbf{W}_h := \{\mathbf{v}_h \in \mathbf{X}_h | \int_\Omega q_h \operatorname{div} \mathbf{v}_h = 0 \quad \forall q_h \in S_h\}$,
(S2) The Babuška-Brezzi condition is satisfied, i.e. a positive constant β exists such that

$$\sup_{\mathbf{v}_h \in \mathbf{X}_h} \frac{(q_h, \operatorname{div} \mathbf{v}_h)}{\|\mathbf{v}_h\|_{\mathbf{W}_0^{1,2}(\Omega)}} \geq \beta \, \|q_h\|_{L^2(\Omega)}$$

for all $q_h \in S_h$

a number of additional conditions hold true which are specified in [29] and [32].

Taylor-Hood elements (i.e. P_2P_1-elements) and P_2P_0-elements are examples in agreement with these conditions. In both cases, $\mathbf{X}_h$ is given as

$$\mathbf{X}_h := \left\{ \mathbf{w} \in (\mathbf{C}_0^0(\bar{\Omega})) : (\mathbf{w})_j|_K \in P_2(K), K \in \mathscr{T}_h, j = 1, \ldots, d \right\}, \quad d = 2, 3.$$

For Taylor-Hood elements, S_h is defined to be the subset of functions in U_h with vanishing mean value. In the case of P_2P_0-elements, S_h is given by the set of ele-

mentwise constant functions with mean value zero. Let us specify the assumptions on initial data and the double-well potential.

Definition 1. Let $\psi \in C^1(\mathbb{R};\mathbb{R}_0^+)$ be given such that ψ' is piecewise C^1 with at most quadratic growth of the derivatives for $|x| \to \infty$. We call $\psi'_{\tau h} \in C^0(\mathbb{R}^2;\mathbb{R})$ an admissible discretization of ψ' if the following is satisfied.

(H1) There is a positive constant C, such that

$$\left|\psi'_{\tau h}(a,b)\right| \leq C\Big(1+|a|^3+|b|^3\Big).$$

(H2) $\psi'_{\tau h}(a,b)(a-b) \geq F(a)-F(b)$ for all $a,b \in \mathbb{R}$.
(H3) $\psi'_{\tau h}(a,b) = F'(a)$ for all $a \in \mathbb{R}$.
(H4) There is a positive constant C such that

$$\left|\psi'_{\tau h}(a,b)-\psi'_{\tau h}(b,c)\right| \leq C\left(a^2+b^2+c^2\right)\left(|a-b|+|b-c|\right)$$

for all $a,b,c \in \mathbb{R}$.

Moreover, we make the following assumptions on initial data and the regularized mass density $\rho(\varphi)$.

(H5) Let initial data $\Phi_0 \in H^2(\Omega;[-1,1])$ and $\mathbf{V}_0 \in \mathbf{W}^{1,2}_{0,\mathrm{div}}(\Omega)$ be given such that we have for discrete initial data $\varphi_h^0 := \mathscr{I}_h\Phi_0$ and $\mathbf{v}_h^0$ – given by the orthogonal projection of $\mathbf{V}_0$ onto $\mathscr{W}_h$ – uniformly in $h>0$ that

$$\int_\Omega \left|\Delta_h\varphi_h^0\right|^2 \leq C\|\Phi_0\|^2_{H^2(\Omega)}$$

and that

$$\int_\Omega \rho(\varphi_h^0)\left|\mathbf{v}_h^0\right|^2 + \frac{1}{2}\int_\Omega \left|\nabla\varphi_h^0\right|^2 + \int_\Omega \mathscr{I}_h F(\varphi_h^0) \leq C\mathscr{E}(\mathbf{V}_0,\Phi_0).$$

Here, the discrete Laplacian $\Delta_h w \in U_h \cap H^1_*(\Omega)$ is defined by

$$(\Delta_h w,\Theta)_h = -\int_\Omega \langle\nabla w,\nabla\Theta\rangle \quad \forall\Theta \in U_h. \tag{45}$$

(H6) Given mass densities $0<\tilde\rho_- \leq \tilde\rho_+ \in \mathbb{R}$ of the fluids involved and an arbitrary, but fixed regularization parameter $\bar\varphi \in \left(\frac{\tilde\rho_-}{\tilde\rho_+-\tilde\rho_-}, \frac{2\tilde\rho_-}{\tilde\rho_+-\tilde\rho_-}\right)$, we define the regularized mass density of the two-phase fluid by a smooth, increasing, strictly positive function ρ of the phase-field φ which satisfies

$$\rho(\varphi)|_{(-1-\bar\varphi,1+\bar\varphi)} = \frac{\tilde\rho_+-\tilde\rho_+}{2}\varphi + \frac{\tilde\rho_-+\tilde\rho_+}{2}, \tag{46}$$

$$\rho(\varphi)\big|_{\left(-\infty,-1-\frac{2\tilde\rho_-}{\tilde\rho_+-\tilde\rho_-}\right)} \equiv const., \tag{47}$$

$$\rho(\varphi)\big|_{\left(1+\frac{2\tilde\rho_-}{\tilde\rho_+-\tilde\rho_-},\infty\right)} \equiv const.. \tag{48}$$

Acknowledgements This work was supported within the DFG Priority Program 1506 "Transport Processes at Fluidic Interfaces".

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