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A Diffuse-Interface Approach for Solid-State Dewetting with Anisotropic Surface Energies

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Abstract

We present a diffuse-interface model for the solid-state dewetting problem with anisotropic surface energies in $\mathbb{R}^d$ for $d \in \{2, 3\}$. The introduced model consists of the anisotropic Cahn–Hilliard equation, with either a smooth or a double-obstacle potential, together with a degenerate mobility function and appropriate boundary conditions on the wall. Upon regularizing the introduced diffuse-interface model, and with the help of suitable asymptotic expansions, we recover as the sharp-interface limit the anisotropic surface diffusion flow for the interface together with an anisotropic Young's law and a zero-flux condition at the contact line of the interface with a fixed external boundary. Furthermore, we show the existence of weak solutions for the regularized model, for both smooth and obstacle potential. Numerical results based on an appropriate finite element approximation are presented to demonstrate the excellent agreement between the proposed diffuse-interface model and its sharp-interface limit.

Keywords Solid-state dewetting · Cahn–Hilliard equation · Anisotropy · Sharp-interface limit · Weak solutions · Finite element method

Mathematics Subject Classification 35K61 · 35K65 · 35C20 · 49J40 · 74E10 · 65M60

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1 Introduction

Deposited solid thin films are unstable and could dewet to form isolated islands on the substrate in order to minimize the total surface energy (Leroy et al. 2016; Thompson 2012). This phenomenon is known as solid-state dewetting (SSD), since the thin films remain in a solid state during the process. SSD has attracted a lot of attention recently and is emerging as a promising route to produce patterns of arrays of particles used in sensor technology, optical and magnetic devices, and catalyst formations, see, e.g., Armelao et al. (2006), Benkouider et al. (2015), Schmidt et al. (2009), Bollani et al. (2019), Salvalaglio et al. (2020), Backofen et al. (2017).

The dominant mass transport mechanism in SSD is surface diffusion (Srolovitz and Safran 1986). This evolution law was first introduced by Mullins (1957) to describe the mass diffusion within interfaces in polycrystalline materials. For surface diffusion, the normal velocity of the interface is proportional to the surface Laplacian of the mean curvature. In the case of SSD, the evolution of the interface that separates the thin film from the surrounding vapor also involves the motion of the contact line, i.e., the region where the film/vapor interface meets the substrate. The equilibrium contact angle is given by Young's law which prescribes a force balance along the substrate. Many efforts have been devoted to SSD problems in recent years. For example, a large body of experiments have revealed that the pattern formations could depend highly on the crystallographic alignments, the film sizes and shapes, as well as the substrate topology, see, e.g., Ye and Thompson (2011), Amram et al. (2012), Thompson (2012), Naffouti et al. (2017), Bollani et al. (2019). In addition, mathematical studies based on different models have been considered in Srolovitz and Safran (1986), Burger (2005), Dornel et al. (2006), Fonseca et al. (2012), Jiang et al. (2012), Naffouti et al. (2017), Boccardo et al. (2022), Jiang and Zhao (2019), Wang et al. (Jan 2015), Jiang et al. (2020), Dziwnik et al. (2017).

In this work, we aim to study the SSD problem with anisotropic surface energies in the diffuse-interface framework. In the isotropic case, diffuse-interface models are based on the Ginzburg–Landau energy

$$\mathcal{E}_{\mathrm{iso}}(\varphi) = \int_{\Omega} \frac{\varepsilon}{2}|\nabla\varphi|^2 + \varepsilon^{-1} F(\varphi)\,\mathrm{d}x, \tag{1.1}$$

where $\Omega \subset \mathbb{R}^d$ is a given domain with $d \in \{2, 3\}$, $\varphi : \Omega \to \mathbb{R}$ is the order parameter, $\varepsilon > 0$ is a small parameter proportional to the thickness of the interfacial layer, and $F(\varphi)$ is the free energy density. The following three choices for F are mainly used in the literature:

(i) The smooth double-well potential (Taylor and Cahn 1994)

$$F(\varphi) = \frac{1}{2}(1-\varphi^2)^2, \tag{1.2a}$$

which has two global minimum points at $\varphi = \pm 1$ and a local maximum point at $\varphi = 0$;

(ii) The logarithmic potential (Cahn and Hilliard 1958)

$$F(\varphi) = \frac{1}{2}\theta\left[(1+\varphi)\,\log(1+\varphi) + (1-\varphi)\,\log(1-\varphi)\right] + \frac{1}{2}(1-\varphi^2), \tag{1.2b}$$

where $\theta > 0$ is the absolute temperature. This potential has two minima $\varphi = \pm(1-\tilde{k}(\theta))$, where $\tilde{k}(\theta)$ is a small positive real number satisfying $\tilde{k}(\theta) \to 0$ as $\theta \to 0$, and its usage enforces φ to attain values within $(-1, 1)$;

(iii) The double-obstacle potential (Blowey and Elliott 1991)

$$F(\varphi) = \begin{cases} \frac{1}{2}(1-\varphi^2) & \text{if } |\varphi| \le 1, \\ \infty & \text{otherwise.} \end{cases} \tag{1.2c}$$

It can be characterized via the *deep quench limit* of the logarithmic potential, i.e., the limit of (1.2b) as $\theta \to 0$.

The (isotropic) Cahn–Hilliard equation can be interpreted as a weighted H^{-1}-gradient flow of the free energy (1.1). It reads as

$$\partial_t \varphi = \nabla \cdot (m(\varphi)\,\nabla \mu), \qquad \mu = -\varepsilon \Delta \varphi + \varepsilon^{-1} F'(\varphi), \tag{1.3}$$

where $m(\varphi)$ is a mobility function, together with Neumann boundary conditions for μ and φ. The Cahn–Hilliard equation was first introduced to study the spinodal decomposition in binary alloys (Cahn and Hilliard 1958; Cahn 1961) and has since then been used to model many other phenomenon, e.g., Abels et al. (2012), Garcke and Novick-Cohen (2000), Khain and Sander (2008), Bertozzi et al. (2006). We note that the double-obstacle potential is not differentiable at $\varphi = \pm 1$, and the definition of the generalized chemical potential in this case becomes

$$\mu \in -\varepsilon \Delta \varphi + \varepsilon^{-1} \partial F(\varphi), \tag{1.4}$$

where $\partial F(\varphi)$ is the Fréchet sub-differential of F at φ and $\Delta\varphi$ has to be understood in a weak sense, see Blowey and Elliott (1991), Barrett et al. (2013). In the case of a constant mobility $m(\varphi) \equiv 1$, (1.3) converges to the Mullins–Sekerka problem (Mullins and Sekerka 1963) as $\varepsilon \to 0$ (Pego 1989; Alikakos et al. 1994). In order to obtain the surface diffusion equation in the sharp-interface limit, a degenerate mobility needs to be chosen. For example, it was shown in Cahn et al. (1996) by a formal asymptotic analysis that the surface diffusion flow is recovered by considering a slow time scale $\tau = O(\varepsilon^{-1}t)$ of (1.3) with $m(\varphi) = (1-\varphi^2)_+$ and with the potential $F(\varphi)$ either chosen as in (1.2c), or as in (1.2b) with $\theta = O(\varepsilon^{\xi})$, $\xi > 0$. When using the smooth double-well potential (1.2a), the situation is less clear. While the limiting motion of surface diffusion is obtained with the choice $m(\varphi) = (1-\varphi^2)^2$ (Voigt 2016; Rätz et al. 2006; Jiang et al. 2012; Dai and Du 2014), using the less degenerate mobility $m(\varphi) = (1-\varphi^2)_+$ may not lead to pure surface diffusion in the limit $\varepsilon \to 0$, since an additional bulk diffusion term is conjectured to be present due to the nonzero-flux contributions (Dai and Du 2014; Lee et al. 2015, 2016). However, in all these

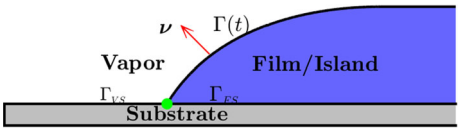

Fig. 1 Sketch of the structure for SSD near the contact line (green point), where the vapor, film and substrate phases meet (Color figure online)

cases, no rigorous proof for the sharp-interface limit or the presence of nonzero-flux contributions is available so far.

A natural generalization of the free energy (1.1) to the case of anisotropic surface energies is given by

$$\mathcal{E}_\gamma(\varphi) = \int_\Omega \frac{\varepsilon}{2}|\gamma(\nabla\varphi)|^2 + \varepsilon^{-1}F(\varphi)\,\mathrm{d}x = \int_\Omega \varepsilon A(\nabla\varphi) + \varepsilon^{-1}F(\varphi)\,\mathrm{d}x, \tag{1.5}$$

see, e.g., Kobayashi (1993), Elliott (1997). Here, $\gamma : \mathbb{R}^d \to [0,\infty)$ is the anisotropic density function, which is positively homogeneous of degree one, and $A := \frac{1}{2}\gamma^2$. This then gives rise to the anisotropic Cahn–Hilliard equation

$$\partial_t\varphi = \nabla\cdot(m(\varphi)\nabla\mu), \qquad \mu = -\varepsilon\nabla\cdot A'(\nabla\varphi) + \varepsilon^{-1}F'(\varphi), \tag{1.6}$$

where A' represents the gradient of the map $A : \mathbb{R}^d \to [0,\infty)$. In contrast to the isotropic case, diffuse-interface models based on (1.5) result in a nonuniform asymptotic interface thickness, which in fact depends on the anisotropic density function $\gamma(\nabla\varphi)$, see Wheeler and McFadden (1996), Wheeler (2006), Bellettini and Paolini (1996), Elliott and Schätzle (1996), Alfaro et al. (2010). To remedy this issue, an alternative energy of the form

$$\widetilde{\mathcal{E}}_\gamma(\varphi) = \int_\Omega |\nabla\varphi|^{-1}\gamma(\nabla\varphi)\left(\frac{\varepsilon}{2}|\nabla\varphi|^2 + \varepsilon^{-1}F(\varphi)\right)\mathrm{d}x \tag{1.7}$$

can be considered, see Torabi et al. (2009), Salvalaglio et al. (2015), so that a constant thickness of the asymptotic interface is achieved. However, the resulting diffuse-interface models based on (1.7) become more nonlinear and are singular at $\nabla\varphi = 0$, which poses great challenges in the mathematical analysis and the stable numerical approximation. Therefore, in this work, we will restrict ourselves to the classical energy in (1.5). We also note that to guarantee that (1.6) converges to the anisotropic surface diffusion flow as $\varepsilon \to 0$, a rescaled anisotropic coefficient needs to be introduced to the degenerate mobility (Rätz et al. 2006; Li et al. 2009). We refer to Sect. 2 below for the precise details.

When it comes to SSD, as shown in Fig. 1, the total surface energy of the system consists of the film/vapor interface energy $\mathcal{E}_{\mathrm{inf}}$ and the substrate energy $\mathcal{E}_{\mathrm{sub}}$,

$$\mathcal{E}_{\mathrm{inf}} = \int_{\Gamma(t)} \gamma(\boldsymbol{\nu})\,\mathrm{d}S, \qquad \mathcal{E}_{\mathrm{sub}} = \gamma_{FS}\int_{\Gamma_{FS}}\mathrm{d}S + \gamma_{VS}\int_{\Gamma_{VS}}\mathrm{d}S, \tag{1.8}$$

where $\Gamma(t)$ is the dynamic film/vapor interface with $\boldsymbol{\nu}$ being the interface normal pointing into the vapor phase, Γ_{FS} and Γ_{VS} are the interfaces between film/substrate

and vapor/substrate, respectively, and γ_{FS} and γ_{VS} are the corresponding surface energy densities. In order to model SSD by the diffuse-interface approach, we associate the vapor phase with $\varphi \approx 1$ and the film phase with $\varphi \approx -1$. Then, the Ginzburg–Landau type energy (1.5), up to a multiplicative constant, will approximate the sharp-interface energy $\mathcal{E}_{\text{inf}}$. Moreover, the contribution to the wall energy $\mathcal{E}_{\text{sub}}$ can be approximated by

$$\mathcal{E}_w(\varphi) = \int_{\Gamma_{FS} \cup \Gamma_{VS}} \frac{\gamma_{VS} + \gamma_{FS}}{2} + (\gamma_{VS} - \gamma_{FS}) G(\varphi) \, \mathrm{d}S, \tag{1.9}$$

where $G(\varphi)$ is a smooth function satisfying $G(\pm 1) = \pm \frac{1}{2}$, see Jiang et al. (2012), Dziwnik et al. (2017), Huang et al. (2019), Backofen et al. (2017) for SSD and (Jacqmin 2000; Qian et al. 2003) for moving contact lines in fluid mechanics.

There are several results on the existence of weak solutions for the degenerate Cahn–Hilliard equation (1.3) with homogeneous boundary conditions or its variants with inhomogeneous boundary conditions, see Elliott and Garcke (1996), Dai and Du (2016), Yin (1992). However, little is known about the anisotropic case except the work in Dziwnik (2019) which focuses on a particular n-fold anisotropy in two space dimensions.

The main aim of this work is to develop a diffuse-interface approach to SSD in the case of anisotropic surface energies based on the energy contributions (1.5) and (1.9). The obtained diffuse-interface model consists of a degenerate anisotropic Cahn–Hilliard equation with appropriate boundary conditions. We study the sharp-interface limit and show the existence of weak solutions to the diffuse-interface model.

The rest of the paper is organized as follows. In Sect. 2, we review a sharp-interface model for SSD and then introduce a diffuse-interface model based on a gradient flow approach. We then derive the sharp-interface limit from a regularized model with the help of asymptotic expansions in Sect. 3. In Sect. 4, we prove the existence of weak solutions to the diffuse-interface model. Numerical tests are presented in Sect. 5, where a comparison between sharp-interface approximations and diffuse-interface approximations is made.

2 Modeling Aspects

In this section, we first review a sharp-interface model for SSD with anisotropic surface energies in two or three space dimensions. Then, we propose a suitable diffuse-interface model to approximate this sharp-interface model. Here, we note that there exist several works on the modeling of SSD using a diffuse-interface approach in the literature. However, these works consider either the isotropic case, e.g., Jiang et al. (2012), Backofen et al. (2017), or the anisotropic case in 2d, e.g., Dziwnik et al. (2017).

2.1 The Sharp-Interface Model

We consider the dewetting of a solid thin film on a flat substrate in $\mathbb{R}^d$ with $d \in \{2, 3\}$, as shown in Fig. 1. We parameterize the interface of $\Gamma(t)$ over the initial interface as follows

$$\mathbf{x}(\cdot, t) \,:\, \Gamma(0) \times [0, T] \to \mathbb{R}^d,$$

where $T > 0$ is a prescribed final time. The induced velocity is then given by

$$\mathbf{V}(\mathbf{x}(\mathbf{q}, t), t) = \partial_t \mathbf{x}(\mathbf{q}, t) \qquad \text{for all} \quad \mathbf{q} \in \Gamma(0), \quad t \in [0, T],$$

where $\Gamma(0)$ is a smooth hypersurface with boundary. The sharp-interface model for SSD (cf. Cahn and Taylor 1994; Taylor and Cahn 1994; Barrett et al. 2010a; Jiang et al. 2020) reads as

$$\mathcal{V} = -\nabla_s \cdot (D(\boldsymbol{\nu})\, \nabla_s \varkappa_\gamma), \tag{2.1a}$$

$$\varkappa_\gamma = -\nabla_s \cdot \gamma'(\boldsymbol{\nu}), \tag{2.1b}$$

which has to hold for all $t \in [0, T]$ and all points on $\Gamma(t)$. Here, $\mathcal{V} = \mathbf{V} \cdot \boldsymbol{\nu}$ is the normal velocity, $\boldsymbol{\nu}$ is the unit normal to $\Gamma(t)$ pointing into the vapor, and ∇_s is the surface gradient operator on $\Gamma(t)$. Besides, $D(\boldsymbol{\nu})$ is an orientation-dependent mobility (cf. Taylor and Cahn 1994). The function D needs to be defined for unit vectors, but here, we extend its domain to $\mathbb{R}^d$ such that it is positively homogeneous of degree one. The term $\varkappa_\gamma$ represents the anisotropic mean curvature, and $\gamma'(\boldsymbol{\nu})$ is the Cahn–Hoffman vector, where γ' denotes the gradient of γ (cf. Hoffman and Cahn 1972). The above equations are subject to the following boundary conditions at the contact line, where the film/vapor interface $\Gamma(t)$ meets the substrate:

- Attachment condition

$$\mathbf{V} \cdot \mathbf{n}_w = 0, \tag{2.2a}$$

- Contact angle condition

$$\gamma'(\boldsymbol{\nu}) \cdot \mathbf{n}_w + \sigma = 0, \tag{2.2b}$$

- Zero-flux condition

$$D(\boldsymbol{\nu})\, \nabla_s \varkappa_\gamma \cdot \mathbf{n}_c = 0, \tag{2.2c}$$

where

$$\sigma = \gamma_{VS} - \gamma_{FS} \tag{2.3}$$

denotes the difference of the substrate energy densities across the contact line. Here, $\mathbf{n}_w$ is the unit normal to the substrate and points in the direction of the substrate,

and $\mathbf{n}_c$ is the conormal vector of $\Gamma(t)$, i.e., it is the outward unit normal to $\partial\Gamma(t)$ and it lies within the tangent plane of $\Gamma(t)$. We observe that (2.2b) enforces an angle condition between the Cahn–Hoffman vector $\gamma'(\boldsymbol{\nu})$ and the substrate unit normal $\mathbf{n}_w$. For example, in the isotropic case, $\gamma(\mathbf{p}) = |\mathbf{p}|$, the Cahn–Hoffman vector reduces to the normal $\boldsymbol{\nu}$, and so if $\sigma = 0$, the condition (2.2b) encodes a 90° contact angle between the film/vapor interface and the substrate.

We assume that the anisotropy function γ that belongs to $C^2\big(\mathbb{R}^d\setminus\{\mathbf{0}\}\big)\cap C(\mathbb{R}^d, \mathbb{R}_{\geq 0})$ is convex and satisfies $\gamma > 0$ on $\mathbb{R}^d \setminus \{\mathbf{0}\}$. We further assume that γ is positively homogeneous of degree one, meaning that

$$\gamma(\lambda\mathbf{p}) = \lambda\gamma(\mathbf{p}) \quad \text{for all } \lambda > 0, \mathbf{p} \in \mathbb{R}^d.$$

This immediately implies $\gamma(\mathbf{0}) = 0$ and the gradient of $\gamma(\mathbf{p})$ satisfies

$$\gamma'(\mathbf{p}) \cdot \mathbf{p} = \gamma(\mathbf{p}) \quad \text{for all } \mathbf{p} \in \mathbb{R}^d \setminus \{\mathbf{0}\}. \tag{2.4}$$

Similarly, the orientation-dependent mobility function $D \in C^2\big(\mathbb{R}^d \setminus \{\mathbf{0}\}\big) \cap C(\mathbb{R}^d, \mathbb{R}_{\geq 0})$ is assumed to satisfy $D > 0$ on $\mathbb{R}^d \setminus \{\mathbf{0}\}$ and

$$D(\lambda\mathbf{p}) = \lambda D(\mathbf{p}) \quad \text{for all } \lambda > 0, \mathbf{p} \in \mathbb{R}^d.$$

Consequently, for the map

$$A : \mathbb{R}^d \to \mathbb{R}, \quad \mathbf{p} \mapsto \tfrac{1}{2}\gamma^2(\mathbf{p}) \tag{2.5}$$

introduced in (1.5), we have $A \in C^2\big(\mathbb{R}^d \setminus \{\mathbf{0}\}\big) \cap C(\mathbb{R}^d, \mathbb{R}_{\geq 0})$. It also follows directly from (2.4) that the relations

$$A(\lambda\mathbf{p}) = \lambda^2 A(\mathbf{p}), \qquad A'(\mathbf{p}) = \gamma(\mathbf{p})\gamma'(\mathbf{p}), \qquad A'(\mathbf{p}) \cdot \mathbf{p} = 2A(\mathbf{p}), \tag{2.6a}$$

$$A'(\lambda\mathbf{p}) = \lambda A'(\mathbf{p}), \qquad A''(\lambda\mathbf{p}) = A''(\mathbf{p}), \qquad A''(\mathbf{p})\mathbf{p} = A'(\mathbf{p}) \tag{2.6b}$$

hold for all $\mathbf{p} \in \mathbb{R}^d \setminus \{\mathbf{0}\}$ and all $\lambda > 0$. Here, A' and A'' denote the gradient and the Hessian of A, respectively.

2.2 The Diffuse-Interface Model

Let $\varphi : \Omega \times [0, T] \to \mathbb{R}$ be an order parameter such that the zero level set $\{\mathbf{x} \in \Omega : \varphi(\mathbf{x}, t) = 0\}$ approximates the film/vapor interface $\Gamma(t)$, $\{\mathbf{x} \in \Omega : \varphi(\mathbf{x}, t) < 0\}$ corresponds to the region occupied by the thin film at time t, whereas $\{\mathbf{x} \in \Omega : \varphi(\mathbf{x}, t) > 0\}$ represents the region occupied by the vapor at time t (see Fig. 2). In addition, $\Gamma_w \subset \partial\Omega$ models the boundary of the substrate. As a combination of (1.5)

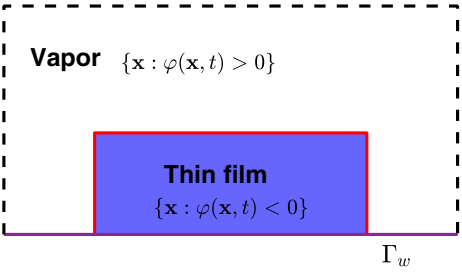

Fig. 2 Geometric setup for SSD in a bounded domain Ω with $\Omega = \overline{\Omega_-}(t) \cup \overline{\Omega_+}(t)$, where $\Omega_-(t) := \{\mathbf{x} \in \Omega : \varphi(\mathbf{x}, t) < 0\}$ and $\Omega_+(t) := \{\mathbf{x} \in \Omega : \varphi(\mathbf{x}, t) > 0\}$

and (1.9), the total free energy of the system is given by

$$\begin{aligned}\mathcal{E}(\varphi) :=& \frac{1}{c_F}\mathcal{E}_\gamma(\varphi) + \mathcal{E}_w(\varphi) - \gamma_{VS}|\Gamma_w| \\ =& \frac{1}{c_F}\int_\Omega \varepsilon A(\nabla\varphi) + \varepsilon^{-1}F(\varphi)\,\mathrm{d}x + \sigma\int_{\Gamma_w} G(\varphi)\,\mathrm{d}S - \frac{\sigma}{2}|\Gamma_w|, \end{aligned} \tag{2.7}$$

where $c_F = \int_{-1}^{1}\sqrt{2F(s)}\,\mathrm{d}s$ and $|\Gamma_w| = \int_{\Gamma_w}\mathrm{d}S$. This choice of c_F ensures that

$$\frac{1}{c_F}\mathcal{E}_\gamma(\varphi) \approx \int_{\Gamma(t)} \gamma(\boldsymbol{\nu})\,\mathrm{d}S$$

for sufficiently small $\varepsilon > 0$. Besides, the constant term $-\gamma_{VS}|\Gamma_w|$ was added to the total energy such that $\mathcal{E}(\varphi)$ now only depends on the single parameter σ (see (2.3)) instead of on γ_{VS} and γ_{FS}. We next derive the diffuse-interface model. To this end, we use the smooth double-well potential

$$F(\varphi) = \frac{1}{2}(1-\varphi^2)^2. \tag{2.8}$$

This implies

$$c_F = \int_{-1}^{1}\sqrt{2F(s)}\,\mathrm{d}s = \frac{4}{3}.$$

We further choose

$$G(\varphi) = \frac{1}{4}(3\varphi - \varphi^3), \tag{2.9}$$

which yields $G(\pm 1) = \pm\frac{1}{2}$ and $G'(\pm 1) = 0$. Let $\psi : \Omega \to \mathbb{R}$ be a sufficiently smooth function. Then, the first variation in the total free energy (2.7) in the direction of ψ can be computed as

$$\lim_{\delta\to 0}\frac{\mathcal{E}(\varphi+\delta\psi)-\mathcal{E}(\varphi)}{\delta} = \frac{1}{c_F}\int_\Omega \varepsilon A'(\nabla\varphi)\cdot\nabla\psi + \varepsilon^{-1}F'(\varphi)\,\psi\,\mathrm{d}x + \sigma\int_{\Gamma_w} G'(\varphi)\,\psi\,\mathrm{d}S$$

$$= \frac{1}{c_F}\int_\Omega [\varepsilon^{-1}F'(\varphi) - \varepsilon\nabla\cdot A'(\nabla\varphi)]\,\psi\,\mathrm{d}x + \frac{1}{c_F}\int_{\partial\Omega\setminus\Gamma_w} \varepsilon A'(\nabla\varphi)\cdot\mathbf{n}\,\psi\,\mathrm{d}S$$
$$+ \frac{1}{c_F}\int_{\Gamma_w}\left[\varepsilon A'(\nabla\varphi)\cdot\mathbf{n}_w + c_F\,\sigma\,G'(\varphi)\right]\psi\,\mathrm{d}S, \tag{2.10}$$

where $\mathbf{n}$ is the outward unit normal to $\partial\Omega\setminus\Gamma_w$ and $\mathbf{n}_w$ is the outward unit normal to Γ_w, as defined previously. The following diffuse-interface model for SSD can be interpreted as a weighted H^{-1}-gradient flow of the energy functional (2.7):

$$\alpha\,\partial_t\varphi = \varepsilon^{-1}\nabla\cdot(m(\varphi)\,\beta(\nabla\varphi)\,\nabla\mu)\,, \qquad \text{in}\quad Q=\Omega\times(0,T], \tag{2.11a}$$
$$\mu = -\varepsilon\nabla\cdot A'(\nabla\varphi) + \varepsilon^{-1}F'(\varphi), \qquad \text{in}\quad Q. \tag{2.11b}$$

Here, $\alpha>0$ is a time scaling coefficient, $m(\varphi)$ is the degenerate mobility given by

$$m(\varphi) = (1-\varphi^2)_+^2 = \begin{cases} 2\,F(\varphi) & \text{if } |\varphi|\le 1,\\ 0 & \text{otherwise,}\end{cases} \tag{2.12}$$

and $\beta(\nabla\varphi)$ is defined as

$$\beta(\nabla\varphi) = \frac{D(\nabla\varphi)}{\gamma(\nabla\varphi)}, \tag{2.13}$$

and so is positively homogeneous of degree zero.

We now write $\Sigma=\partial\Omega\times(0,T]$ and $\Sigma_w=\Gamma_w\times(0,T]$. On Σ_w, we impose the boundary conditions

$$m(\varphi)\,\beta(\nabla\varphi)\nabla\mu\cdot\mathbf{n}_w = 0, \qquad \varepsilon A'(\nabla\varphi)\cdot\mathbf{n}_w + c_F\,\sigma\,G'(\varphi) = 0. \tag{2.14a}$$

Here, the first equation is the zero-flux condition on the boundary, whereas the second equation guarantees the integral over Γ_w in (2.10) vanishes. Moreover, on $\Sigma\setminus\Sigma_w$, we impose the natural boundary conditions

$$m(\varphi)\,\beta(\nabla\varphi)\nabla\mu\cdot\mathbf{n} = 0, \qquad A'(\nabla\varphi)\cdot\mathbf{n} = 0. \tag{2.14b}$$

Remark 2.1 It is also possible to consider the double-obstacle potential (1.2c) along with the mobility $m(\varphi)=(1-\varphi^2)_+$. Then, the corresponding diffuse-interface model consists of (2.11a) and the variational inclusion

$$\mu \in -\varepsilon\nabla\cdot A'(\nabla\varphi) + \varepsilon^{-1}\partial F(\varphi). \tag{2.15}$$

instead of (2.11b).

3 The Sharp-Interface Limit

We consider the smooth double-well potential introduced in (2.8) and regularize the coefficients $m(\varphi)$ and $\beta(\nabla\varphi)$ of the diffuse-interface model (2.11) with the help of the interfacial parameter ε by defining

$$m^\varepsilon(\varphi) := \varepsilon^r + m(\varphi) = \varepsilon^r + (1-\varphi^2)_+^2, \tag{3.1}$$

$$\beta^\varepsilon(\nabla\varphi) := \sqrt{\frac{d_1^2\varepsilon^r + D^2(\nabla\varphi)}{\gamma_0^2\varepsilon^r + \gamma^2(\nabla\varphi)}}, \tag{3.2}$$

where $r \geq 2$. The regularized diffuse-interface model is then given by

$$\alpha\,\partial_t\varphi^\varepsilon = \varepsilon^{-1}\nabla\cdot\left(m^\varepsilon(\varphi^\varepsilon)\,\beta^\varepsilon(\nabla\varphi^\varepsilon)\,\nabla\mu^\varepsilon\right) \quad \text{in } Q, \tag{3.3a}$$

$$\mu^\varepsilon = -\varepsilon\nabla\cdot A'(\nabla\varphi^\varepsilon) + \varepsilon^{-1}F'(\varphi^\varepsilon) \quad \text{in } Q, \tag{3.3b}$$

$$m^\varepsilon(\varphi^\varepsilon)\,\beta^\varepsilon(\nabla\varphi^\varepsilon)\nabla\mu^\varepsilon\cdot\mathbf{n}_w = 0 \quad \text{on } \Sigma_w, \tag{3.3c}$$

$$\varepsilon A'(\nabla\varphi^\varepsilon)\cdot\mathbf{n}_w + c_F\,\sigma\,G'(\varphi^\varepsilon) = 0 \quad \text{on } \Sigma_w, \tag{3.3d}$$

$$m^\varepsilon(\varphi^\varepsilon)\,\beta^\varepsilon(\nabla\varphi^\varepsilon)\nabla\mu^\varepsilon\cdot\mathbf{n} = 0 \quad \text{on } \Sigma\setminus\Sigma_w, \tag{3.3e}$$

$$\varepsilon A'(\nabla\varphi^\varepsilon)\cdot\mathbf{n} = 0 \quad \text{on } \Sigma\setminus\Sigma_w. \tag{3.3f}$$

We note that the introduction of the three regularization terms ε^r in (3.1) and (3.2) allows for a mathematical analysis of (3.3) in Sect. 4 below. In fact, on defining

$$\gamma_0 := \min_{|\mathbf{p}|=1}\gamma(\mathbf{p}) > 0, \qquad \gamma_1 := \max_{|\mathbf{p}|=1}\gamma(\mathbf{p}) > 0,$$

$$d_0 := \min_{|\mathbf{p}|=1} D(\mathbf{p}) > 0, \qquad d_1 := \max_{|\mathbf{p}|=1} D(\mathbf{p}) > 0,$$

we have

$$\varepsilon^r \leq m^\varepsilon(\varphi) \leq \varepsilon^r + 1 \quad \text{and} \quad \frac{d_0}{\gamma_1} \leq \beta^\varepsilon(\nabla\varphi) \leq \frac{d_1}{\gamma_0}.$$

Moreover, by choosing $r \geq 2$, we ensure that the sharp-interface limit of (3.3) is unchanged compared to the limit of (2.11).

We now formally derive the sharp-interface limit of the regularized model (2.11) via the method of matched asymptotic expansions. We suppose that for $\varepsilon > 0$, $(\varphi^\varepsilon, \mu^\varepsilon)$ is the solution of the regularized diffuse-interface model (3.3). Then, we write

$$\Gamma^\varepsilon(t) := \left\{\mathbf{x}\in\Omega \mid \varphi^\varepsilon(\mathbf{x},t) = 0\right\} \quad \text{and} \quad \Lambda^\varepsilon(t) := \Gamma^\varepsilon(t)\cap\Gamma_w \tag{3.4}$$

to denote the interface and the contact line, respectively. We further assume that their limits as $\varepsilon \to 0$ are given by $\Gamma(t)$ and $\Lambda(t)$, respectively. We introduce a local parameterization for $\Gamma(t)$ on an open subset $\mathcal{O}\subset\mathbb{R}^{d-1}$ by

$$\mathbf{r}(\mathbf{s},t) : \mathcal{O}\times[0,T] \to \mathbb{R}^d. \tag{3.5}$$

Our asymptotic analysis for the interface dynamics will follow similar techniques in the literature for degenerate Cahn-Hilliard equations, see, e.g., Cahn et al. (1996), Dai and Du (2014), for the isotropic case and Rätz et al. (2006), Dziwnik et al. (2017) for the anisotropic case in 2d.

3.1 Outer Expansions

Away from the interface and the contact line, we assume that the following ansatz holds

$$\varphi^\varepsilon(\mathbf{x},t) = \varphi_0(\mathbf{x},t) + \varepsilon\varphi_1(\mathbf{x},t) + \varepsilon^2\varphi_2(\mathbf{x},t) + \cdots, \tag{3.6a}$$

$$\mu^\varepsilon(\mathbf{x},t) = \varepsilon^{-1}\,\mu_{-1}(\mathbf{x},t) + \mu_0(\mathbf{x},t) + \varepsilon\mu_1(\mathbf{x},t) + \varepsilon^2\mu_2(\mathbf{x},t) + \cdots. \tag{3.6b}$$

Moreover, in view of (3.1) and (3.2), we know that

$$m^\varepsilon(\varphi^\varepsilon) = m(\varphi_0) + \varepsilon\, m'(\varphi_0)\,\varphi_1 + O(\varepsilon^2), \tag{3.7a}$$

$$\beta^\varepsilon(\nabla\varphi^\varepsilon) = \beta(\nabla\varphi_0) + \varepsilon\,\beta'(\nabla\varphi_0)\cdot\nabla\varphi_1 + O(\varepsilon^2), \tag{3.7b}$$

since $r \geq 2$ and $\beta^\varepsilon(\mathbf{p}) = \beta(\mathbf{p}) + O(\varepsilon^r)$, where β' denotes the gradient of β. Plugging the expansions (3.6) and (3.7) into (3.3a) and (3.3b) gives

$$0 = \nabla\cdot(\beta(\nabla\varphi_0)\,m(\varphi_0)\,\nabla\mu_{-1}), \qquad \mu_{-1} = F'(\varphi_0).$$

As the energy (1.5) is expected to be bounded at leading order, it needs to hold $F(\varphi_0) = 0$. This means that φ_0 attains only the values -1 and 1. Hence, $\mu_{-1} = 0$. We now define

$$\Omega_+(t) := \big\{\mathbf{x}\in\Omega \mid \varphi_0(\mathbf{x},t) = 1\big\}, \qquad \Omega_-(t) := \big\{\mathbf{x}\in\Omega \mid \varphi_0(\mathbf{x},t) = -1\big\},$$

as the outer regions, meaning that $\varphi_0 = \pm 1$ in $\Omega_\pm(t)$.

3.2 Inner Expansions

In the inner region near the interface $\Gamma(t)$, we introduce the annular neighborhood

$$\mathcal{N}(t) := \Big\{\mathbf{x}\in\Omega \;:\; |\mathrm{d}(\mathbf{x},t)| < \delta\Big\}, \qquad \delta > 0,$$

where $\mathrm{d}(\mathbf{x},t)$ represents the signed distance of $\mathbf{x}$ to $\Gamma(t)$, defined to be positive in $\Omega_+(t)$. Assuming $\Gamma(t)$ to be sufficiently smooth, we find a $\delta > 0$ such that for every $\mathbf{x}\in\mathcal{N}(t)$, there exist unique vectors $\mathbf{r}(\mathbf{x},t)$ and $\mathbf{s}(\mathbf{x},t)$ such that

$$\mathbf{x} = \mathbf{r}(\mathbf{s}(\mathbf{x},t),t) + \mathrm{d}(\mathbf{x},t)\,\boldsymbol{\nu}(\mathbf{s}(\mathbf{x},t),t). \tag{3.8}$$

Here, $\boldsymbol{\nu}(\mathbf{s},t)$ is the unit normal vector on $\Gamma(t)$ at $\mathbf{r}(\mathbf{s},t)$ pointing into $\Omega_+(t)$.

Due to rapid changes of φ^ε in normal direction, we introduce the stretched variable $\rho(\mathbf{x},t)=\varepsilon^{-1}\mathrm{d}(\mathbf{x},t)$. Any scalar function $b(\mathbf{x},t)$ can be expressed in the new coordinate system as $b(\mathbf{x},t)=\overline{b}(\mathbf{s}(\mathbf{x},t),\rho(\mathbf{x},t),t)$. For any vector field $\mathbf{b}(\mathbf{x},t)$, we use an analogous notation. Without loss of generality, we assume that $\{\mathbf{t}_1,\ \mathbf{t}_2,\cdots,\mathbf{t}_{d-1}\}$ forms an orthonormal basis of the tangent space of $\Gamma(t)$ at the point $\mathbf{r}(\mathbf{s},t)$ such that

$$\mathbf{t}_i\cdot\mathbf{t}_j=\delta_{ij},\qquad \mathbf{t}_j=\partial_{s_j}\mathbf{r},\qquad \partial_{s_j}\mathbf{t}_j=-\kappa_j\,\boldsymbol{\nu}\quad\text{for}\quad \mathbf{s}=(s_1,s_2,\cdots,s_{d-1})^T,$$

where κ_j is the principal curvature of $\Gamma(t)$ at the point $\mathbf{r}(\mathbf{s},t)$ in the direction of $\mathbf{t}_j$. As in Dai and Du (2014), we obtain the identities

$$\nabla\mathrm{d}=\varepsilon\,\nabla\rho=\boldsymbol{\nu}(\mathbf{s},t)\ \text{and}\ \nabla s_j=\frac{1}{1+\varepsilon\,\rho\,\kappa_j(\mathbf{s},t)}\mathbf{t}_j(\mathbf{s},t),\quad 1\le j\le d-1,\ \text{in}\,\mathcal{N}(t).$$

Therefore, using the new coordinates, we calculate

$$\partial_t b=\partial_t\overline{b}+\sum_{j=1}^{d-1}\partial_{s_j}\overline{b}\,\partial_t s_j+\partial_\rho\overline{b}\,\partial_t\rho=\partial_t^\Gamma\overline{b}-\varepsilon^{-1}\mathcal{V}\,\partial_\rho\overline{b},\tag{3.9a}$$

$$\nabla b=\nabla\rho\,\partial_\rho\overline{b}+\sum_{j=1}^{d-1}\partial_{s_j}\overline{b}\nabla s_j=\varepsilon^{-1}\,\boldsymbol{\nu}\,\partial_\rho\overline{b}+\nabla_s\overline{b}+O(\varepsilon),\tag{3.9b}$$

$$\nabla\cdot\mathbf{b}=\nabla\rho\cdot\partial_\rho\overline{\mathbf{b}}+\sum_{j=1}^{d-1}\partial_{s_j}\overline{\mathbf{b}}\cdot\nabla s_j=\varepsilon^{-1}\boldsymbol{\nu}\cdot\partial_\rho\overline{\mathbf{b}}+\nabla_s\cdot\overline{\mathbf{b}}+O(\varepsilon),\tag{3.9c}$$

where $\nabla_s=\sum_{j=1}^{d-1}\mathbf{t}_j\,\partial_{s_j}$ denotes the surface gradient operator on $\Gamma(t)$,

$$\partial_t^\Gamma\overline{b}=\partial_t\overline{b}+\sum_{j=1}^{d-1}\partial_{s_j}\overline{b}\,\partial_t s_j,$$

and $\mathcal{V}$ is the velocity of $\Gamma(t)$ in the direction of $\boldsymbol{\nu}$, i.e., $\mathcal{V}=-\partial_t\mathrm{d}=-\varepsilon\,\partial_t\rho$.

In the inner region, we assume the following expansions

$$\varphi^\varepsilon=\Phi_0(\mathbf{s},\rho,t)+\varepsilon\Phi_1(\mathbf{s},\rho,t)+\varepsilon^2\Phi_2(\mathbf{s},\rho,t)+\cdots,\tag{3.10a}$$

$$\mu^\varepsilon=\varepsilon^{-1}M_{-1}(\mathbf{s},\rho,t)+M_0(\mathbf{s},\rho,t)+\varepsilon M_1(\mathbf{s},\rho,t)+\varepsilon^2M_2(\mathbf{s},\rho,t)+\cdots.\tag{3.10b}$$

In particular, on assuming $\partial_\rho\Phi_0>0$, we have, similarly to (3.7), that

$$m^\varepsilon(\nabla\varphi^\varepsilon)=m(\Phi_0)+\varepsilon\,m'(\Phi^0)\,\Phi_1+O(\varepsilon^2),\tag{3.11a}$$

$$\beta^\varepsilon(\nabla\varphi^\varepsilon)=\beta(\boldsymbol{\nu})+\varepsilon\,\beta'(\boldsymbol{\nu})\cdot\nabla_s\Phi_0+O(\varepsilon^2),\tag{3.11b}$$

where we have used the fact that β is positively homogeneous of order zero.

Plugging (3.10) and (3.11) into (3.3a), we obtain the leading order term

$$0 = \partial_\rho\big(\beta(\boldsymbol{\nu})m(\Phi_0)\partial_\rho M_{-1}\big), \tag{3.12}$$

which implies that $m(\Phi_0)\partial_\rho M_{-1}$ is independent of ρ, i.e., it can be expressed as

$$m(\Phi_0)\,\partial_\rho\, M_{-1} = J(\mathbf{s}, t).$$

In addition, using the matching condition

$$\lim_{\rho\to\pm\infty} \Phi_0(\rho) = \pm 1, \tag{3.13}$$

we infer $J(\mathbf{s}, t) = 0$ due to the degenerate mobility $m(\Phi_0)$. Since $m(s) > 0$ if $s \in (-1, 1)$, we thus conclude that M_{-1} is independent of ρ. By the matching condition $\lim_{\rho\to\pm\infty} M_{-1}(\mathbf{s}, t) = \mu_{-1}$, we obtain

$$M_{-1} = M_{-1}(\mathbf{s}, t) \equiv 0.$$

For the terms of order $O(\frac{1}{\varepsilon^3})$, we obtain

$$0 = \partial_\rho\left(\beta(\boldsymbol{\nu})m(\Phi_0)\partial_\rho M_0\right).$$

Repeating the above line of argument, we deduce

$$\partial_\rho M_0 = 0, \qquad M_0 = M_0(\mathbf{s}, t). \tag{3.14}$$

Using the fact that $M_{-1} = 0$ and $\partial_\rho M_0 = 0$, we then have the following expansions

$$\begin{aligned}
&\nabla\cdot(\beta^\varepsilon(\nabla\varphi^\varepsilon)\,m^\varepsilon(\varphi^\varepsilon)\nabla\mu^\varepsilon)\\
&\quad= \frac{1}{\varepsilon}\,\partial_\rho(\beta(\boldsymbol{\nu})\,m(\Phi_0)\,\partial_\rho M_1)\\
&\qquad+ \partial_\rho(\beta'(\boldsymbol{\nu})\cdot\nabla_s\Phi_0\,m(\Phi_0)\,\partial_\rho M_1 + \beta(\boldsymbol{\nu})m'(\Phi_0)\Phi_1\,\partial_\rho M_1)\\
&\qquad+ \partial_\rho(\beta(\boldsymbol{\nu})\,m(\Phi_0)\,\partial_\rho\,M_2) + \nabla_s\cdot(\beta(\boldsymbol{\nu})\,m(\Phi_0)\,\nabla_s M_0) + O(\varepsilon).
\end{aligned} \tag{3.15}$$

Considering the order $O(\frac{1}{\varepsilon^2})$ of (3.3a), we obtain that

$$0 = \partial_\rho\left(\beta(\boldsymbol{\nu})\,m(\Phi_0)\,\partial_\rho M_1\right). \tag{3.16}$$

Similarly, by using the matching conditions, we arrive at

$$M_1 = M_1(\mathbf{s}, t). \tag{3.17}$$

At $O(\frac{1}{\varepsilon})$, using $\partial_\rho M_1 = 0$ and (3.15), we have

$$-\alpha\,\mathcal{V}\partial_\rho\Phi_0 = \partial_\rho\left(\beta(\boldsymbol{\nu})\,m(\Phi_0)\,\partial_\rho M_2\right) + \nabla_s\cdot(\beta(\boldsymbol{\nu})\,m(\Phi_0)\,\nabla_s M_0). \tag{3.18}$$

We next consider the expansion of (3.3b). Using the identities in (2.6) and assuming $\partial_\rho \Phi_0 > 0$, we expand the anisotropic term $A'(\nabla \Phi^\varepsilon)$ as follows:

$$A'(\nabla \Phi^\varepsilon) = A'\left(\frac{1}{\varepsilon}\partial_\rho \Phi^\varepsilon\, \boldsymbol{\nu} + \nabla_s \Phi^\varepsilon + O(\varepsilon)\right) = \frac{1}{\varepsilon}\partial_\rho \Phi^\varepsilon\, A'(\boldsymbol{\nu}) + A''(\boldsymbol{\nu})\nabla_s \Phi^\varepsilon + O(\varepsilon).$$

This then yields

$$\begin{aligned}
\nabla \cdot A'(\nabla \Phi^\varepsilon) &= \frac{1}{\varepsilon}\partial_\rho [A'(\nabla \Phi^\varepsilon)] \cdot \boldsymbol{\nu} + \nabla_s \cdot A'(\nabla \Phi^\varepsilon) \\
&= \frac{1}{\varepsilon}\partial_\rho \left(\frac{1}{\varepsilon}\partial_\rho \Phi^\varepsilon\, 2A(\boldsymbol{\nu}) + A'(\boldsymbol{\nu}) \cdot \nabla_s \Phi^\varepsilon\right) \\
&\quad + \nabla_s \cdot \left(\frac{1}{\varepsilon}\partial_\rho \Phi^\varepsilon A'(\boldsymbol{\nu}) + A''(\boldsymbol{\nu})\nabla_s \Phi^\varepsilon\right) + O(\varepsilon) \\
&= \frac{2}{\varepsilon^2}\partial_{\rho\rho} \Phi^\varepsilon\, A(\boldsymbol{\nu}) + \frac{1}{\varepsilon}\left(A'(\boldsymbol{\nu}) \cdot \partial_\rho(\nabla_s \Phi^\varepsilon) + \nabla_s \cdot (\partial_\rho \Phi^\varepsilon\, A'(\boldsymbol{\nu}))\right) + O(1).
\end{aligned}$$

Now, plugging (3.10) into (3.3b), we obtain for the leading order term that

$$2A(\boldsymbol{\nu})\partial_{\rho\rho}\Phi_0 - F'(\Phi_0) = M_{-1} = 0. \tag{3.19}$$

Using the translation identity $\Phi_0(0) = 0$, we then obtain

$$\Phi_0(\rho) = \tanh\left(\frac{\rho}{\gamma(\boldsymbol{\nu})}\right), \quad -\infty < \rho < +\infty. \tag{3.20}$$

Similarly, the $O(1)$ term resulting from (3.3b) implies

$$2A(\boldsymbol{\nu})\partial_{\rho\rho}\Phi_1 + A'(\boldsymbol{\nu}) \cdot \partial_\rho(\nabla_s \Phi_0) + \nabla_s \cdot (\partial_\rho \Phi_0\, A'(\boldsymbol{\nu})) - F''(\Phi_0)\Phi_1 = -M_0(\mathbf{s}, t). \tag{3.21}$$

Multiplying (3.21) by $\partial_\rho \Phi_0$ and then integrating from $-\infty$ to ∞ with respect to ρ yields

$$\begin{aligned}
&\int_{-\infty}^{+\infty} \left(A'(\boldsymbol{\nu}) \cdot \partial_\rho(\nabla_s \Phi_0) + \nabla_s \cdot (\partial_\rho \Phi_0\, A'(\boldsymbol{\nu}))\right) \partial_\rho \Phi_0 \, \mathrm{d}\rho \\
&+ \int_{-\infty}^{+\infty} \left(2A(\boldsymbol{\nu})\partial_{\rho\rho}\Phi_1 \partial_\rho \Phi_0 - F''(\Phi_0)\Phi_1 \partial_\rho \Phi_0\right) \mathrm{d}\rho = -M_0 \int_{-\infty}^{+\infty} \partial_\rho \Phi_0 \, \mathrm{d}\rho.
\end{aligned} \tag{3.22}$$

Differentiating (3.19) with respect to ρ gives

$$2A(\boldsymbol{\nu})\partial_{\rho\rho\rho}\Phi_0 - F''(\Phi_0)\partial_\rho \Phi_0 = 0.$$

Therefore, since $\lim_{\rho\to\pm\infty}\partial_\rho\Phi_0 = 0$ and $\lim_{\rho\to\pm\infty}\Phi_1 = 0$, we compute

$$\begin{aligned}&\int_{-\infty}^{+\infty}\left(2A(\boldsymbol{\nu})\partial_{\rho\rho}\Phi_1\partial_\rho\Phi_0 - F''(\Phi_0)\Phi_1\partial_\rho\Phi_0\right)\mathrm{d}\rho\\ &\quad=\int_{-\infty}^{+\infty}\left(2A(\boldsymbol{\nu})\partial_{\rho\rho\rho}\Phi_0 - F''(\Phi_0)\partial_\rho\Phi_0\right)\Phi_1\,\mathrm{d}\rho = 0\end{aligned}$$

via integration by parts. Then, using (3.20) and the matching condition in (3.13), we can reformulate (3.22) as

$$\int_{-\infty}^{+\infty}\left(A'(\boldsymbol{\nu})\cdot\partial_\rho(\nabla_s\Phi_0) + \nabla_s\cdot(\partial_\rho\Phi\, A'(\boldsymbol{\nu}))\right)\partial_\rho\Phi_0\,\mathrm{d}\rho = -2M_0(\mathbf{s},t). \quad (3.23)$$

It further follows from (3.20) that $\partial_\rho(\nabla_s\Phi_0) = \nabla_s(\partial_\rho\Phi_0)$. We thus have

$$\int_{-\infty}^{+\infty}\nabla_s\cdot[A'(\boldsymbol{\nu})(\partial_\rho\Phi_0)^2]\,\mathrm{d}\rho = -2M_0(\mathbf{s},t),$$

which yields

$$M_0(s,t) = -\frac{1}{2}\nabla_s\cdot\left(A'(\boldsymbol{\nu})\int_{-\infty}^{+\infty}(\partial_\rho\Phi_0)^2\,\mathrm{d}\rho\right) = -\frac{1}{2}c_{_F}\nabla_s\cdot\gamma'(\boldsymbol{\nu}) = \frac{1}{2}c_{_F}\varkappa_\gamma, \quad (3.24)$$

where $\varkappa_\gamma = -\nabla_s\cdot\gamma'(\boldsymbol{\nu})$ is the weighted mean curvature defined in (2.1b).

We now return to (3.18) and integrate it with respect to ρ from $-\infty$ to $+\infty$. Using the fact that $\lim_{\rho\to\pm\infty} m(\Phi_0)\partial_\rho M_2 = 0$, we get

$$-2\,\alpha\,\mathcal{V} = \nabla_s\cdot\left(\beta(\boldsymbol{\nu})\int_{-\infty}^{\infty}m(\Phi_0)\,\mathrm{d}\rho\,\nabla_s M_0\right) = c_{_F}\nabla_s\cdot[D(\boldsymbol{\nu})\nabla_s M_0],$$

where we recall (3.20) and also use the identities

$$\beta(\boldsymbol{\nu}) = \frac{D(\boldsymbol{\nu})}{\gamma(\boldsymbol{\nu})} \quad\text{and}\quad \int_{-\infty}^{+\infty}m(\Phi_0)\,\mathrm{d}\rho = \int_{-\infty}^{+\infty}2\,F(\Phi_0(\rho))\,\mathrm{d}\rho = c_{_F}\gamma(\boldsymbol{\nu}).$$

We thus obtain

$$\mathcal{V} = -\frac{c_{_F}^2}{4\,\alpha}\nabla_s\cdot[D(\boldsymbol{\nu})\nabla_s\varkappa_\gamma] \quad\text{with}\quad \varkappa_\gamma = -\nabla_s\cdot\gamma'(\boldsymbol{\nu}). \quad (3.25)$$

3.3 Expansions Near the Intersection with the Substrate

We next study the expansions near the intersection with the substrate using the technique discussed in Dziwnik et al. (2017), Owen et al. (1990).

3.3.1 The Boundary Layer Near the Wall

In the boundary layer near Γ_w, we first introduce the variable $\eta = \varepsilon^{-1}\,\mathrm{d}_w(\mathbf{x})$, where $\mathrm{d}_w(\mathbf{x})$ represents the distance from $\mathbf{x}$ to the wall Γ_w. Then, for a scalar function $b(\mathbf{x}, t)$, we can write it as $b(\mathbf{x}, t) = \widehat{b}(\eta, \mathbf{y}, t)$, where $\mathbf{y}$ is the $(d-1)$-dimensional coordinate system that is orthogonal to η. This implies

$$\nabla b = \nabla_{\mathbf{y}} \widehat{b} - \varepsilon^{-1} \partial_\eta \widehat{b}\, \mathbf{n}_w.$$

We consider the expansions

$$\varphi^\varepsilon = \widehat{\varphi}_0(\eta, \mathbf{y}, t) + \varepsilon \widehat{\varphi}_1(\eta, \mathbf{y}, t) + \varepsilon^2 \widehat{\varphi}_2(\eta, \mathbf{y}, t) + \cdots, \tag{3.26}$$

$$\mu^\varepsilon = \widehat{\mu}_0(\eta, \mathbf{y}, t) + \varepsilon \widehat{\mu}_1(\eta, \mathbf{y}, t) + \varepsilon^2 \widehat{\mu}_2(\eta, \mathbf{y}, t) + \cdots, \tag{3.27}$$

and plug them into (3.3a) and (3.3b). The leading order terms yield

$$\partial_\eta \left(\widehat{\beta}_0\, m(\widehat{\varphi}_0)\, \partial_\eta \widehat{\mu}_0 \right) = 0, \tag{3.28a}$$

$$\partial_\eta [A'(-\partial_\eta \widehat{\varphi}_0\, \mathbf{n}_w)] \cdot \mathbf{n}_w + F'(\widehat{\varphi}_0) = 0, \tag{3.28b}$$

where $\widehat{\beta}_0 = \beta(-\partial_\eta \widehat{\varphi}_0\, \mathbf{n}_w)$. At the boundary $\eta = 0$, it holds

$$-A'(-\partial_\eta \widehat{\varphi}_0\, \mathbf{n}_w) \cdot \mathbf{n}_w + c_{_F}\, \sigma\, G'(\widehat{\varphi}_0) = 0, \tag{3.29a}$$

$$\widehat{\beta}_0\, m(\widehat{\varphi}_0) \partial_\eta \widehat{\mu}_0 = 0. \tag{3.29b}$$

Thus, from (3.28a) and (3.29b), we obtain

$$m(\widehat{\varphi}_0) \partial_\eta \widehat{\mu}_0 = 0.$$

Multiplying (3.28b) by $\partial_\eta \widehat{\varphi}_0$ and using the identities in (2.6), we arrive at

$$\begin{aligned} 0 &= -\partial_{\eta\eta}\, \widehat{\varphi}_0\, \mathbf{n}_w \cdot A''(-\partial_\eta \widehat{\varphi}_0\, \mathbf{n}_w)\, \partial_\eta \widehat{\varphi}_0\, \mathbf{n}_w + F'(\widehat{\varphi}_0) \partial_\eta \widehat{\varphi}_0 \\ &= \partial_{\eta\eta} \widehat{\varphi}_0\, \mathbf{n}_w \cdot A'(-\partial_\eta \widehat{\varphi}_0\, \mathbf{n}_w) + F'(\widehat{\varphi}_0) \partial_\eta \widehat{\varphi}_0. \end{aligned} \tag{3.30}$$

Integrating (3.30) over η leads to

$$F(\widehat{\varphi}_0) = A(-\partial_\eta \widehat{\varphi}_0\, \mathbf{n}_w) + c(\mathbf{y}, t) = (\partial_\eta \widehat{\varphi}_0)^2\, A(-\mathbf{n}_w), \tag{3.31}$$

where $c(\mathbf{y}, t) = 0$ due to the matching condition when $\eta \to \infty$. This implies

$$\partial_\eta \widehat{\varphi}_0 = \begin{cases} -\sqrt{\frac{F(\widehat{\varphi}_0)}{A(-\mathbf{n}_w)}} & \text{if} \quad \partial_\eta \widehat{\varphi}_0 < 0, \\ +\sqrt{\frac{F(\widehat{\varphi}_0)}{A(-\mathbf{n}_w)}} & \text{if} \quad \partial_\eta \widehat{\varphi}_0 > 0. \end{cases} \tag{3.32}$$

3.3.2 The Inner Layer Near the Contact Line

We assume that a local parameterization of the contact line $\Lambda(t)$ is given by

$$\mathbf{r}_w(s_w, t) : \mathcal{O}_w \times [0, T] \to \mathbb{R}^d, \tag{3.33}$$

where in the case $d = 2$, we simply set $\mathcal{O}_w = \{0\}$. For a contact point $\mathbf{x}_c \in \Lambda(t)$, we then introduce an interior layer near it. Precisely, for any $\mathbf{x}$ in the plane that contains $\mathbf{x}_c$ and is spanned by $\mathbf{n}_s$ and $\mathbf{n}_w$, we write

$$\xi = \varepsilon^{-1} (\mathbf{x} - \mathbf{x}_c) \cdot \mathbf{n}_s, \qquad \eta = -\varepsilon^{-1} (\mathbf{x} - \mathbf{x}_c) \cdot \mathbf{n}_w,$$

where $\mathbf{n}_s$ is the unit normal to $\Lambda(t)$ on the wall Γ_w and pointing into $\Omega_+(t)$. For a scalar function $b(\mathbf{x}, t)$, we can rewrite it as $b(\mathbf{x}, t) = \widetilde{b}(s_w, \xi, \eta, t)$. In a similar manner to (3.9), we compute

$$\partial_t b = -\varepsilon^{-1} \partial_\xi \widetilde{b} \, (\partial_t \mathbf{x}_c \cdot \mathbf{n}_s) + \partial_t^\Lambda \widetilde{b}, \tag{3.34}$$

$$\nabla b = \varepsilon^{-1} \, (\partial_\xi \widetilde{b} \, \mathbf{n}_s - \partial_\eta \widetilde{b} \, \mathbf{n}_w) + \nabla_{s_w} \widetilde{b} + O(\varepsilon), \tag{3.35}$$

$$\nabla \cdot \mathbf{b} = \varepsilon^{-1} \, (\partial_\xi \widetilde{\mathbf{b}} \cdot \mathbf{n}_s - \partial_\eta \widetilde{\mathbf{b}} \cdot \mathbf{n}_w) + \nabla_{s_w} \cdot \widetilde{\mathbf{b}} + O(\varepsilon), \tag{3.36}$$

where $\nabla_t^\Lambda \widetilde{b} = \partial_t \widetilde{b} + \partial_t s_w \cdot \nabla_{s_w} \widetilde{b}$. We then consider the expansions

$$\varphi^\varepsilon = \widetilde{\varphi}_0(s_w, \xi, \eta, t) + \varepsilon \widetilde{\varphi}_1(s_w, \xi, \eta, t) + \varepsilon^2 \widetilde{\varphi}_2(s_w, \xi, \eta, t) + \cdots, \tag{3.37}$$

$$\mu^\varepsilon = \widetilde{\mu}_0(s_w, \xi, \eta, t) + \varepsilon \widetilde{\mu}_1(s_w, \xi, \eta, t) + \varepsilon^2 \widetilde{\mu}_2(s_w, \xi, \eta, t) + \cdots, \tag{3.38}$$

and plug them into (3.3a) and (3.3b). By defining $\nabla_c = \mathbf{n}_s \, \partial_\xi - \mathbf{n}_w \, \partial_\eta$, the leading order term yields

$$\nabla_c \cdot \big(\widetilde{\beta}_0 \, m(\widetilde{\varphi}_0) \nabla_c \widetilde{\mu}_0\big) = 0, \tag{3.39a}$$

$$\partial_\xi \big(A'(\nabla_c \widetilde{\varphi}_0) \cdot \mathbf{n}_s\big) - \partial_\eta \big(A'(\nabla_c \widetilde{\varphi}_0) \cdot \mathbf{n}_w\big) = F'(\widetilde{\varphi}_0), \tag{3.39b}$$

where $\widetilde{\beta}_0 = \beta(\nabla_c \widetilde{\varphi}_0)$. Similarly, the leading order terms of the boundary conditions (3.3c) and (3.3d) give

$$\widetilde{\beta}_0 \, m(\widetilde{\varphi}_0) \partial_\eta \widetilde{\mu}_0 = 0, \tag{3.40a}$$

$$A'(\nabla_c \widetilde{\varphi}_0) \cdot \mathbf{n}_w + c_{_F} \, \sigma \, G'(\widetilde{\varphi}_0) = 0. \tag{3.40b}$$

Besides, we have the matching condition

$$\lim_{\xi \to \pm\infty} \widetilde{\varphi}_0 = \lim_{\mathbf{y} \to \mathbf{y}(x_c^\pm)} \widehat{\varphi}_0(\mathbf{y}, \eta) = \widehat{\varphi}_0^\pm. \tag{3.41}$$

Now, multiplying (3.39b) by $\partial_\xi \widetilde{\varphi}_0$ and integrating the resulting equation in a box $R := [-\xi_1, \xi_1] \times [0, \eta_1]$, we get

$$\begin{aligned}&\int_{-\xi_1}^{\xi_1}\int_0^{\eta_1} \partial_\xi \widetilde{\varphi}_0 \left[\partial_\xi\big(A'(\nabla_c\widetilde{\varphi}_0)\cdot \mathbf{n}_s\big) - \partial_\eta\big(A'(\nabla_c\widetilde{\varphi}_0)\cdot \mathbf{n}_w\big)\right] \mathrm{d}\eta\mathrm{d}\xi\\ &\quad = \int_{-\xi_1}^{\xi_1}\int_0^{\eta_1} \partial_\xi \widetilde{\varphi}_0\, F'(\widetilde{\varphi}_0)\,\mathrm{d}\eta\mathrm{d}\xi,\end{aligned}$$

which can be rewritten as

$$\begin{aligned}&\int_0^{\eta_1}\int_{-\xi_1}^{\xi_1} \partial_\xi \left[F(\widetilde{\varphi}_0) + A(\nabla_c\widetilde{\varphi}_0) - \partial_\xi\widetilde{\varphi}_0\, A'(\nabla_c\widetilde{\varphi}_0)\,\cdot \mathbf{n}_s\right]\mathrm{d}\xi\,\mathrm{d}\eta\\ &\quad + \int_{-\xi_1}^{\xi_1}\int_0^{\eta_1} \partial_\eta\left[\partial_\xi\widetilde{\varphi}_0\, A'(\nabla_c\widetilde{\varphi}_0)\cdot \mathbf{n}_w\right]\mathrm{d}\eta\mathrm{d}\xi = 0,\end{aligned} \tag{3.42}$$

by using the identity

$$\begin{aligned}&-\partial_\xi\widetilde{\varphi}_0\,\partial_\xi[A'(\nabla_c\widetilde{\varphi}_0)\cdot\mathbf{n}_s] - \partial_\xi\partial_\eta\widetilde{\varphi}_0\, A'(\nabla_c\widetilde{\varphi}_0)\cdot\mathbf{n}_w\\ &\quad = \partial_\xi\left[A(\nabla_c\widetilde{\varphi}_0) - \partial_\xi\widetilde{\varphi}_0\, A'(\nabla_c\widetilde{\varphi}_0)\cdot\mathbf{n}_s\right].\end{aligned}$$

For the first integral in (3.42), applying Gauss's theorem and using the matching condition in (3.41) as well as the fact $\lim_{\xi\to+\infty}\partial_\xi\widetilde{\varphi}_0 = 0$, we have

$$\begin{aligned}&\lim_{\xi_1,\eta_1\to+\infty}\int_0^{\eta_1}\left[F(\widetilde{\varphi}_0) + A(\nabla_c\widetilde{\varphi}_0) - \partial_\xi\widetilde{\varphi}_0\, A'(\nabla_c\widetilde{\varphi}_0)\,\cdot\mathbf{n}_s\right]_{-\xi_1}^{\xi_1}\mathrm{d}\eta\\ &\quad = \int_0^{+\infty} F(\widehat{\varphi}_0^+) + A(-\partial_\eta\widehat{\varphi}_0^+\,\mathbf{n}_w)\,\mathrm{d}\eta - \int_0^{+\infty} F(\widehat{\varphi}_0^-) + A(-\partial_\eta\widehat{\varphi}_0^-\,\mathbf{n}_w)\,\mathrm{d}\eta\\ &\quad = 2\int_0^{+\infty} F(\widehat{\varphi}_0^+)\,\mathrm{d}\eta - 2\int_0^{+\infty} F(\widehat{\varphi}_0^-)\,\mathrm{d}\eta\\ &\quad = 2\sqrt{A(-\mathbf{n}_w)}\Big(\int_0^{+\infty}\sqrt{F(\widehat{\varphi}_0^+)}\partial_\eta\Phi_0^+\,\mathrm{d}\eta + \int_0^{+\infty}\sqrt{F(\widehat{\varphi}_0^-)}\partial_\eta\Phi_0^-\,\mathrm{d}\eta\Big) = 0,\end{aligned} \tag{3.43}$$

where we have used (3.31) and (3.32).

We then apply Gauss's theorem to the second integral in (3.42). Recalling the boundary condition (3.40b), we obtain

$$\begin{aligned}&\int_{-\xi_1}^{\xi_1}\left[\partial_\xi\widetilde{\varphi}_0\, A'(\nabla_c\widetilde{\varphi}_0)\cdot\mathbf{n}_w\right]\big|_{\eta_1}\mathrm{d}\xi - \int_{-\xi_1}^{\xi_1}\left[\partial_\xi\widetilde{\varphi}_0\, A'(\nabla_c\widetilde{\varphi}_0)\cdot\mathbf{n}_w\right]\big|_0\mathrm{d}\xi\\ &\quad = \int_{-\xi_1}^{\xi_1}\left[\partial_\xi\widetilde{\varphi}_0\, A'(\nabla_c\widetilde{\varphi}_0)\cdot\mathbf{n}_w\right]\big|_{\eta_1}\mathrm{d}\xi + c_{_F}\,\sigma\int_{-\xi_1}^{\xi_1}\partial_\xi\widetilde{\varphi}_0\, G'(\widetilde{\varphi}_0)\,\mathrm{d}\xi = I + II.\end{aligned} \tag{3.44}$$

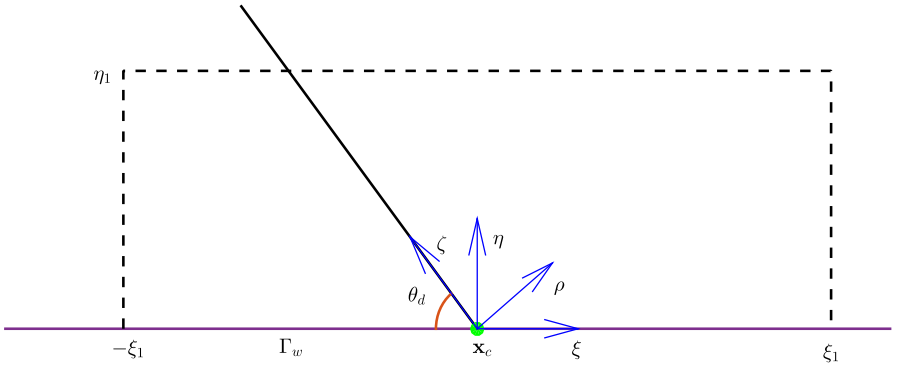

Fig. 3 Sketch of the local coordinates (ξ, η) and (ρ, ζ) at a contact point $\mathbf{x}_c$, where $\theta_d \in (0, \pi)$ is the contact angle

Sending $\xi_1 \to +\infty$ and recalling (2.9), we obtain

$$\lim_{\xi_1 \to +\infty} II = \lim_{\xi_1 \to +\infty} c_F\, \sigma \int_{-\xi_1}^{\xi_1} \partial_\xi \widetilde{\varphi}_0\, g(\widetilde{\varphi}_0)\, \mathrm{d}\xi = c_F\, \sigma\, (G(1) - G(-1)) = c_F\, \sigma. \tag{3.45}$$

Next, we rewrite the term I in terms of the new coordinate system (ρ, ζ), which can be regarded as a transformation from (η, ξ) with a counterclockwise rotation of θ_d in the plane (see Fig. 3). Precisely, it holds that

$$\rho = \xi \sin\theta_d + \eta \cos\theta_d, \qquad \zeta = -\xi \cos\theta_d + \eta \sin\theta_d, \tag{3.46a}$$

and thus,

$$\partial_\xi = \partial_\rho \sin\theta_d - \partial_\zeta \cos\theta_d, \qquad \partial_\eta = \partial_\rho \cos\theta_d + \partial_\zeta \sin\theta_d. \tag{3.46b}$$

Moreover, we have

$$\nabla_c = \mathbf{n}_s\, \partial_\xi - \mathbf{n}_w\, \partial_\eta = \boldsymbol{\nu}\, \partial_\rho - \mathbf{n}_c\, \partial_\zeta, \qquad \mathbf{n}_c = \sin\theta_d\, \mathbf{n}_w + \cos\theta_d\, \mathbf{n}_s, \tag{3.46c}$$

where $\mathbf{n}_c$ is the conormal vector of $\Gamma(t)$ at $\mathbf{x}_c$. By (3.46), we can recast the term I as

$$I = \int_{-\xi_1 + \eta_1 \cos\theta_d}^{\xi_1 \sin\theta_d + \eta_1 \cos\theta_d} \left[\partial_\rho \widetilde{\varphi}_0 - \partial_\zeta \widetilde{\varphi}_0 \cot\theta_d\right] A'(\partial_\rho \widetilde{\varphi}_0 \boldsymbol{\nu} - \partial_\zeta \widetilde{\varphi}_0\, \mathbf{n}_c) \cdot \mathbf{n}_w\, \mathrm{d}\rho. \tag{3.47}$$

By the matching condition $\lim_{\zeta \to +\infty} \widetilde{\varphi}_0 = \Phi_0(\rho)$, we have $\lim_{\zeta \to +\infty} \partial_\zeta \widetilde{\varphi}_0 = 0$. Then, it follows directly that

$$\lim_{\xi_1, \eta_1 \to +\infty} I = \int_{-\infty}^{+\infty} (\partial_\rho \Phi_0)^2 A'(\boldsymbol{\nu}) \cdot \mathbf{n}_w\, \mathrm{d}\rho = \frac{c_F\, A'(\boldsymbol{\nu}) \cdot \mathbf{n}_w}{\gamma(\boldsymbol{\nu})} = c_F\, \gamma'(\boldsymbol{\nu}) \cdot \mathbf{n}_w. \tag{3.48}$$

Collecting the results in (3.43), (3.45) and (3.48) yields that

$$\gamma'(\boldsymbol{\nu}) \cdot \mathbf{n}_w + \sigma = 0, \tag{3.49}$$

which is exactly the anisotropic Young's law in (2.2b).

We next derive the zero-flux condition. Similarly to the above, we integrate (3.39a) over the box R. Applying Gauss's theorem and using the boundary condition (3.40a) gives rise to

$$\begin{aligned} 0 &= \int_0^{\eta_1} \int_{-\xi_1}^{\xi_1} \partial_\xi [\widetilde{\beta}_0\, m(\widetilde{\varphi}_0)\, \partial_\xi \widetilde{\mu}_0] + \partial_\eta [\widetilde{\beta}_0\, m(\widetilde{\varphi}_0)\, \partial_\eta \widetilde{\mu}_0]\, \mathrm{d}\xi \mathrm{d}\eta \\ &= \int_0^{\eta_1} \big[\widetilde{\beta}_0\, m(\widetilde{\varphi}_0)\, \partial_\xi \widetilde{\mu}_0\big]\big|_{-\xi_1}^{\xi_1} \mathrm{d}\eta + \int_{-\xi_1}^{\xi_1} \big[\widetilde{\beta}_0\, m(\widetilde{\varphi}_0)\, \partial_\eta \widetilde{\mu}_0\big]\big|_{\eta_1} \mathrm{d}\xi = III + IV. \end{aligned} \tag{3.50}$$

Taking $\xi_1 \to \infty$ and using fact $\lim_{\xi \to \pm\infty} \widetilde{\varphi}_0 = \pm 1$, as well as $m(\widetilde{\varphi}_0) = 0$, we get $III = 0$. On recalling (3.46), as well as the matching conditions,

$$\lim_{\zeta \to +\infty} \widetilde{\varphi}_0 = \Phi_0(\rho) = \tanh\Big(\frac{\rho}{\gamma(\boldsymbol{\nu})}\Big), \quad \lim_{\zeta \to +\infty} \widetilde{\mu}_0 = M_0(\mathbf{s}, t) = \varkappa_\gamma, \quad \lim_{\zeta \to +\infty} \partial_\zeta \widetilde{\varphi}_0 = 0,$$

we get in the case of $\xi_1, \eta_1 \to \infty$ that

$$0 = \int_{-\infty}^{\infty} \big[m(\Phi_0)\, \beta(\boldsymbol{\nu}) \partial_\zeta \varkappa_\gamma\big]\, \mathrm{d}\rho = -\beta(\boldsymbol{\nu}) \int_{-\infty}^{\infty} m(\Phi_0)\, \mathrm{d}\rho\, \mathbf{n}_c \cdot \nabla_s \varkappa_\gamma.$$

This yields the zero-flux condition

$$D(\boldsymbol{\nu})\, \mathbf{n}_c \cdot \nabla_s \varkappa_\gamma = 0. \tag{3.51}$$

In addition, the attachment condition in (2.2a) follows naturally.

In summary, we thus obtain the following system of equations as the sharp-interface limit of the regularized diffuse-interface model (3.3):

$$\mathcal{V} = -\frac{c_F^2}{4\,\alpha} \nabla_s \cdot [D(\boldsymbol{\nu}) \nabla_s \varkappa_\gamma] \quad \text{with} \quad \mathcal{V} = \mathbf{V} \cdot \boldsymbol{\nu} \quad \text{and} \quad \varkappa_\gamma = -\nabla_s \cdot \gamma'(\boldsymbol{\nu}) \qquad \text{on} \quad \Gamma(t), \tag{3.52a}$$

$$\mathbf{V} \cdot \mathbf{n}_w = 0, \quad \gamma'(\boldsymbol{\nu}) \cdot \mathbf{n}_w + \sigma = 0, \quad D(\boldsymbol{\nu})\, \mathbf{n}_c \cdot \nabla_s \varkappa_\gamma = 0 \qquad \text{on} \quad \Lambda(t). \tag{3.52b}$$

Remark 3.1 In the case of the double-obstacle potential (1.2c) and the degenerate mobility $m(\varphi) = (1 - \varphi^2)_+$, we could obtain (3.52a) in a similar manner. But the

leading order inner solution (3.20) should be replaced by

$$\Phi_0(\rho) = \begin{cases} \sin(\frac{\rho}{\gamma(\boldsymbol{\nu})}) & \text{if} \quad \rho \in [-\frac{\pi}{2}\gamma(\boldsymbol{\nu}), \frac{\pi}{2}\gamma(\boldsymbol{\nu})], \\ -1 & \text{if} \quad \rho < -\frac{\pi}{2}\gamma(\boldsymbol{\nu}), \\ 1 & \text{if} \quad \rho > \frac{\pi}{2}\gamma(\boldsymbol{\nu}). \end{cases} \tag{3.53}$$

This yields $c_{_F} = \frac{\pi}{2}$ in (3.52a). The boundary conditions in (3.52b) can be derived similarly. It is also possible to consider the logarithmic potential (see (1.2b)) along with the mobility $m(\varphi) = (1-\varphi^2)_+$. If $\theta = O(\varepsilon^\xi)$ for some $\xi > 0$, it can be shown by means of the techniques from Cahn et al. (1996) that the same desired sharp-interface limit is obtained.

4 Analysis of the Diffuse-Interface Model

In this section, we analyze a general class of diffuse-interface models of the type

$$\alpha\, \partial_t \varphi = \nabla \cdot \big(M(\nabla\varphi, \varphi)\nabla\mu\big) \qquad \text{in } Q, \tag{4.1a}$$
$$\mu = -\varepsilon \nabla \cdot A'(\nabla\varphi) + \varepsilon^{-1} F'(\varphi) \qquad \text{in } Q, \tag{4.1b}$$
$$\nabla\mu \cdot \mathbf{n} = 0 \qquad \text{on } \Sigma, \tag{4.1c}$$
$$\varepsilon A'(\nabla\varphi) \cdot \mathbf{n} + c_{_F}\, \sigma\, G'(\varphi) = 0 \qquad \text{on } \Sigma_w, \tag{4.1d}$$
$$\varepsilon A'(\nabla\varphi) \cdot \mathbf{n} = 0 \qquad \text{on } \Sigma \setminus \Sigma_w, \tag{4.1e}$$
$$\varphi|_{t=0} = \varphi_0 \qquad \text{in } \Omega, \tag{4.1f}$$

where $\alpha, \varepsilon, c_{_F} \in \mathbb{R}_{>0}$ and $\sigma \in \mathbb{R}$ are given constants. In contrast to the previous sections, the potential $F : \mathbb{R} \to \mathbb{R}$ and $G : \mathbb{R} \to \mathbb{R}$, $A : \mathbb{R}^d \to \mathbb{R}$ and $M : \mathbb{R}^d \times \mathbb{R} \to \mathbb{R}$ are general functions satisfying certain conditions that will be specified in Sect. 4.1. If A, F, G, m^ε and β^ε are chosen as in (2.5), (2.8), (2.9), (3.1) and (3.2), respectively, and if M is defined by $M(\mathbf{p}, s) := \beta^\varepsilon(\mathbf{p}) m^\varepsilon(s)$ for all $\mathbf{p} \in \mathbb{R}^d$ and $s \in \mathbb{R}$, then the system (4.1) is exactly the model (3.3) that was introduced in Sect. 3. The total free energy functional $\mathcal{E} : H^1(\Omega) \to \mathbb{R}$ associated with the system (4.1), up to an additive constant, reads as

$$\mathcal{E}(\varphi) := \frac{1}{c_{_F}} \int_\Omega \varepsilon A(\nabla\varphi) + \varepsilon^{-1} F(\varphi)\, \mathrm{d}x + \sigma \int_{\Gamma_w} G(\varphi)\, \mathrm{d}S. \tag{4.2}$$

It is also possible to consider the system (4.1) for F being the double-obstacle potential, which can be expressed as

$$F : \mathbb{R} \to [0, \infty], \qquad F(s) = F_0(s) + I_{[-1,1]}(s), \tag{4.3}$$

where the function

$$F_0 : \mathbb{R} \to [0, \infty), \qquad F_0(s) = \tfrac{1}{2}(1 - \varphi^2), \tag{4.4}$$

represents its regular part, and

$$I : \mathbb{R} \to [0, \infty], \qquad I_{[-1,1]}(s) = \begin{cases} 0 & \text{if } |s| \le 1, \\ +\infty & \text{if } |s| > 1 \end{cases} \tag{4.5}$$

denotes the indicator functional of the interval $[-1, 1]$. In this case, (4.1b) needs to be represented by a variational inequality, see (4.18b).

4.1 Notation and Preliminaries

Notation. In this section, we use the following notation: For any $1 \le p \le \infty$ and $k \ge 0$, the standard Lebesgue and Sobolev spaces on Ω are denoted by $L^p(\Omega)$ and $W^{k,p}(\Omega)$. Their standard norms are written as $\|\cdot\|_{L^p(\Omega)}$ and $\|\cdot\|_{W^{k,p}(\Omega)}$. In the case $p = 2$, these spaces are Hilbert spaces, and we write $H^k(\Omega) = W^{k,2}(\Omega)$. Here, we identify $H^0(\Omega)$ with $L^2(\Omega)$. For the Lebesgue and Sobolev spaces on $\partial\Omega$, we use an analogous notation. For any Banach space X, its dual space is denoted by X', and the associated duality pairing by $\langle \cdot\,,\, \cdot \rangle_X$. If X is a Hilbert space, we write $(\cdot, \cdot)_X$ to denote its inner product. We further define

$$\langle f \rangle_\Omega := \frac{1}{|\Omega|} \langle f\,,\, 1 \rangle_{H^1(\Omega)} \quad \text{for} \quad f \in H^1(\Omega)'$$

as the generalized spatial mean of f, where $|\Omega|$ denotes the d-dimensional Lebesgue measure of Ω. With the usual identification $L^1(\Omega) \subset H^1(\Omega)'$, it holds that $\langle f \rangle_\Omega = \frac{1}{|\Omega|} \int_\Omega f \,\mathrm{d}x$ if $f \in L^1(\Omega)$. In addition, we introduce

$$\begin{aligned} H^1_{(m)}(\Omega) &:= \left\{ u \in H^1(\Omega) \,\middle|\, \langle u \rangle_\Omega = m \right\} \qquad \text{for any } m \in \mathbb{R}, \\ H^{-1}_{(0)}(\Omega) &:= \left\{ f \in \left(H^1(\Omega)\right)' \,\middle|\, \langle f \rangle_\Omega = 0 \right\}. \end{aligned}$$

We point out that for every $m \in \mathbb{R}$, $H^1_{(m)}(\Omega)$ is an affine subspace of the Hilbert space $H^1(\Omega)$. In the case $m = 0$, it is even a closed linear subspace, meaning that $H^1_{(0)}(\Omega)$ is also a Hilbert space.

General assumptions We make the following general assumptions that are supposed to hold throughout this section.

A1 The set $\Omega \subset \mathbb{R}^d$ with $d \in \{2, 3\}$ is a bounded Lipschitz domain. Moreover, $T > 0$ denotes an arbitrary final time.

A2 The function $G : \mathbb{R} \to \mathbb{R}$ is non-negative and twice continuously differentiable. Moreover, there exists an exponent $q \in [2, 4)$, as well as positive constants C_G and $C_{G'}$, such that

$$G(s) \le C_G(1 + |s|^q) \quad \text{and} \quad \left|G'(s)\right| \le C_{G'}(1 + |s|^{q-1})$$

for all $s \in \mathbb{R}$.

A3 "The function $A : \mathbb{R}^d \to \mathbb{R}$ is continuously differentiable, positively homogeneous of degree 2 and positive on $\mathbb{R}^d$ 0. Hence there exist constants $A_0, A_1 \in \mathbb{R}$ with $0 < A_0 \leq A_1$ such that"

$$A_0 |\mathbf{p}|^2 \leq A(\mathbf{p}) \leq A_1 |\mathbf{p}|^2 \quad \text{for all } \mathbf{p} \in \mathbb{R}^d.$$

The gradient $A' : \mathbb{R}^d \to \mathbb{R}^d$ is strongly monotone, i.e., there exists a constant $a_0 > 0$ such that

$$\big(A'(\mathbf{p}) - A'(\mathbf{q})\big) \cdot (\mathbf{p} - \mathbf{q}) \geq a_0 |\mathbf{p} - \mathbf{q}|^2 \quad \text{for all } \mathbf{p}, \mathbf{q} \in \mathbb{R}^d,$$

which implies that A is strongly convex and thus strictly convex. Moreover, there exists a constant $a_1 > 0$ such that

$$\big|A'(\mathbf{p})\big| \leq a_1 |\mathbf{p}| \quad \text{for all } \mathbf{p} \in \mathbb{R}^d.$$

A4 The function $M : \mathbb{R}^d \times \mathbb{R} \to \mathbb{R}$ is continuous and there exist constants $M_0, M_1 \in \mathbb{R}$ with $0 < M_0 \leq M_1$ such that

$$M_0 \leq M(\mathbf{p}, s) \leq M_1 \quad \text{for all } \mathbf{p} \in \mathbb{R}^d \text{ and } s \in \mathbb{R}.$$

Remark 4.1 (a) We point out that the choices

$$G(s) := \frac{1}{4}(3s - s^3) \qquad \text{for all } s \in \mathbb{R} \qquad \big(\text{cf. (2.9)}\big),$$
$$M(\mathbf{p}, s) := \beta^\varepsilon(\mathbf{p})\, m^\varepsilon(s)$$

with

$$m^\varepsilon(s) := \varepsilon^r + (1 - s^2)_+^2 \qquad \text{for all } s \in \mathbb{R} \qquad \big(\text{cf. (3.1)}\big),$$
$$\beta^\varepsilon(\mathbf{p}) := \sqrt{\frac{d_1^2\, \varepsilon^{2r} + D^2(\mathbf{p})}{\gamma_0^2 \varepsilon^{2r} + \gamma^2(\mathbf{p})}} \qquad \text{for all } \mathbf{p} \in \mathbb{R}^d \qquad \big(\text{cf. (3.2)}\big),$$

are admissible as they satisfy the conditions imposed in A2 (with $q = 3$) and A4.

(b) Suppose that the function γ that was introduced in Sect. 2.1 additionally satisfies the following convexity condition: There exists a constant $\alpha_0 > 0$ such that

$$\gamma''(\mathbf{p})\mathbf{q} \cdot \mathbf{q} \geq \alpha_0 |\mathbf{q}|^2 \quad \text{for all } \mathbf{p}, \mathbf{q} \in \mathbb{R}^d \text{ with } |\mathbf{p}| = 1 \text{ and } \mathbf{p} \cdot \mathbf{q} = 0, \tag{4.6}$$

where γ'' represents the Hessian of γ. Thus, the function

$$A : \mathbb{R}^d \to \mathbb{R}, \quad A(\mathbf{p}) = \tfrac{1}{2}\gamma^2(\mathbf{p})$$

is admissible as it satisfies all conditions imposed in assumption A3. In particular, as shown in Gräser et al. (2013), the convexity condition (4.6) ensures that A' is strongly monotone.

A special inner product on $H^{-1}_{(0)}(\Omega)$. We now introduce a certain inner product on the function space $H^{-1}_{(0)}(\Omega)$ based on the solution operator of a suitable elliptic problem. Therefore, let $a \in L^\infty(\Omega)$ be a uniformly positive function, i.e., there exist $a_0, a_1 \in \mathbb{R}$ with $0 < a_0 < a_1$ such that

$$a_0 \leq a \leq a_1 \quad \text{a.e. in } \Omega.$$

Then, for every $f \in H^{-1}_{(0)}(\Omega)$, there exists a unique weak solution $u_f \in H^1_{(0)}(\Omega)$ of the elliptic boundary value problem

$$-\nabla \cdot \big(a \nabla u\big) = f \qquad \text{in } \Omega, \tag{4.7a}$$

$$\nabla u \cdot \mathbf{n} = 0 \qquad \text{on } \partial\Omega, \tag{4.7b}$$

meaning that

$$\int_\Omega a \nabla u_f \cdot \nabla \zeta \, \mathrm{d}x = \big\langle f \, , \, \zeta \big\rangle_{H^1} \qquad \text{for all } \zeta \in H^1(\Omega). \tag{4.8}$$

We can thus define a solution operator

$$S_a : H^{-1}_{(0)}(\Omega) \to H^1_{(0)}(\Omega), \quad f \mapsto S_a(f) := u_f. \tag{4.9}$$

We next define the bilinear form

$$\big(\cdot \, , \, \cdot\big)_{S_a} : H^{-1}_{(0)}(\Omega) \times H^{-1}_{(0)}(\Omega) \to \mathbb{R}, \quad \big(f \, , \, g\big)_{S_a} := \int_\Omega a \, \nabla S_a(f) \cdot \nabla S_a(g) \, \mathrm{d}x, \tag{4.10}$$

which defines an inner product on $H^{-1}_{(0)}(\Omega)$ since a is uniformly positive and $\nabla S_a(f) = 0$ a.e. in Ω already implies $f = 0$ a.e. in Ω. Its induced norm is given by

$$\|\cdot\|_{S_a} : H^{-1}_{(0)}(\Omega) \to \mathbb{R}, \quad \|f\|_{S_a} := \big(f \, , \, f\big)^{1/2}_{S_a}. \tag{4.11}$$

We point out that on the space $H^{-1}_{(0)}(\Omega)$, the norm $\|\cdot\|_{S_a}$ is equivalent to the standard operator norm $\|\cdot\|_{(H^1(\Omega))'}$. The bilinear form $(\cdot\,,\,\cdot)_{S_a}$ also defines an inner product on the space $H^1_{(0)}(\Omega)$. Moreover, $\|\cdot\|_{S_a}$ is also a norm on $H^1_{(0)}(\Omega)$ but the space is not complete with respect to this norm.

4.2 Existence of Weak Solutions

For ease of presentation, in what follows, we simply fix $\alpha = \varepsilon = \sigma = c_F = 1$, since the precise choice of these values has no impact on the mathematical analysis.

4.2.1 Weak Solutions for Smooth Potentials

In this subsection, we make the following assumption on the potential F:

F1 The potential $F : \mathbb{R} \to \mathbb{R}$ is continuously differentiable. Moreover, there exists an exponent $p \in [2, 6)$, as well as non-negative constants B_F, C_F and $C_{F'}$ such that

$$-B_F \le F(s) \le C_F(1 + |s|^p) \quad \text{and} \quad \big|F'(s)\big| \le C_{F'}(1 + |s|^{p-1}).$$

for all $s \in \mathbb{R}$.

Obviously, the smooth double-well potential introduced in (1.2a) fulfills F1 with $p = 4$. However, the logarithmic potential (see (1.2b)) and the double-obstacle potential (see (1.2c)) do not satisfy this assumption.

A weak solution of the general diffuse-interface model (4.1) is then defined as follows.

Definition 4.2 Suppose that the assumptions A1–A4 and F1 are fulfilled, and let $\varphi_0 \in H^1(\Omega)$ be any initial datum. Then, the pair (φ, μ) is called a weak solution to system (4.1) if the following properties hold:

(i) The functions φ and μ have the following regularity:

$$\varphi \in C^{0,1/4}\big([0, T]; L^2(\Omega)\big) \cap L^\infty\big(0, T; H^1(\Omega)\big) \cap H^1\big(0, T; H^1(\Omega)'\big),$$
$$\mu \in L^2\big(0, T; H^1(\Omega)\big).$$

(ii) The pair (φ, μ) satisfies the weak formulations

$$\big\langle \partial_t \varphi\,,\, \zeta \big\rangle_{H^1(\Omega)} = -\int_\Omega M(\nabla\varphi, \varphi)\, \nabla\mu \cdot \nabla\zeta \,\mathrm{d}x, \tag{4.12a}$$

$$\int_\Omega \mu\, \eta \,\mathrm{d}x = \int_\Omega A'(\nabla\varphi) \cdot \nabla\eta + F'(\varphi)\, \eta \,\mathrm{d}x + \int_{\Gamma_w} G'(\varphi)\, \eta \,\mathrm{d}S \tag{4.12b}$$

a.e. on $[0, T]$ for all test functions $\zeta, \eta \in H^1(\Omega)$. Moreover, φ satisfies the initial condition

$$\varphi(0) = \varphi_0 \qquad \text{a.e. in } \Omega. \tag{4.13}$$

(iii) The pair (φ, μ) satisfies the weak energy dissipation law

$$\mathcal{E}\big(\varphi(t)\big) + \frac{1}{2}\int_0^t \int_\Omega M(\nabla\varphi, \varphi)\, |\nabla\mu|^2 \,\mathrm{d}x\,\mathrm{d}t \le \mathcal{E}(\varphi_0) \qquad \text{for almost all } t \in [0, T]. \tag{4.14}$$

The existence of such a weak solution is ensured by the following theorem.

Theorem 4.3 *Suppose that the assumptions A1–A4 and F1 are fulfilled, and let* $\varphi_0 \in H^1(\Omega)$ *be any initial datum. Then, there exists a weak solution* (φ, μ) *to the system* (4.1) *in the sense of Definition* 4.2.

The proof of this theorem is presented in Sect. 4.3.

In the next subsection, we intend to prove the existence of a weak solution to the diffuse-interface model (4.1) for the double-obstacle potential (1.2c). Our strategy is to approximate the double-obstacle potential by a sequence of regular potentials. To this end, in Corollary 4.4, we will present an additional uniform estimate for $F'(\varphi)$, where (φ, μ) is a weak solution to (4.1) with a regular potential F satisfying the following assumption:

F2 The potential $F : \mathbb{R} \to \mathbb{R}$ is twice continuously differentiable and there exist constants $c_0, c_1 \geq 0$ such that

$$-c_0 \leq F''(s) \leq c_1 \quad \text{for all } s \in \mathbb{R}. \tag{4.15}$$

We point out that if F2 is fulfilled, then F1 holds with $p = 2$.

Corollary 4.4 *Suppose that the assumptions A1–A4 and F2 are fulfilled. Let* $\varphi_0 \in H^1(\Omega)$ *be any initial datum satisfying* $\left|\langle \varphi_0 \rangle_\Omega\right| \leq 1 - \kappa$ *for some* $\kappa \in (0, 1]$*, and let* (φ, μ) *be a corresponding weak solution. Then, there exists a constant* $c > 0$ *depending only on* φ_0, $\mathcal{E}(\varphi_0)$, c_0 *and the constants in A1–A4, but not on* c_1*, such that*

$$\left\| F'(\varphi) \right\|^2_{L^2(Q)} \leq \frac{c}{\kappa^2} \big(1 + \|F\|^2_{L^\infty([-R,R])}\big), \tag{4.16}$$

where $R := \left|\langle \varphi_0 \rangle_\Omega\right| + \frac{\kappa}{2} < 1$.

Remark 4.5 In Corollary 4.4, the assumption $\left|\langle \varphi_0 \rangle_\Omega\right| \leq 1 - \kappa$ is made in order to ensure $R \leq 1$, which is crucial for later use. However, without this assumption, a similar estimate can be derived if $R > 1$ is allowed. For instance, choosing $R := \left|\langle \varphi_0 \rangle_\Omega\right| + 1$, we obtain the estimate

$$\left\| F'(\varphi) \right\|^2_{L^2(Q)} \leq c\big(1 + \|F\|^2_{L^\infty([-R,R])}\big) \tag{4.17}$$

instead of (4.16) even without the mean value assumption.

4.2.2 Weak Solutions for the Double-Obstacle Potential

In this subsection, we assume that $F = F_0 + I_{[-1,1]}$ is the double-obstacle potential as introduced in (4.3). Then, a weak solution of the general diffuse-interface model (4.1) is defined as follows.

Definition 4.6 Suppose that the assumptions A1–A4 are fulfilled, and let $\varphi_0 \in H^1(\Omega)$ be any initial datum satisfying $|\varphi_0| \leq 1$ a.e. in Ω. Then, the pair (φ, μ) is called a weak solution to system (4.1) if the following properties hold:

(i) The functions φ and μ have the following regularity:

$$\varphi \in C^{0,1/4}\big([0,T];L^2(\Omega)\big) \cap L^\infty\big(0,T;H^1(\Omega)\big) \cap H^1\big(0,T;H^1(\Omega)'\big),$$
$$\mu \in L^2\big(0,T;H^1(\Omega)\big).$$

(ii) It holds that $|\varphi| \leq 1$ a.e. in Q and the pair (φ,μ) satisfies the weak formulation

$$\big\langle \partial_t \varphi\,,\,\zeta\big\rangle_{H^1(\Omega)} = -\int_\Omega M(\nabla\varphi,\varphi)\,\nabla\mu\cdot\nabla\zeta\,\mathrm{d}x, \tag{4.18a}$$

for all $\zeta \in H^1(\Omega)$ as well as the variational inequality

$$\begin{aligned}\iint_Q \mu\,(\varphi-\eta)\,\mathrm{d}x\,\mathrm{d}t \geq \iint_Q A'(\nabla\varphi)\cdot(\nabla\varphi-\nabla\eta) + F_0'(\varphi)(\varphi-\eta)\,\mathrm{d}x\,\mathrm{d}t \\ + \iint_{\Sigma_w} G'(\varphi)\,(\varphi-\eta)\,\mathrm{d}S\,\mathrm{d}t\end{aligned} \tag{4.18b}$$

for all $\eta \in L^2(0,T;H^1(\Omega))$ with $|\eta| \leq 1$ a.e. in Q. Moreover, φ satisfies the initial condition

$$\varphi(0) = \varphi_0 \qquad \text{a.e. in } \Omega. \tag{4.19}$$

(iii) The pair (φ,μ) satisfies the weak energy dissipation law

$$\mathcal{E}\big(\varphi(t)\big) + \frac{1}{2}\int_0^t\int_\Omega M(\nabla\varphi,\varphi)\,|\nabla\mu|^2\,\mathrm{d}x\,\mathrm{d}t \leq \mathcal{E}(\varphi_0) \qquad \text{for almost all } t\in[0,T]. \tag{4.20}$$

The existence of such a weak solution is ensured by the following theorem.

Theorem 4.7 *Suppose that the assumptions A1–A4 are fulfilled, and let $\varphi_0 \in H^1(\Omega)$ be any initial datum satisfying $|\varphi_0| \leq 1$ a.e. in Ω and $\big|\langle\varphi_0\rangle_\Omega\big| \leq 1-\kappa$ for some $\kappa \in (0,1]$. Then, there exists a weak solution (φ,μ) to the system (4.1) in the sense of Definition 4.6.*

The idea behind the proof of Theorem 4.7 is to approximate the double-obstacle potential by a sequence $(F_n)_{n\in\mathbb{N}}$ of regular potentials where for each $n\in\mathbb{N}$, F_n is a regular potential fulfilling the condition F2. Therefore, Corollary 4.4 can be applied to derive a suitable uniform bound on the terms involving F_n'. We point out that the same strategy could be used to construct a weak solution to the diffuse-interface model (4.1) in the case that F is the logarithmic potential (1.2b).

4.3 Proofs

4.3.1 Proof of Theorem 4.3

The proof is divided into five steps.

Step 1: Implicit time discretization. Let $N \in \mathbb{N}$ be arbitrary. We define $\tau := T/N$ as our time step size. Let now $n \in \{0, ..., N-1\}$ be arbitrary. We now define functions φ^n with $n = 0, ..., N$ by the following recursion:

- The zeroth iterate is defined as the initial datum, i.e., $\varphi^0 := \varphi_0$.
- If for some $n \in \{0, ..., N-1\}$, the n-th iterate φ^n is already constructed, we choose $\varphi^{n+1} \in H^1_{(m)}$ as a minimizer of the functional

$$J_n : H^1_{(m)}(\Omega) \to \mathbb{R}, \quad J_n(\varphi) := \frac{1}{2\tau} \left\| \varphi - \varphi^n \right\|^2_{S_a} + \mathcal{E}(\varphi). \tag{4.21}$$

  Here, $\mathcal{E}$ is the energy functional defined in (4.2), with $\varepsilon = \sigma = c_F = 1$, and $\|\cdot\|_{S_a}$ is the norm defined in (4.11) with a being chosen as

$$a := M(\nabla\varphi^n, \varphi^n). \tag{4.22}$$

  This choice is actually possible since the function M is assumed to be bounded and uniformly positive (see A4). The existence of a minimizer of the functional J_n will be established in Step 2.

The idea behind this construction is that the first variation in the functional J_n at the point φ^{n+1} is zero since φ^{n+1} is a minimizer of J_n. This means that

$$\left(\frac{\varphi^{n+1} - \varphi^n}{\tau}, \eta \right)_{S_a} + \int_\Omega A'(\nabla\varphi^{n+1}) \cdot \nabla\eta + F'(\varphi^{n+1})\, \eta \, \mathrm{d}x + \int_{\Gamma_w} G'(\varphi^{n+1})\, \eta \, \mathrm{d}S = 0 \tag{4.23}$$

for all test functions $\eta \in H^1_{(0)}(\Omega)$. We now define

$$\mu^{n+1} := S_a \left(-\frac{\varphi^{n+1} - \varphi^n}{\tau} \right) + c^{n+1} \in H^1(\Omega), \tag{4.24}$$

with

$$c^{n+1} := \frac{1}{|\Omega|} \left(\int_\Omega F'(\varphi^{n+1})\, \mathrm{d}x + \int_{\Gamma_w} G'(\varphi^{n+1})\, \mathrm{d}S \right) \tag{4.25}$$

and a being chosen as in (4.22). Recalling the definition of the inner product $(\cdot\,, \cdot)_{S_a}$ (see (4.10)), we infer from (4.23) that

$$\int_\Omega \mu^{n+1}\, \eta \, \mathrm{d}x = \int_\Omega A'(\nabla\varphi^{n+1}) \cdot \nabla\eta + F'(\varphi^{n+1})\, \eta \, \mathrm{d}x + \int_{\Gamma_w} G'(\varphi^{n+1})\, \eta \, \mathrm{d}S \tag{4.26}$$

for all $\eta \in H^1_{(0)}(\Omega)$. Due to the choice of the constant c^{n+1}, a straightforward computation reveals that (4.26) remains true even for all test functions $\eta \in H^1(\Omega)$. This

means that for every $n \in \{0, ..., N-1\}$, the pair $(\varphi^{n+1}, \mu^{n+1})$ satisfies the equations

$$\left\langle \frac{\varphi^{n+1} - \varphi^n}{\tau}, \zeta \right\rangle_{H^1(\Omega)} = -\int_\Omega M(\nabla\varphi^n, \varphi^n)\nabla\mu^{n+1} \cdot \nabla\zeta \, \mathrm{d}x, \tag{4.27a}$$

$$\int_\Omega \mu^{n+1} \eta \, \mathrm{d}x = \int_\Omega A'(\nabla\varphi^{n+1}) \cdot \nabla\eta + F'(\varphi^{n+1}) \eta \, \mathrm{d}x + \int_{\Gamma_w} G'(\varphi^{n+1}) \eta \, \mathrm{d}S \tag{4.27b}$$

for all test functions $\zeta, \eta \in H^1(\Omega)$. Here, (4.27a) follows directly from the construction of μ^{n+1} in (4.24) and the definition of the solution operator S_a (see (4.9)). The system (4.27) can be interpreted as a time-discrete approximation of the weak formulation (4.12).

The time-discrete approximate solution now needs to be extended onto the whole time interval $[0, T]$. The *piecewise constant extension* (φ_N, μ_N) is defined as

$$\big(\varphi_N, \mu_N\big)(\cdot, t) := \begin{cases} (\varphi_0, \mu_0) & \text{if } t \le 0, \\ (\varphi^n, \mu^n) & \text{if } t \in \big((n-1)\tau, n\tau\big], n \in \{1, ..., N\}, \end{cases} \tag{4.28}$$

whereas the *piecewise linear extension* $(\overline{\varphi}_N, \overline{\mu}_N)$ is defined as

$$(\overline{\varphi}_N, \overline{\mu}_N)(\cdot, t) := \lambda(\varphi^n, \mu^n) + (1-\lambda)(\varphi^{n-1}, \mu^{n-1}) \tag{4.29}$$

for $t = \lambda n\tau + (1-\lambda)(n-1)\tau$ with $n \in \{1, ..., N\}$ and $\lambda \in [0, 1]$.

Henceforth, the letter C will denote generic positive constants that may depend only on φ_0 and the constants introduced in A2–A4 and F1 but not on n, N or τ. These constants may also change their value from line to line.

Step 2: Existence of a minimizer to the functional J_n. We now prove that the functional J_n introduced in (4.21) actually possesses a minimizer. Therefore, we employ the direct method of the calculus of variations.

For any $\varphi \in H^1_{(m)}(\Omega)$, we obtain

$$\|\varphi\|_{L^2(\Omega)} \le \big\|\langle\varphi\rangle_\Omega\big\|_{L^2(\Omega)} + \big\|\varphi - \langle\varphi\rangle_\Omega\big\|_{L^2(\Omega)} \le C\big(1 + \|\nabla\varphi\|_{L^2(\Omega)}\big)$$

by means of Poincaré's inequality. This directly implies

$$\|\varphi\|_{H^1(\Omega)} \le c_*\big(1 + \|\nabla\varphi\|_{L^2(\Omega)}\big) \quad \text{for all } \varphi \in H^1_{(m)}(\Omega) \tag{4.30}$$

for some positive constant c_* depending only on m and Ω. Recalling the assumptions on A (see A3), that $F \ge -B_F$ (see F1) and that $G \ge 0$ (see A2), we use Poincaré's inequality to derive the estimate

$$\begin{aligned} J_n(\varphi) &\ge \int_\Omega A(\nabla\varphi) \, \mathrm{d}x - B_F|\Omega| \ge A_0 \|\nabla\varphi\|^2_{L^2(\Omega)} - B_F|\Omega| \\ &\ge \frac{A_0}{c_*^2} \|\varphi\|^2_{H^1(\Omega)} - A_0 - B_F|\Omega| \end{aligned} \tag{4.31}$$

for all $\varphi \in H^1_{(m)}(\Omega)$. This means that J_n is coercive and bounded from below. Hence, the infimum

$$\mathcal{I} := \inf_{H^1_{(m)}(\Omega)} J_n$$

exists, and consequently, there also exists a corresponding minimizing sequence $(\varphi_k)_{k\in\mathbb{N}}$ with

$$J_n(\varphi_k) \to \mathcal{I} \quad \text{as } k \to \infty \quad \text{and} \quad J_n(\varphi_k) \leq \mathcal{I} + 1 \quad \text{for all } k \in \mathbb{N}.$$

Now, (4.31) directly implies that $(\varphi_k)_{k\in\mathbb{N}}$ is bounded in $H^1_{(m)}(\Omega)$. Using the Banach–Alaoglu theorem, the compact embeddings $H^1_{(m)}(\Omega) \hookrightarrow L^p(\Omega)$ and $H^1_{(m)}(\Omega) \hookrightarrow L^q(\partial\Omega)$, we infer that there exists a function $\overline{\varphi} \in H^1_{(m)}(\Omega)$ such that

$$\begin{aligned} \varphi_k \to \overline{\varphi} \quad &\text{weakly in } H^1_{(m)}(\Omega), \text{ strongly in } L^p(\Omega) \text{ and in } L^q(\partial\Omega), \\ &\text{pointwise a.e. in } \Omega, \text{ and pointwise a.e. on } \partial\Omega \end{aligned} \tag{4.32}$$

along a non-relabeled subsequence. Since A is continuous and convex (see A3), we infer

$$\int_\Omega A(\nabla\overline{\varphi})\,\mathrm{d}x \leq \liminf_{k\to\infty} \int_\Omega A(\nabla\varphi_k)\,\mathrm{d}x \tag{4.33}$$

due to weak lower semicontinuity. Recalling the growth conditions on F and G (see F1 and A2) and the convergences in (4.32), we apply Lebesgue's general convergence theorem (see Alt 2016, [Section 3.25]) to conclude

$$\int_\Omega F(\varphi_k)\,\mathrm{d}x \to \int_\Omega F(\overline{\varphi})\,\mathrm{d}x \quad \text{and} \quad \int_{\Gamma_w} G(\varphi_k)\,\mathrm{d}S \to \int_{\Gamma_w} G(\overline{\varphi})\,\mathrm{d}S \tag{4.34}$$

as $k \to \infty$. Combining (4.33) and (4.34), we obtain

$$J_n(\overline{\varphi}) \leq \liminf_{k\to\infty} J_n(\varphi_k) = \mathcal{I}.$$

This proves that $\overline{\varphi}$ is a minimizer of the functional J_n.

Step 3: A priori estimates for the piecewise constant extension. We now claim that the piecewise constant extension (φ_N, μ_N) fulfills the uniform priori estimate

$$\|\varphi_N\|_{L^\infty(0,T;H^1(\Omega))} + \|\mu_N\|_{L^2(0,T;H^1(\Omega))} \leq C. \tag{4.35}$$

To prove (4.35), we exploit the recursive construction of the time-discrete approximate solution. Since for any $n \in \{0, ..., N-1\}$, φ^{n+1} was chosen to be a minimizer

of the functional J_n, we have

$$\frac{1}{2\tau}\left\|\varphi^{n+1}-\varphi^n\right\|_{S_a}^2+\mathcal{E}(\varphi^{n+1})=J_n(\varphi^{n+1})\le J_n(\varphi^n)=\mathcal{E}(\varphi^n) \tag{4.36}$$

for all $n\in\{0,\dots,N-1\}$. By a simple induction, we thus infer

$$\mathcal{E}(\varphi^n)\le\mathcal{E}(\varphi_0)\quad\text{for all } n\in\{0,\dots,N-1\}. \tag{4.37}$$

Recalling the assumptions on A (see A3) and that the potentials F and G are bounded from below (see A2 and F1), we use estimate (4.30) and (4.37) to obtain

$$\left\|\varphi^{n+1}\right\|_{H^1(\Omega)}^2\le C+C\left\|\nabla\varphi^{n+1}\right\|_{L^2(\Omega)}^2\le C+C\int_\Omega A(\nabla\varphi^{n+1})\le C+C\mathcal{E}(\varphi^{n+1})\le C \tag{4.38}$$

for all $n\in\{0,\dots,N-1\}$. By the definition of φ_N, this directly implies

$$\|\varphi_N\|_{L^\infty(0,T;H^1(\Omega))}\le C. \tag{4.39}$$

For any $n\in\{1,\dots,N\}$, we now set $t_n:=n\tau$. By the definition of the piecewise constant extension, we have

$$\varphi_N(t)=\varphi(t_n)=\varphi^n\quad\text{and}\quad\mu_N(t)=\mu(t_n)=\mu^n \tag{4.40}$$

for all $t\in(t_{n-1},t_n]$. Recalling the priori estimate (4.36) and the definition of μ^n (see (4.24)), we obtain

$$\begin{aligned}
&\mathcal{E}\big(\varphi_N(t_n)\big)+\frac{1}{2}\int_{t_{n-1}}^{t_n}\int_\Omega M\big(\nabla\varphi_N(s-\tau),\varphi_N(s-\tau)\big)\,|\nabla\mu_N(s)|^2\,\mathrm{d}x\,\mathrm{d}s\\
&\quad=\mathcal{E}\big(\varphi_N(t_n)\big)+\frac{1}{2\tau^2}\int_{t_{n-1}}^{t_n}\|\varphi_N(s)-\varphi_N(s-\tau)\|_{S_a}^2\,\mathrm{d}s\\
&\quad=\mathcal{E}\big(\varphi_N(t_n)\big)+\frac{1}{2\tau}\|\varphi_N(t_n)-\varphi_N(t_n-\tau)\|_{S_a}^2\\
&\quad\le\mathcal{E}\big(\varphi_N(t_{n-1})\big)
\end{aligned}$$

for all $n\in\{0,\dots,N-1\}$. Hence, by induction, we get

$$\mathcal{E}\big(\varphi_N(t_n)\big)+\frac{1}{2}\int_0^{t_n}\int_\Omega M\big(\nabla\varphi_N(s-\tau),\varphi_N(s-\tau)\big)\,|\nabla\mu_N(s)|^2\,\mathrm{d}x\,\mathrm{d}s\le\mathcal{E}(\varphi_0)$$

for all $n \in \{0, \dots, N-1\}$. Now, for any $t \in (0, T]$, we find an index $n \in \{0, \dots, N-1\}$ such that $t \in (t_{n-1}, t_n]$. Recalling (4.40), we eventually conclude that

$$\mathcal{E}\big(\varphi_N(t)\big) + \frac{1}{2}\int_0^t \int_\Omega M\big(\nabla\varphi_N(s-\tau), \varphi_N(s-\tau)\big)\, |\nabla\mu_N(s)|^2 \,\mathrm{d}x\,\mathrm{d}s \le \mathcal{E}(\varphi_0) \tag{4.41}$$

for all $t \in [0, T]$. In particular, choosing $t = T$, we obtain the uniform bound

$$\|\nabla\mu_N\|^2_{L^2(0,T;L^2(\Omega))} \le C. \tag{4.42}$$

We now test (4.27b) with the constant function $\eta \equiv 1/|\Omega|$. Using the growth assumptions from F1, the continuous embeddings $H^1(\Omega) \hookrightarrow L^5(\Omega)$ and $H^1(\Omega) \hookrightarrow L^3(\partial\Omega)$, as well as the uniform bound (4.39), we derive the estimate

$$\begin{aligned}
\big|\langle\mu_N(t)\rangle_\Omega\big| &\le \frac{1}{|\Omega|}\left(\int_\Omega \big|F'\big(\varphi_N(t)\big)\big| \,\mathrm{d}x + \int_{\Gamma_w} \big|G'\big(\varphi_N(t)\big)\big| \,\mathrm{d}S\right)\\
&\le C\big(1 + \|\varphi_N(t)\|^5_{L^5(\Omega)} + \|\varphi_N(t)\|^3_{L^3(\partial\Omega)}\big)\\
&\le C\big(1 + \|\varphi_N\|^5_{L^\infty(0,T;H^1(\Omega))} + \|\varphi_N\|^3_{L^\infty(0,T;H^1(\Omega))}\big) \le C.
\end{aligned}$$

Applying Poincaré's inequality, we thus obtain

$$\begin{aligned}
\|\mu_N(t)\|_{L^2(\Omega)} &\le \big\|\langle\mu_N(t)\rangle_\Omega\big\|_{L^2(\Omega)} + \big\|\mu_N - \langle\mu_N(t)\rangle_\Omega\big\|_{L^2(\Omega)}\\
&\le C\big(1 + \|\nabla\mu_N(t)\|_{L^2(\Omega)}\big).
\end{aligned} \tag{4.43}$$

Combining (4.42) and (4.43), this yields

$$\|\mu_N\|_{L^2(0,T;H^1(\Omega))} \le C. \tag{4.44}$$

Due to (4.39) and (4.44), the a priori estimate (4.35) is now established.

Step 4: A priori estimate for the piecewise linear extension. We next claim that for all $s, t \in [0, T]$,

$$\big\|\overline{\varphi}_N(t) - \overline{\varphi}_N(s)\big\|_{L^2(\Omega)} \le C\,|t-s|^{\frac{1}{4}}, \tag{4.45a}$$

$$\big\|\overline{\varphi}_N(t) - \varphi_N(t)\big\|_{L^2(\Omega)} \le C\tau^{\frac{1}{4}}, \tag{4.45b}$$

$$\big\|\partial_t\overline{\varphi}_N\big\|_{L^2(0,T;H^1(\Omega)')} \le C. \tag{4.45c}$$

In particular, the first estimate means that the piecewise linear extension $\overline{\varphi}_N$ is Hölder continuous in time.

To prove these inequalities, we first infer from (4.27a) and the definition of the piecewise linear extension (see (4.29)) that

$$\big\langle\partial_t\overline{\varphi}_N(\tau)\,,\,\zeta\big\rangle_{H^1(\Omega)} = -\int_\Omega \nabla\mu_N(\tau)\cdot\nabla\zeta \,\mathrm{d}x \tag{4.46}$$

for almost all $\tau \in [0,T]$ and all $\zeta \in H^1(\Omega)$. Let now $\xi \in L^2(0,T;H^1(\Omega))$ be arbitrary. We test (4.46) with $\xi(\tau)$ and integrate the resulting equation with respect to τ from 0 to T. Then, using Hölder's inequality as well as the a priori estimate (4.35), we obtain

$$\left| \int_0^T \left\langle \partial_t \overline{\varphi}_N(\tau)\,,\, \xi \right\rangle_{H^1(\Omega)} \mathrm{d}t \right| \leq \|\mu_N\|_{L^2(0,T;H^1(\Omega))}\, \|\xi\|_{L^2(0,T;H^1(\Omega))} \leq C\, \|\xi\|_{L^2(0,T;H^1(\Omega))}\,. \tag{4.47}$$

Taking the supremum over all $\xi \in L^2(0,T;H^1(\Omega))$ with $\|\xi\|_{L^2(0,T;H^1(\Omega))} \leq 1$, this proves estimate (4.45c).

Next, let $s,t \in [0,T]$ be arbitrary. Without loss of generality, we assume $s < t$. Integrating (4.46) with respect to τ from s to t, choosing $\zeta = \overline{\varphi}_N(t) - \overline{\varphi}_N(s)$, and using Hölder's inequality, we derive the estimate

$$\begin{aligned} \left\|\overline{\varphi}_N(t) - \overline{\varphi}_N(s)\right\|_{L^2(\Omega)}^2 &\leq \left\|\nabla\overline{\varphi}_N(t) - \nabla\overline{\varphi}_N(s)\right\|_{L^2(\Omega)} \int_s^t \|\nabla\mu_N(\tau)\|_{L^2(\Omega)}\, \mathrm{d}\tau \\ &\leq 2\, \|\varphi_N\|_{L^\infty(0,T;H^1(\Omega))}\, \|\mu_N\|_{L^2(0,T;L^2(\Omega))}\, |s-t|^{\frac{1}{2}}\,. \end{aligned} \tag{4.48}$$

In view of the a priori estimate (4.35), this proves (4.45a).

Let now $t \in [0,T]$ be arbitrary. Then, we find $\lambda \in [0,1]$ and $n \in \{1,\ldots,N\}$ such that $t = \lambda n\tau + (1-\lambda)(n-1)\tau$. We thus obtain

$$\begin{aligned} \left\|\overline{\varphi}_N(t) - \varphi_N(t)\right\|_{L^2(\Omega)} &= \left\|\lambda\varphi^n + (1-\lambda)\varphi^{n-1} - \varphi^n\right\|_{L^2(\Omega)} \\ &= (1-\lambda)\left\|\varphi^n - \varphi^{n-1}\right\|_{L^2(\Omega)} \\ &= (1-\lambda)\left\|\varphi_N\big(n\tau\big) - \varphi_N\big((n-1)\tau\big)\right\|_{L^2(\Omega)}\,. \end{aligned}$$

Applying (4.45a) with $t = n\tau$ and $s = (n-1)\tau$, we conclude (4.45b). This means that all estimates in (4.45) are established.

Step 5: Convergence to a weak solution. In view of the uniform a priori estimate (4.35), the Banach–Alaoglu theorem implies the existence of functions $\varphi \in L^\infty(0,T;H^1(\Omega))$ and $\mu \in L^2(0,T;H^1(\Omega))$ such that

$$\varphi_N \to \varphi \qquad \text{weakly}-^* \text{ in } L^\infty(0,T;H^1(\Omega)), \tag{4.49}$$

$$\mu_N \to \mu \qquad \text{weakly in } L^2(0,T;H^1(\Omega)), \tag{4.50}$$

as $N \to \infty$, along a non-relabeled subsequence. We further know that

$$\left\|\overline{\varphi}_N\right\|_{L^\infty(0,T;H^1(\Omega))} \leq \|\varphi_N\|_{L^\infty(0,T;H^1(\Omega))} \leq C.$$

In combination with the uniform estimate (4.45c), we use the Banach–Alaoglu theorem to infer $\varphi \in H^1(0,T;H^1(\Omega)')$ with

$$\overline{\varphi}_N \to \varphi \quad \text{weakly in } H^1(0,T;H^1(\Omega)') \tag{4.51}$$

as $N \to \infty$, up to subsequence extraction. Moreover, due to the compact embeddings $H^1(\Omega) \hookrightarrow L^p(\Omega)$ and $H^1(\Omega) \hookrightarrow L^q(\partial\Omega)$, we apply the Aubin–Lions lemma to obtain

$$\overline{\varphi}_N \to \varphi \quad \text{strongly in } C([0,T];L^p(\Omega)) \cap C([0,T];L^q(\partial\Omega)). \tag{4.52}$$

By passing to the limit in estimate (4.45a), we conclude $\varphi \in C^{0,1/4}([0,T],L^2(\Omega))$. This means that the functions φ and μ satisfy the regularity conditions of Definition 4.2(i). Using the estimate (4.45b), we directly deduce from (4.52) that

$$\begin{aligned} \varphi_N \to \varphi \quad &\text{strongly in } L^\infty(0,T;L^p(\Omega)) \cap L^\infty(0,T;L^q(\partial\Omega)), \\ &\text{a.e. in } \Omega, \text{ and a.e. on } \partial\Omega, \end{aligned} \tag{4.53}$$

as $N \to \infty$, after another subsequence extraction.

From the time-discrete weak formulation (4.27), we infer that the piecewise constant extension (φ_N,μ_N) and the piecewise linear extension $(\overline{\varphi}_N,\overline{\mu}_N)$ satisfy the approximate weak formulation

$$\int_0^T \big\langle \partial_t \overline{\varphi}_N(t)\,,\,\xi \big\rangle_{H^1(\Omega)}\,\mathrm{d}t = -\iint_Q M\big(\nabla\varphi_N(t-\tau),\varphi_N(t-\tau)\big)\,\nabla\mu_N(t)\cdot\nabla\xi\,\mathrm{d}x\,\mathrm{d}t, \tag{4.54a}$$

$$\iint_Q \mu_N\,\vartheta\,\mathrm{d}x\,\mathrm{d}t = \iint_Q A'(\nabla\varphi_N)\cdot\nabla\vartheta + F'(\varphi_N)\,\vartheta\,\mathrm{d}x\,\mathrm{d}t + \iint_{\Sigma_w} G'(\varphi_N)\,\vartheta\,\mathrm{d}S\,\mathrm{d}t \tag{4.54b}$$

for all test functions $\xi,\vartheta \in L^2(0,T;H^1(\Omega))$. Recalling the growth conditions on F' and G' from F1 and A2, as well as the priori estimate (4.35), we infer that the sequence $(F'(\varphi_N))_{N\in\mathbb{N}}$ is bounded in $L^\infty(0,T;L^{6/5}(\Omega))$ and the sequence $(G'(\varphi_N))_{N\in\mathbb{N}}$ is bounded in $L^\infty(0,T;L^{4/3}(\partial\Omega))$. Hence, according to the Banach–Alaoglu theorem, there exist functions $f^* \in L^\infty(0,T;L^{6/5}(\Omega))$ and $g^* \in L^\infty(0,T;L^{4/3}(\partial\Omega))$ such that

$$\begin{aligned} F'(\varphi_N) &\to f^* && \text{weakly} - ^* \text{ in } L^\infty(0,T;L^{6/5}(\Omega)), \\ G'(\varphi_N) &\to g^* && \text{weakly} - ^* \text{ in } L^\infty(0,T;L^{4/3}(\partial\Omega)), \end{aligned}$$

as $N \to \infty$, along a non-relabeled subsequence. Moreover, the convergences in (4.53) directly imply $F'(\varphi_N) \to F'(\varphi)$ a.e. in Ω and $G'(\varphi_N) \to G'(\varphi)$ a.e. on $\partial\Omega$. By a convergence principle based on Egorov's theorem (see DiBenedetto 2002, [Proposition 9.2c]), we now infer $f^* = F'(\varphi)$ a.e. in Ω and $g^* = G'(\varphi)$ a.e. on $\partial\Omega$. This

means that

$$F'(\varphi_N) \to F'(\varphi) \qquad \text{weakly} - * \text{ in } L^\infty(0,T;L^{6/5}(\Omega)), \tag{4.55}$$

$$G'(\varphi_N) \to G'(\varphi) \qquad \text{weakly} - * \text{ in } L^\infty(0,T;L^{4/3}(\partial\Omega)), \tag{4.56}$$

as $N \to \infty$. Testing the approximate weak formulation (4.54b) with $\vartheta = \varphi_N - \varphi$ and employing the strong monotonicity condition on A' from A3, we obtain

$$\begin{aligned} a_0 \left\| \nabla\varphi_N - \nabla\varphi \right\|_{L^2(Q)}^2 &\le \iint_Q \big(A'(\nabla\varphi_N) - A'(\nabla\varphi) \big) \cdot \big(\nabla\varphi_N - \nabla\varphi \big) \,\mathrm{d}x \,\mathrm{d}t \\ &= \iint_Q \mu_N \, (\varphi_N - \varphi) \,\mathrm{d}x \,\mathrm{d}t - \iint_Q F'(\varphi_N) \, (\varphi_N - \varphi) \,\mathrm{d}x \,\mathrm{d}t \\ &\quad - \iint_{\Sigma_w} G'(\varphi_N) \, (\varphi_N - \varphi) \,\mathrm{d}S \,\mathrm{d}t \\ &\quad - \iint_Q A'(\nabla\varphi) \cdot \big(\nabla\varphi_N - \nabla\varphi \big) \,\mathrm{d}x \,\mathrm{d}t . \end{aligned} \tag{4.57}$$

Using the convergences (4.50), (4.53), (4.55) and (4.56) along with the weak-strong convergence principle, we infer that the right-hand side of the above estimate tends to zero. We thus conclude that

$$\nabla\varphi_N \to \nabla\varphi \quad \text{strongly in } L^2(Q) \text{ and a.e. in } \Omega \tag{4.58}$$

as $N \to \infty$, up to subsequence extraction. In view of the growth condition on A' from A3, Lebesgue's general convergence theorem further reveals that

$$A'(\nabla\varphi_N) \to A'(\nabla\varphi) \quad \text{strongly in } L^2(Q;\mathbb{R}^d). \tag{4.59}$$

Due to the convergences (4.50), (4.55), (4.56) and (4.59), we can now pass to the limit in (4.54b) to conclude that

$$\iint_Q \mu \, \vartheta \,\mathrm{d}x \,\mathrm{d}t = \iint_Q A'(\nabla\varphi) \cdot \nabla\vartheta + F'(\varphi) \, \vartheta \,\mathrm{d}x \,\mathrm{d}t + \iint_{\Sigma_w} G'(\varphi) \, \vartheta \,\mathrm{d}S \,\mathrm{d}t \tag{4.60}$$

holds for all $\vartheta \in L^2(0,T;H^1(\Omega))$.

We now fix an arbitrary time $t_0 \in (0,T]$. Since $\tau = T/N \to 0$ as $N \to \infty$, we may assume (without loss of generality) that N is chosen large enough to ensure $t - \tau \in [0,T]$ for all $t \in [t_0,T]$. We have

$$\begin{aligned} &\left\| \nabla\varphi_N(t-\tau) - \nabla\varphi(t) \right\|_{L^2(t_0,T;L^2(\Omega))}^2 \\ &\quad \le C \left\| \nabla\varphi_N(t-\tau) - \nabla\varphi(t-\tau) \right\|_{L^2(t_0,T;L^2(\Omega))}^2 + C \left\| \nabla\varphi(t-\tau) - \nabla\varphi(t) \right\|_{L^2(t_0,T;L^2(\Omega))}^2 \\ &\quad \le C \left\| \nabla\varphi_N(t) - \nabla\varphi(t) \right\|_{L^2(0,T;L^2(\Omega))}^2 + C \left\| \nabla\varphi(t-\tau) - \nabla\varphi(t) \right\|_{L^2(t_0,T;L^2(\Omega))}^2 \end{aligned} \tag{4.61}$$

for almost all $t \in [t_0, T]$. Here, from the second to the third line, we used the change of variables $s = t - \tau$ and the fact that $[t_0 - \tau, T - \tau] \subset [0, T]$ to estimate the first summand. Now, as $N \to \infty$, the first summand in the third line of (4.61) tends to zero because of (4.58), whereas the second summand tends to zero since due to mean-continuity in $L^p(Q)$ (see, e.g., Alt 2016, [Section 4.15]). This proves

$$\nabla \varphi_N(\cdot\,, \cdot - \tau) \to \nabla \varphi \quad \text{strongly in } L^2(\Omega \times [t_0, T]) \tag{4.62}$$

as $N \to \infty$. Since $t_0 \in (0, T]$ was arbitrary, we deduce

$$\nabla \varphi_N(\cdot\,, \cdot - \tau) \to \nabla \varphi \quad \text{a.e. in } Q \tag{4.63}$$

as $N \to \infty$, after extracting a subsequence. Proceeding similarly, and using the strong convergence $\varphi_N \to \varphi$ in $L^2(Q)$ (which directly follows from (4.53)), we further obtain

$$\varphi_N(\cdot\,, \cdot - \tau) \to \varphi \quad \text{a.e. in } Q \tag{4.64}$$

as $N \to \infty$. Using (4.63) and (4.64) along with Lebesgue's dominated convergence theorem, we infer

$$M\big(\nabla \varphi_N(\cdot\,, \cdot - \tau), \varphi_N(\cdot\,, \cdot - \tau)\big)\, \nabla \zeta \quad \to \quad M(\nabla \varphi, \varphi)\, \nabla \zeta \tag{4.65}$$

strongly in $L^2(Q)$, as $N \to \infty$, up to subsequence extraction. Employing the weak-strong convergence principle, we can thus pass to the limit $N \to \infty$ in the approximate weak formulation (4.54a) to obtain

$$\int_0^T \langle \partial_t \varphi\,,\, \zeta \rangle_{H^1(\Omega)}\, \mathrm{d}t = -\iint_Q M(\nabla \varphi, \varphi)\, \nabla \mu \cdot \nabla \zeta \, \mathrm{d}x \, \mathrm{d}t \tag{4.66}$$

for all $\zeta \in L^2(0, T; H^1(\Omega))$. Combining (4.60) and (4.66), we eventually conclude that the pair (φ, μ) satisfies the weak formulation (4.12). Moreover, as a direct consequence of the convergence (4.52), φ satisfies the initial condition (4.13). This means that all conditions of Definition 4.2(ii) are fulfilled.

Recalling the growth conditions on F and G from F1 and A2, as well as the convergences in (4.53), we apply Lebesgue's general convergence theorem (see Alt 2016, [Section 3.25]) to conclude

$$F(\varphi_N) \to F(\varphi) \qquad \text{strongly in } L^1(Q), \tag{4.67}$$

$$G(\varphi_N) \to G(\varphi) \qquad \text{strongly in } L^1(Q). \tag{4.68}$$

Then, from the convergences (4.58),(4.67) and (4.68), we infer that

$$\mathcal{E}\big(\varphi_N(t)\big) \to \mathcal{E}\big(\varphi(t)\big) \quad \text{for almost all } t \in [0, T], \tag{4.69}$$

as $N \to \infty$. Recalling (4.50) and (4.65), we use the weak-strong convergence principle to infer

$$\sqrt{M\big(\nabla\varphi_N(\cdot\,,\,\cdot-\tau),\varphi_N(\cdot\,,\,\cdot-\tau)\big)}\,\nabla\mu_N \to \sqrt{M(\nabla\varphi,\varphi)}\,\nabla\mu \qquad \text{weakly in } L^2(Q) \tag{4.70}$$

as $N \to \infty$. We now use the convergences (4.69) and (4.70), the weak lower semicontinuity of the $L^2(Q)$-norm, as well as the discrete energy inequality (4.41), to derive the estimate

$$\begin{aligned}
&\mathcal{E}\big(\varphi(t)\big) + \frac{1}{2}\int_0^t \int_\Omega M\big(\nabla\varphi(s),\varphi(s)\big)\,|\nabla\mu(s)|^2 \,\mathrm{d}x\,\mathrm{d}s \\
&\leq \liminf_{N\to\infty} \mathcal{E}\big(\varphi_N(t)\big) + \liminf_{N\to\infty} \frac{1}{2}\int_0^t \int_\Omega M\big(\nabla\varphi_N(s-\tau),\varphi_N(s-\tau)\big)\,|\nabla\mu_N(s)|^2 \,\mathrm{d}x\,\mathrm{d}s \\
&\leq \liminf_{N\to\infty} \bigg[\mathcal{E}\big(\varphi_N(t)\big) + \frac{1}{2}\int_0^t \int_\Omega M\big(\nabla\varphi_N(s-\tau),\varphi_N(s-\tau)\big)\,|\nabla\mu_N(s)|^2 \,\mathrm{d}x\,\mathrm{d}s\bigg] \\
&\leq \mathcal{E}(\varphi_0)
\end{aligned} \tag{4.71}$$

for almost all $t \in [0,T]$. This proves the weak energy dissipation law (4.14), and thus, the condition in Definition 4.2(iii) is fulfilled.

We eventually conclude that the pair (φ,μ) is a weak solution to system (4.1) in the sense of Definition 4.2. Hence, the proof is complete. □

4.3.2 Proof of Corollary 4.4

Let (φ,μ) be a weak solution to the system (4.1), whose existence is guaranteed by Theorem 4.3. By a straightforward computation, we notice that

$$\big\|F'(\varphi)\big\|^2_{L^2(Q)} = \int_0^T \int_\Omega (F'(\varphi))^2 \,\mathrm{d}x\,\mathrm{d}t \leq 2I_1 + \frac{2}{|\Omega|} I_2, \tag{4.72}$$

where

$$I_1 := \int_0^T \int_\Omega \big(F'(\varphi) - \langle F'(\varphi)\rangle_\Omega\big)^2 \,\mathrm{d}x\,\mathrm{d}t \quad \text{and} \quad I_2 := \int_0^T \bigg(\int_\Omega \big|F'(\varphi)\big|\,\mathrm{d}x\bigg)^2 \,\mathrm{d}t.$$

Hence, in the following, we intend to prove (4.16) by deriving suitable bounds on the terms I_1 and I_2. The letter C will denote generic positive constants depending only on φ_0, $\mathcal{E}(\varphi_0)$, c_0 and the constants in A1–A4, but not on c_1.

Let $\eta \in H^1(\Omega)$ be arbitrary. Since A is convex (see A3), we know that

$$A'(\nabla\varphi)\cdot\nabla(\eta-\varphi) \leq A(\nabla\eta) - A(\nabla\varphi) \quad \text{a.e. in } Q.$$

Testing the weak formulation (4.12b) with $\eta - \varphi$ instead of η and using the above estimate, we thus infer that the variational inequality

$$\int_\Omega F'(\varphi)(\varphi - \eta)\,\mathrm{d}x \le \int_\Omega \mu(\varphi - \eta)\,\mathrm{d}x + \int_\Omega A(\nabla\eta) - A(\nabla\varphi)\,\mathrm{d}x - \int_{\Gamma_w} G'(\varphi)(\varphi - \eta)\,\mathrm{d}S \tag{4.73}$$

holds a.e. in $[0, T]$ for all $\eta \in H^1(\Omega)$. Moreover, since (φ, μ) is a weak solution of (4.1), it satisfies the weak energy inequality (4.14). Using Poincaré's inequality, we infer

$$\|\varphi\|_{L^\infty(0,T;H^1(\Omega))} + \|\mu\|_{L^2(0,T;H^1(\Omega))} \le C. \tag{4.74}$$

Step 1: We first derive an estimate for the term I_1. Therefore, we choose

$$\eta := \varphi - \delta\big(F'(\varphi) - \langle F'(\varphi)\rangle_\Omega\big) \tag{4.75}$$

for sufficiently small $\delta > 0$ which ensures $1 - \delta F''(\varphi) > 0$. Since $F'(\varphi) \in L^\infty(0, T; H^1(\Omega))$ due to (4.15), we know that $\eta \in L^\infty(0, T; H^1(\Omega))$. Recalling that A is positively homogeneous of degree 2, we obtain

$$\begin{aligned} A\big(\nabla\eta\big) - A(\nabla\varphi) &= A\big(\nabla\varphi - \delta F''(\varphi)\nabla\varphi\big) - A(\nabla\varphi) \\ &= \big(1 - \delta F''(\varphi)\big)^2 A(\nabla\varphi) - A(\nabla\varphi) \\ &= \big(-2F''(\varphi) + \delta^2 F''(\varphi)^2\big)A(\nabla\varphi) \end{aligned} \tag{4.76}$$

a.e. in Q. We now test the variational inequality (4.73) with η. After dividing the resulting inequality by δ, we use (4.76) to deduce

$$\begin{aligned} \int_\Omega \big(F'(\varphi) - \langle F'(\varphi)\rangle_\Omega\big)^2\,\mathrm{d}x &= \int_\Omega F'(\varphi)\big(F'(\varphi) - \langle F'(\varphi)\rangle_\Omega\big)\,\mathrm{d}x \\ &\le \int_\Omega \big(\mu - \langle\mu\rangle_\Omega\big)\big(F'(\varphi) - \langle F'(\varphi)\rangle_\Omega\big)\,\mathrm{d}x \\ &\quad - \int_{\Gamma_w} G'(\varphi)\big(F'(\varphi) - \langle F'(\varphi)\rangle_\Omega\big)\,\mathrm{d}S \\ &\quad + \int_\Omega \big(-2F''(\varphi) + \delta^2 F''(\varphi)^2\big)A(\nabla\varphi)\,\mathrm{d}x \end{aligned}$$

a.e. in $[0, T]$. Recalling that F2 implies that F1 holds with $p = 2$, we derive the estimate

$$\big|\langle F'(\varphi)\rangle_\Omega\big| \le C + C\int_\Omega |\varphi|\,\mathrm{d}x \le C + C\,\|\varphi\|_{L^\infty(0,T;L^1(\Omega))} \le C$$

a.e. in $[0, T]$. Hence, using the growth condition on G' from A2 and the continuous embedding $H^1(\Omega) \hookrightarrow L^4(\partial\Omega)$, we deduce

$$\begin{aligned}
&\left| \int_{\Gamma_w} G'(\varphi)\big(F'(\varphi) - \big\langle F'(\varphi)\big\rangle_\Omega\big)\,\mathrm{d}S \right| \\
&\quad \le \int_{\Gamma_w} \big|G'(\varphi)\big|\,\big(\,\big|F'(\varphi)\big| + C\big)\,\mathrm{d}S \\
&\quad \le \int_{\Gamma_w} \big(C + C\,|\varphi|^3\big)\big(C + C\,|\varphi|\,\big)\,\mathrm{d}S \le C + C\int_{\Gamma_w} |\varphi|^4\,\mathrm{d}S \\
&\quad \le C + C\,\|\varphi\|^4_{L^4(\partial\Omega)} \le C + C\,\|\varphi\|^4_{H^1(\Omega)}
\end{aligned} \tag{4.77}$$

a.e. in $[0, T]$. Sending $\delta \to 0$ and using the growth condition from A3, the condition $-F'' \le c_0$ (cf. (4.15)) as well as Poincaré's inequality and Young's inequality, we infer

$$\int_\Omega \big(F'(\varphi) - \big\langle F'(\varphi)\big\rangle_\Omega\big)^2\,\mathrm{d}x \le C\big(1 + \|\varphi\|^4_{H^1(\Omega)} + \|\mu\|^2_{H^1(\Omega)}\big)$$

a.e. in $[0, T]$. Integrating this inequality with respect to time from 0 to T, and using estimate (4.74), we eventually conclude the bound

$$I_1 \le C. \tag{4.78}$$

Step 2: We now derive a suitable estimate for the term I_2. Let $\lambda \in L^\infty([0, T])$ be any function that will be fixed later. We set

$$\eta := \varphi - \delta(\varphi - \langle\varphi\rangle_\Omega) \tag{4.79}$$

for some $\delta > 0$. Testing the variational formulation with this η, dividing the resulting equation by δ, and recalling that A is positively homogeneous of degree 2, we derive the estimate

$$\begin{aligned}
&\int_\Omega F'(\varphi)(\lambda - \langle\varphi\rangle_\Omega)\,\mathrm{d}x \\
&\quad = \int_\Omega F'(\varphi)(\lambda - \varphi)\,\mathrm{d}x + \int_\Omega F'(\varphi)(\varphi - \langle\varphi\rangle_\Omega)\,\mathrm{d}x \\
&\quad \le \int_\Omega F'(\varphi)(\lambda - \varphi)\,\mathrm{d}x + \int_\Omega (\mu - \langle\mu\rangle_\Omega)\varphi\,\mathrm{d}x - \int_{\Gamma_w} G'(\varphi)(\varphi - \langle\varphi\rangle_\Omega)\,\mathrm{d}S \\
&\qquad + \delta(\delta - 2)\int_\Omega A(\nabla\varphi)\,\mathrm{d}x.
\end{aligned} \tag{4.80}$$

Since $F'' + c_0 \geq 0$ due to (4.15), we know that the function $s \mapsto F(s) + \frac{1}{2}c_0 s^2$ is convex. We thus have

$$\begin{aligned} F(\lambda) + \tfrac{1}{2}c_0\lambda^2 &\geq F(\varphi) + \tfrac{1}{2}c_0\varphi^2 + \big(F'(\varphi) + c_0\varphi\big)(\lambda - \varphi) \\ &\geq \big(F'(\varphi) + c_0\varphi\big)(\lambda - \varphi) \end{aligned}$$

a.e. in Q. Using this estimate, as well as Young's inequality, we now get

$$\int_\Omega F'(\varphi)(\lambda - \varphi)\,\mathrm{d}x \leq \int_\Omega F(\lambda)\,\mathrm{d}x + \int_\Omega \tfrac{3}{2}c_0\varphi^2 + c_0\lambda^2\,\mathrm{d}x \tag{4.81}$$

almost everywhere in $[0, T]$. Sending $\delta \to 0$ in (4.80) and using the above estimate, the growth conditions from A2 and A3, the continuous embedding $H^1(\Omega) \hookrightarrow L^4(\partial\Omega)$, as well as Poincaré's inequality, we infer

$$\int_\Omega F'(\varphi)(\lambda - \langle\varphi\rangle_\Omega)\,\mathrm{d}x \leq C\,\|F(\lambda)\|_{L^\infty([0,T])} + C\big(1 + \|\varphi\|^4_{H^1(\Omega)} + \|\mu\|_{H^1(\Omega)}\,\|\varphi\|_{H^1(\Omega)}\big). \tag{4.82}$$

We now fix λ as

$$\lambda(t) := \begin{cases} \langle\varphi(t)\rangle_\Omega + \frac{\kappa}{2} & \text{if } \big\langle F'\big(\varphi(t)\big)\big\rangle_\Omega \geq 0, \\ \langle\varphi(t)\rangle_\Omega - \frac{\kappa}{2} & \text{if } \big\langle F'\big(\varphi(t)\big)\big\rangle_\Omega < 0. \end{cases} \tag{4.83}$$

for all $t \in [0, T]$. Testing (4.12a) with $\zeta \equiv 1$ and integrating the resulting equation with respect to time, we infer $\langle\varphi(t)\rangle_\Omega = \langle\varphi_0\rangle_\Omega$ for all $t \in [0, T]$. In view of (4.82), we thus get

$$\frac{\kappa}{2}\int_\Omega \big|F'(\varphi)\big|\,\mathrm{d}x \leq C\,\|F(\lambda)\|_{L^\infty([0,T])} + C\big(1 + \|\varphi\|^4_{H^1(\Omega)} + \|\mu\|_{H^1(\Omega)}\,\|\varphi\|_{H^1(\Omega)}\big). \tag{4.84}$$

a.e. in $[0, T]$. We now multiply this estimate by $\frac{2}{\kappa}$ and take the square on both sides. Integrating the resulting inequality with respect to time and using the uniform estimate (4.74), we eventually conclude

$$\begin{aligned} I_2 &\leq C\kappa^{-2}\,\|F\|^2_{L^\infty([-R,R])} + C\kappa^{-2}\big(1 + \|\varphi\|^8_{H^1(\Omega)} + \|\mu\|^2_{H^1(\Omega)}\,\|\varphi\|^2_{H^1(\Omega)}\big) \\ &\leq C\kappa^{-2}\,\|F\|^2_{L^\infty([-R,R])} + C. \end{aligned} \tag{4.85}$$

We finally plug the estimates (4.78) for I_1 and (4.85) for I_2 into (4.72). This proves (4.16), and thus, the proof of Corollary 4.4 is complete. □

4.3.3 Proof of Theorem 4.7

The proof is split into three steps.

Step 1: Approximation of the double-obstacle potential by smooth potentials. To prove the assertion, we approximate the double-obstacle potential F by a sequence of regular potentials $(F_n)_{n\in\mathbb{N}}$. Therefore, we define the function

$$J : \mathbb{R} \to [0,\infty), \quad s \mapsto \begin{cases} 6s^2 + 20s + 17 & \text{if } s \le -2, \\ (s+1)^4 & \text{if } -2 < s < -1, \\ 0 & \text{if } -1 \le s \le 1, \\ (s-1)^4 & \text{if } 1 < s < 2, \\ 6s^2 - 20s + 17 & \text{if } s \ge 2, \end{cases}$$

and for any $n \in \mathbb{N}$, we set

$$F_n : \mathbb{R} \to [0,\infty), \quad s \mapsto F_0(s) + nJ(s). \tag{4.86}$$

By this construction, we have $J \in C^2(\mathbb{R};[0,\infty))$, J is convex, and $F_n = F_0$ on $[-1,1]$ for all $n \in \mathbb{N}$. It is straightforward to check that for all $n \in \mathbb{N}$, the approximate potential F_n satisfies the assumption F2 with $c_0 = 1$ and $c_1 = 12n$. It thus follows that F1 is satisfied with $p = 2$ and $B_F = \frac{3}{2}$. In the remainder of this proof, it will be crucial that the constants B_F and c_0 are independent of n. For any $n \in \mathbb{N}$, we further define the approximate energy functional by

$$\mathcal{E}_n : H^1(\Omega) \to \mathbb{R}, \quad \mathcal{E}_n(\varphi) := \int_\Omega A(\nabla\varphi) + F_n(\varphi)\,\mathrm{d}x + \int_{\Gamma_w} G(\varphi)\,\mathrm{d}S. \tag{4.87}$$

Step 2: A priori estimates for the sequence of approximate solutions. We now conclude from Theorem 4.3 that for every $n \in \mathbb{N}$, there exists a weak solution (φ_n, μ_n) of the system (4.1) to the potential F_n in the sense of Definition 4.2. In the following, the letter C will denote generic positive constants that may depend on φ_0, κ and the constants in A1–A4 but not on the approximation index n.

As the weak solutions (φ_n, μ_n) satisfy the weak energy dissipation law (4.14) written for $\mathcal{E}_n$, we deduce the estimate

$$\begin{aligned} &\frac{1}{2}\int_\Omega |\nabla\varphi_n(t)|^2\,\mathrm{d}x - B_F|\Omega| + \frac{1}{2}M_0\int_0^t\int_\Omega |\nabla\mu_n(s)|^2\,\mathrm{d}x\,\mathrm{d}s \\ &\quad\le \mathcal{E}_n\big(\varphi_n(t)\big) + \frac{1}{2}\int_0^t\int_\Omega M\big(\nabla\varphi_n(s),\varphi_n(s)\big)\,|\nabla\mu_n(s)|^2\,\mathrm{d}x\,\mathrm{d}s \\ &\quad\le \mathcal{E}_n(\varphi_0) \le C\,\|\nabla\varphi_0\|^2_{L^2(\Omega)} + C\,\|F_0\|_{L^\infty([-1,1])} \le C \end{aligned}$$

for almost all $t \in [0, T]$ and all $n \in \mathbb{N}$. As B_F is independent of n, we use Poincaré's inequality to conclude the uniform bound

$$\|\varphi_n\|_{L^\infty(0,T;H^1(\Omega))} + \|\mu_n\|_{L^2(0,T;H^1(\Omega))} \leq C. \tag{4.88}$$

Integrating the weak formulation (4.12a) written for (φ_n, μ_n) with respect to time from 0 to T, we now use (4.88) to derive the uniform estimate

$$\|\partial_t \varphi_n\|_{L^2(0,T;H^1(\Omega)')} \leq C. \tag{4.89}$$

Furthermore, Corollary 4.4 provides the estimate

$$\big\|F_n'(\varphi)\big\|_{L^2(Q)}^2 \leq \frac{c}{\kappa^2}\big(1 + \|F_n\|_{L^\infty([-R,R])}^2\big), \tag{4.90}$$

where $R = \big|\langle \varphi_0 \rangle_\Omega\big| + \frac{\kappa}{2} < 1$. Here, the constant c depends only on φ_0, $\mathcal{E}_n(\varphi_0)$, $c_0 = 1$ and the constants in A1–A4. Since $F_n = F_0$ on $[-1, 1]$, we know that $F_n(\varphi_0) = F_0(\varphi_0)$ for all $n \in \mathbb{N}$. Consequently, $\mathcal{E}_n(\varphi_0)$ does not depend on n, and thus, c is independent of n. We infer the uniform bound

$$\big\|F_n'(\varphi_n)\big\|_{L^2(Q)}^2 \leq \frac{c}{\kappa^2}\big(1 + \|F_0\|_{L^\infty([-1,1])}^2\big) \leq C. \tag{4.91}$$

Using (4.88), we further get

$$\big\|F_0'(\varphi_n)\big\|_{L^2(Q)} = \|\varphi_n\|_{L^2(Q)} \leq C\,\|\varphi_n\|_{L^\infty(0,T;L^2(\Omega))} \leq C. \tag{4.92}$$

Combining (4.91) and (4.92), we now conclude

$$\big\|J'(\varphi_n)\big\|_{L^2(Q)} \leq \frac{1}{n}\Big(\big\|F_0'(\varphi_n)\big\|_{L^2(Q)} + \big\|F_n'(\varphi_n)\big\|_{L^2(Q)}\Big) \leq \frac{C}{n}. \tag{4.93}$$

Step 3: Convergence to a weak solution. In view of the uniform estimates (4.88) and (4.89), we now use the continuous embedding $H^1(\Omega) \hookrightarrow L^4(\partial\Omega)$, the Banach–Alaoglu theorem, and the Aubin–Lions lemma along with the compact embeddings $H^1(\Omega) \hookrightarrow L^2(\Omega)$ and $H^1(\Omega) \hookrightarrow L^r(\partial\Omega)$ for $r \in [1, 4)$ to conclude the existence of functions φ and μ such that

$$\partial_t \varphi_n \to \partial_t \varphi \quad \text{weakly in } L^2(0, T; H^1(\Omega)'), \tag{4.94}$$

$$\begin{aligned} \varphi_n \to \varphi \quad & \text{weakly}-^* \text{ in } L^\infty(0, T; H^1(\Omega)) \text{ and in } L^\infty(0, T; L^4(\partial\Omega)), \\ & \text{strongly in } C([0, T]; L^2(\Omega)), \text{ a.e. in } Q, \\ & \text{strongly in } C([0, T]; L^r(\partial\Omega)) \text{ and a.e. on } \Sigma, \end{aligned} \tag{4.95}$$

$$\mu_n \to \mu \quad \text{weakly in } L^2(0, T; H^1(\Omega)), \tag{4.96}$$

for all $r \in [1, 4)$ as $n \to \infty$, after extraction of a subsequence. Using the uniform bound (4.93) along with the Banach–Alaoglu theorem, as well as the pointwise–a.e. convergence stated in (4.95), we deduce

$$J'(\varphi_n) \to 0 \qquad \text{strongly in } L^2(Q), \tag{4.97a}$$
$$J'(\varphi_n) \to J'(\varphi) \qquad \text{a.e. in } Q, \tag{4.97b}$$

as $n \to \infty$. As the strong limit in $L^2(Q)$ and the pointwise limit coincide, we have $J'(\varphi) = 0$ a.e. in Q. Since $J'(s) = 0$ if $|s| \leq 1$ and $\left|J'(s)\right| > 0$ if $|s| > 1$, we conclude

$$|\varphi| \leq 1 \qquad \text{a.e. in } Q.$$

As $F_0'(\varphi_n) = -\varphi_n$, the convergence

$$F_0'(\varphi_n) \to F_0'(\varphi) \qquad \text{weakly in } L^2(Q) \text{ and a.e. in } Q, \tag{4.98}$$

follows directly from (4.95). Moreover, using the growth condition on G' (see A2), (4.95) and Lebesgue's general convergence theorem (see Alt 2016, [Section 3.25]), we obtain

$$G'(\varphi_n) \to G'(\varphi) \qquad \text{strongly in } L^{4/3}(\Sigma) \text{ and a.e. on } \Sigma, \tag{4.99}$$

as $n \to \infty$, after another subsequence extraction. Arguing as in the proof of Theorem 4.3, we exploit the strong monotonicity condition on A' from A3 to further derive the convergences

$$\nabla\varphi_n \to \nabla\varphi \qquad \text{strongly in } L^2(Q) \text{ and a.e. in } Q, \tag{4.100}$$
$$A'(\nabla\varphi_n) \to A'(\nabla\varphi) \qquad \text{strongly in} L^2(Q;\mathbb{R}^d), \tag{4.101}$$

as $n \to \infty$, up to subsequence extraction. Combining (4.95) and (4.100), we eventually get

$$M(\nabla\varphi_n, \varphi_n) \to M(\nabla\varphi, \varphi) \qquad \text{a.e. in} Q. \tag{4.102}$$

Let now $n \in \mathbb{N}$ be arbitrary and let $\zeta \in H^1(\Omega)$ and $\eta \in L^2(0, T; H^1(\Omega))$ with $|\eta| \leq 1$ a.e. in Q be an arbitrary test functions. This already implies that $J'(\eta) = 0$ a.e. in Q. Moreover, since J is convex its derivative J' is monotonically increasing. We thus have

$$J'(\varphi_n)(\varphi_n - \eta) \geq J'(\eta)(\varphi_n - \eta) = 0 \quad \text{a.e. in} Q. \tag{4.103}$$

We now recall that the weak solution (φ_n, μ_n) satisfies the weak formulation (4.12) written for (φ_n, μ_n) instead of (φ, μ). The weak formulation (4.12a) written for

(φ_n, μ_n) and tested with ζ reads as

$$\big\langle \partial_t \varphi_n \,,\, \zeta \big\rangle_{H^1(\Omega)} = -\int_\Omega M(\nabla\varphi_n, \varphi_n)\, \nabla\mu \cdot \nabla\zeta \,\mathrm{d}x. \tag{4.104}$$

Testing the weak formulation (4.12b) written for (φ_n, μ_n) with $\varphi_n - \eta$, integrating with respect to time from 0 to T, and employing estimate (4.103), we obtain

$$\begin{aligned}\iint_Q \mu_n\,(\varphi_n - \eta)\,\mathrm{d}x\,\mathrm{d}t \geq \iint_Q A'(\nabla\varphi_n)\cdot(\nabla\varphi_n - \nabla\eta) + F_0'(\varphi_n)\,(\varphi_n - \eta)\,\mathrm{d}x\,\mathrm{d}t \\ + \iint_{\Sigma_w} G'(\varphi_n)\,(\varphi_n - \eta)\,\mathrm{d}S\,\mathrm{d}t. \end{aligned} \tag{4.105}$$

Using the convergences (4.94)–(4.102), Lebesgue's dominated convergence theorem, as well as the weak-strong convergence principle, we pass to the limit $n \to \infty$ in (4.104) and (4.105). This proves that the pair (φ, μ) satisfies the weak formulation (4.18a) for all $\zeta \in H^1(\Omega)$, as well as the variational inequality (4.18b) for all $\eta \in L^2(0,T; H^1(\Omega))$ with $|\eta| \leq 1$ a.e. in Q. Moreover, (4.95) directly implies that φ satisfies the initial condition (4.19). This means that all conditions of Definition 4.6(ii) are verified.

Proceeding similarly as in Step 4 of the proof of Theorem 4.3, and using the weak formulation (4.18a), we can show a posteriori that φ is Hölder continuous in time in the sense that $\varphi \in C^{0,1/4}([0,T]; L^2(\Omega))$. In combination with (4.94)–(4.96), this proves that all conditions of Definition 4.6(i) are fulfilled.

Recalling that $|\varphi| \leq 1$ a.e. in Q, we use (4.95) along with Lebesgue's general convergence theorem (see Alt 2016, [Section 3.25]) to conclude

$$\int_\Omega F(\varphi)\,\mathrm{d}x = \int_\Omega F_0(\varphi)\,\mathrm{d}x = \lim_{n\to\infty} \int_\Omega F_0(\varphi_n)\,\mathrm{d}x \leq \liminf_{n\to\infty} \int_\Omega F_n(\varphi_n)\,\mathrm{d}x$$

a.e. in $[0,T]$. Using the convergences (4.95), (4.96), (4.100) and (4.102), we now proceed similarly as in Step 5 of the proof of Theorem 4.3 (cf. (4.71)) to verify that the pair (φ, μ) satisfies the weak energy dissipation law (4.20). This means that Definition 4.6(iii) is also fulfilled.

In summary, we conclude that the pair (φ, μ) is a weak solution to system (4.1) (with F being the double-obstacle potential) in the sense of Definition 4.6. Hence, the proof of Theorem 4.7 is complete. □

5 Numerical Results

In this section, we present numerical comparisons between the diffuse-interface model (3.3) and its sharp-interface limit (3.52).

For the sharp-interface computations, (**SI**), we employ the parametric finite element approximation from Bao et al. (2023), which uses piecewise linear finite elements and relies crucially on the stable approximation of the anisotropy introduced in Barrett et al.

(2008a, b), see also Bao and Zhao (2022). Here, we recall that this stable approximation is designed for anisotropy functions of the form

$$\gamma(\mathbf{p}) = \sum_{\ell=1}^{L} \sqrt{\Lambda_\ell \mathbf{p} \cdot \mathbf{p}}, \tag{5.1}$$

where Λ_ℓ, $\ell = 1, \dots, L$, are symmetric and positive definite matrices. We refer to Barrett et al. (2008a), Barrett et al. (2008b), Barrett et al. (2010b), Bao and Zhao (2022), Bao et al. (2023) for details. Clearly, for (5.1), the assumption A3 is satisfied, recall Remark 4.1.

For the diffuse-interface approximations, (**DI**), we adapt the finite element discretizations from Barrett et al. (2014) to the system (3.3). To this end, we assume that Ω is a polyhedral domain and let $\mathcal{T}_h$ be a regular triangulation of Ω into disjoint open simplices. Associated with $\mathcal{T}_h$ is the piecewise linear finite element space

$$S^h = \left\{ \zeta \in C^0(\overline{\Omega}) : \zeta_{|o} \in P_1(o) \, \forall o \in \mathcal{T}_h \right\},$$

where we denote by $P_1(o)$ the set of all affine linear functions on o, cf. Ciarlet (1978). We also let $(\cdot, \cdot)$ denote the L^2-inner product on Ω, and let $(\cdot, \cdot)^h$ be the usual mass lumped L^2-inner product on Ω associated with $\mathcal{T}_h$. In a similar fashion, we let $\langle \cdot, \cdot \rangle^h_{\Gamma_w}$ denote the mass lumped L^2-inner product on Γ_w. Finally, Δt denotes a chosen uniform time step size.

Our fully discrete finite element approximation of (3.3) is then given as follows. For $n \geq 0$, let $\varphi_h^n \in S^h$ be given. Then, find $(\varphi_h^{n+1}, \mu_h^{n+1}) \in S^h \times S^h$ such that

$$\alpha \left(\frac{\varphi_h^{n+1} - \varphi_h^n}{\Delta t}, \chi \right)^h + \varepsilon^{-1} \big(m^\varepsilon(\varphi_h^n) \beta^\varepsilon(\nabla \varphi_h^n) \nabla \mu_h^{n+1}, \nabla \chi \big) = 0, \tag{5.2a}$$

$$\varepsilon \big(B(\nabla \varphi_h^n) \nabla \varphi_h^{n+1}, \nabla \eta \big) + \varepsilon^{-1} \big(F'(\varphi_h^{n+1}), \eta \big)^h + c_F \sigma \langle G'(\varphi_h^{n+1}), \eta \rangle^h_{\Gamma_w} = (\mu_h^{n+1}, \eta)^h \tag{5.2b}$$

for all $(\chi, \eta) \in S^h \times S^h$. The above scheme utilizes the linearization $B(\mathbf{p})\mathbf{p} = A'(\mathbf{p})$ for anisotropies of the form (5.1), which was first introduced in Barrett et al. (2013). In particular, the symmetric positive definite matrices B are defined by

$$B(\mathbf{p}) = \begin{cases} \gamma(\mathbf{p}) \displaystyle\sum_{\ell=1}^{L} \frac{\Lambda_\ell}{\sqrt{\Lambda_\ell \mathbf{p} \cdot \mathbf{p}}} & \mathbf{p} \neq \mathbf{0}, \\ L \displaystyle\sum_{\ell=1}^{L} \Lambda_\ell & \mathbf{p} = \mathbf{0}. \end{cases} \tag{5.3}$$

We stress that the induced semi-implicit discretization of $A'(\nabla \varphi)$ in (5.2b) ensures that our numerical method is stable. In fact, using the techniques in Barrett et al. (2013), Barrett et al. (2014), and on employing semi-implicit approximations of $F'(\varphi)$ and

$G'(\varphi)$ based on convex/concave splittings of F and G, an unconditional stability result can be shown. However, for the purposes of this paper, we prefer the simpler approximation (5.2). We also note that extending the scheme (5.2) to the case of the obstacle potential (1.2c), when (5.2b) needs to be replaced with a variational inequality, is straightforward. We refer to Barrett et al. (2013), Barrett et al. (2014) for the precise details.

We implemented the scheme (5.2), and its obstacle potential variant, with the help of the finite element toolbox ALBERTA, see (Schmidt and Siebert 2005). To increase computational efficiency, we employ adaptive meshes, which have a finer mesh size $h_f = \frac{\sqrt{2}}{N_f}$ within the diffuse interfacial regions and a coarser mesh size $h_c = \frac{\sqrt{2}}{N_c}$ away from them, with $N_f, N_c \in \mathbb{N}$, see Baňas and Nürnberg (2008), Barrett et al. (2004) for a more detailed description. The nonlinear systems of equations arising from (5.2) at each time step are solved with a Newton method, where we employ the sparse factorization package UMFPACK, see Davis (2004), for the solution of the linear systems at each iteration. In the case of the double-obstacle potential, we employ the solution method from Baňas and Nürnberg (2008), Barrett et al. (2014).

In all our computations, we fix the mobility $D(\boldsymbol{\nu}) = 1$ and, up to possible rotations, use the anisotropy

$$\gamma(\mathbf{p}) = \sum_{\ell=1}^{d} \sqrt{(1-\delta^2)\, p_\ell^2 + \delta^2 |\mathbf{p}|^2}, \qquad \mathbf{p} = (p_1, \cdots, p_d)^T, \tag{5.4}$$

which can be regarded as a smoothed ℓ^1-norm, with a small regularization parameter $\delta > 0$. Note that, (5.4) is a special case of (5.1). For the (**DI**) computations, we choose for the potential F either (1.2a), so that $c_F = \frac{4}{3}$, or (1.2c), so that $c_F = \frac{\pi}{2}$. We let G be defined by (2.9), while the regularized mobility functions are defined via (3.1) and (3.2), with $r = 2$ and $\gamma_0 = d_1 = 1$. We also choose $\alpha = \frac{c_F^2}{4}$ so that (3.25) is consistent with (2.1a). Finally, unless otherwise stated, we use the smooth potential (1.2a) for our (**DI**) computations.

5.1 2d Results

In numerical simulations of solid-state dewetting problems, it is often of interest whether a thin film of material breaks up into islands. For example, in two space dimensions and in the isotropic case with a 90° contact angle condition, it has been observed that elongated films undergo pinch-off once the aspect ratio of length versus height goes beyond a critical value $R_0 \approx 127.9$, (Dornel et al. 2006; Wang et al. Jan 2015). For nonzero values of σ, the critical value behaves like $R_0 \approx 96.6/\sin(\frac{1}{2}\arccos\sigma) - 8.66$, (Dornel et al. 2006).

it turns out that the anisotropy γ can have a dramatic influence on the critical value R_0. To investigate this numerically, we simulate the evolution of small thin films, starting from an initial interface in the form of the upper half of a tube with aspect ratio $R = L/H$, and fix $H = 0.3$. We consider the following four example situations:

(a) an island of $R = 15$ with anisotropy $\gamma(\mathcal{R}(\frac{\pi}{4})\mathbf{p})$ and $\sigma = \cos\frac{5\pi}{6}$;

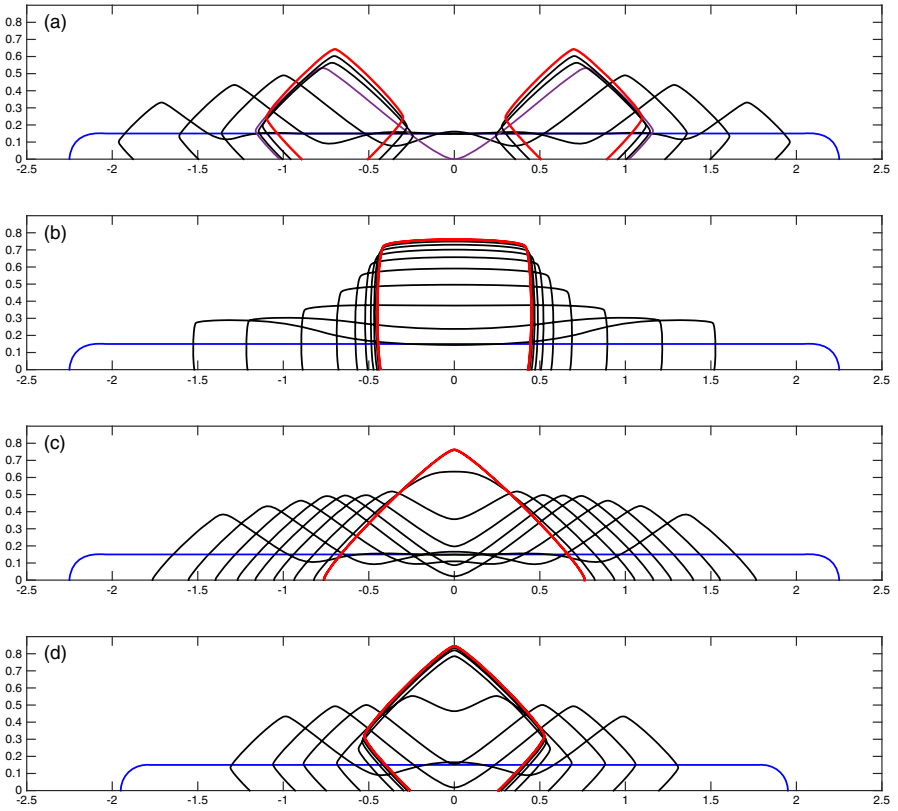

Fig. 4 Evolution of small island films toward the equilibrium (red line) for the SI approximations. **a** Plots at $t = 0, 0.002, 0.01, 0.02, 0.030878, 0.0319, 0.0339, 0.1$, where the island occurs pinch-off at $t = 0.030878$; **b–d** are the plots at $t = 0, 0.01, 0.02, \cdots, 0.1$ (Color figure online)

(b) an island of $R = 15$ with anisotropy $\gamma(\mathbf{p})$ and $\sigma = \cos\frac{5\pi}{6}$;
(c) an island of $R = 15$ with anisotropy $\gamma(\mathcal{R}(\frac{\pi}{4})\mathbf{p})$ and $\sigma = \cos\frac{\pi}{2}$;
(d) an island of $R = 13$ with anisotropy $\gamma(\mathcal{R}(\frac{\pi}{4})\mathbf{p})$ and $\sigma = \cos\frac{5\pi}{6}$,

where $\mathcal{R}(\theta)$ is the rotation matrix with an angle θ, and $\gamma(\mathbf{p})$ is given by (5.4) with $d = 2, \delta = 0.1$. We note that anisotropies with a fourfold symmetry like our choices above are often used in two-dimensional models for materials with a cubic crystalline surface energy (Liu and Metiu 1993; McFadden et al. 2000; Zhang and Gladwell 2003).

Plots of the interface profiles for the SI approximations are presented in Fig. 4a–d for the four examples, respectively, where the approximated polygonal curve consists of 2048 line segments, and the time step size is fixed as 10^{-6}. From these figures, we can observe the influence of the anisotropy γ, the contact energy density difference σ, and the aspect ratio R of the thin film on the evolution. In particular, comparing the evolutions in Fig. 4a and d, we see that the critical value R_0 for break-up to occur appears to satisfy $13 < R_0 \leq 15$, which is much smaller than in the isotropic case.

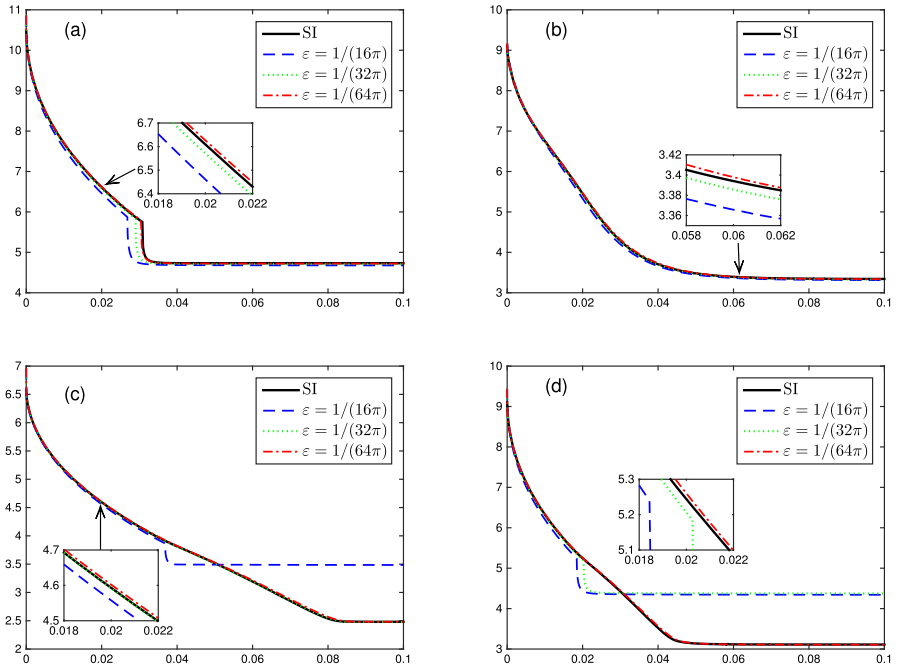

Fig. 5 The time history of the energy for the DI and SI approximations in the four different examples using the double smooth potential

Moreover, we see that either rotating the anisotropy, Fig. 4b, or changing the contact angle, Fig. 4c, ensures that no break-up occurs, meaning that $R_0 > 15$ in both cases.

Let us remark that the pinch-off observed in Fig. 4a represents a singularity for the parametric description on which the SI approximations are based. Hence, we perform a heuristical topological change, from a single curve to two separate curves, once an inner vertex of the polygonal curve touches the substrate. In what follows, we will use the computations in Fig. 4 as reference solutions for our DI approximations, in order to empirically confirm our theoretical results from Sect. 3.

For our DI approximations, we consider the computational domain $\Omega = [0, 3] \times [0, 1]$, on which for symmetry reasons, we only compute the right half of the evolving thin film. As interfacial parameters, we consider $\varepsilon = 1/(2^{4+i}\pi)$, for $i = 0, \ldots, 2$, and choose the discretization parameters as $N_f = 2^{8+i}$, $N_c = 2^{5+i}$, $\Delta t = 10^{-3}/2^{4+2i}$. These spatial adaptive discretization parameters allow for a sufficient resolution of the diffuse-interface, while the temporal discretization parameters yield an excellent agreement with the SI approximations. In fact, in Fig. 5, we show the energy plots of the DI approximations and compare them with the corresponding SI approximations for the four different examples from Fig. 4. We observe that for sufficiently small values of ε, there is excellent agreement between the SI and DI evolutions, in line with our asymptotic analysis in Sect. 3. What is interesting to note is that for Example (a), the pinch-off time predicted by the DI computations is too early when ε is not small, and this can be explained by the fact that the wider interfacial region "sees" contact

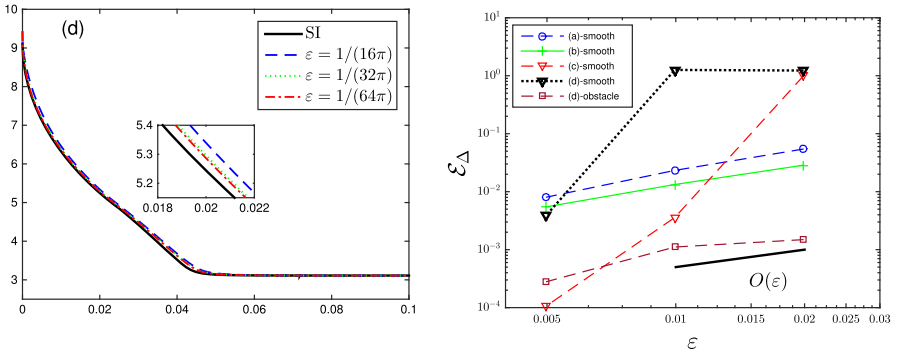

Fig. 6 Left panel: The time history of the energy for the DI and SI approximations in Example (d) using the obstacle potential (1.2c). Right panel: The errors $\mathcal{E}_\Delta$ of the energy at the final time $T = 0.1$ between the SI and DI approximations plotted against ε. Here, "(d)-obstacle" refers to Example (d) with the obstacle potential, while the remaining graphs are for Examples (a)–(d) with the smooth potential

with the substrate earlier, leading to the break-up into two islands. For the same reason, in Examples (c) and (d), the DI computations for $\varepsilon = 1/(16\pi)$ erroneously predict a pinch-off, leading to a larger final energy. But once ε is sufficiently small, no pinch-off occurs, in agreement with the SI evolutions.

We note that using the double-obstacle potential (1.2c) leads to very similar results. As an example, we show the evolution of the discrete energies for Example (d) in Fig. 6. In addition, in order to also have a quantitative comparison between our SI and DI computations, in the same figure, we also present plots of the energy difference $\mathcal{E}_\Delta$ between the final SI and DI solutions against ε. The presented results suggest that the DI energies of the final states approach the corresponding SI energy with $O(\varepsilon)$. Note that, the three instances where $\mathcal{E}_\Delta \geq 10^{-1}$ correspond to cases where the DI computations wrongly predict a pinch-off. Moreover, in practice, we observe that the contact angles between DI and SI at the final time agree very well, with the error being of order 10^{-3} throughout.

The qualitative behavior of the DI and SI approximations is compared in Figs. 7, 8, 9, 10. In all four examples, we note an excellent agreement between the two different approaches. This is particularly noteworthy in Example (a) with the occurrence of a topological change, which is not covered by our asymptotic analysis.

5.2 3d Results

In 3d, we compare our SI and DI approximations for the evolution of an initially spherical island for the anisotropy $\gamma(\mathcal{R}_x(\frac{\pi}{4})\mathcal{R}_y(\frac{\pi}{4})\mathbf{p})$, where $\gamma(\mathbf{p})$ is given by (5.4) with $d = 3$, $\delta = 0.1$, and where $\mathcal{R}_x(\theta)$, $\mathcal{R}_y(\theta)$ are rotation matrices which rotate a vector through an angle θ within the (y, z)- and (x, z)-planes, respectively. The initial interface is chosen to be a semisphere of radius 0.4, attached to the (x, y)-plane, and we let $\sigma = \cos(\frac{5\pi}{6})$.

For the SI computation, we consider a polyhedral surface with 8256 triangles and 4225 vertices, and a time step size 10^{-4}. For our DI approximations, on the other

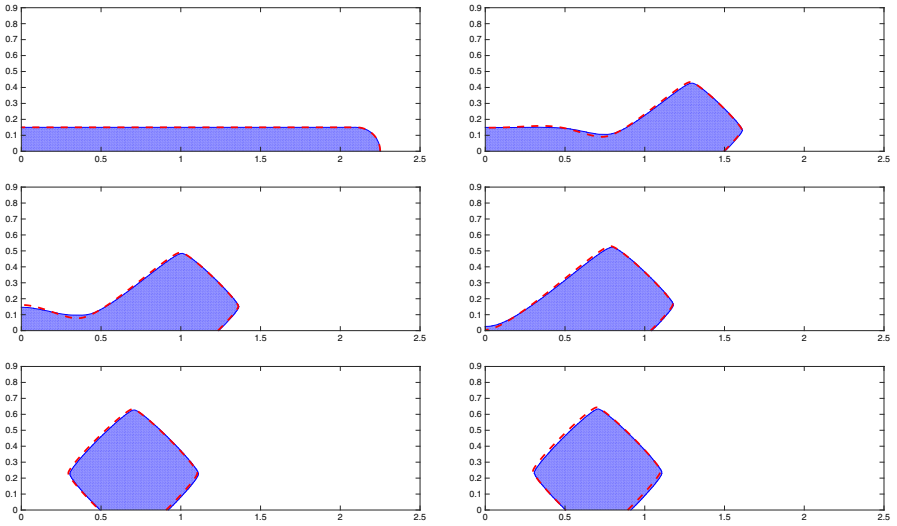

Fig. 7 [Example (a)] Interface profiles at times $t = 0, 0.01, 0.02, 0.03, 0.04, 0.1$ for the DI approximations with $\varepsilon = 1/(64\pi)$, and the red dash line represents the SI approximations (Color figure online)

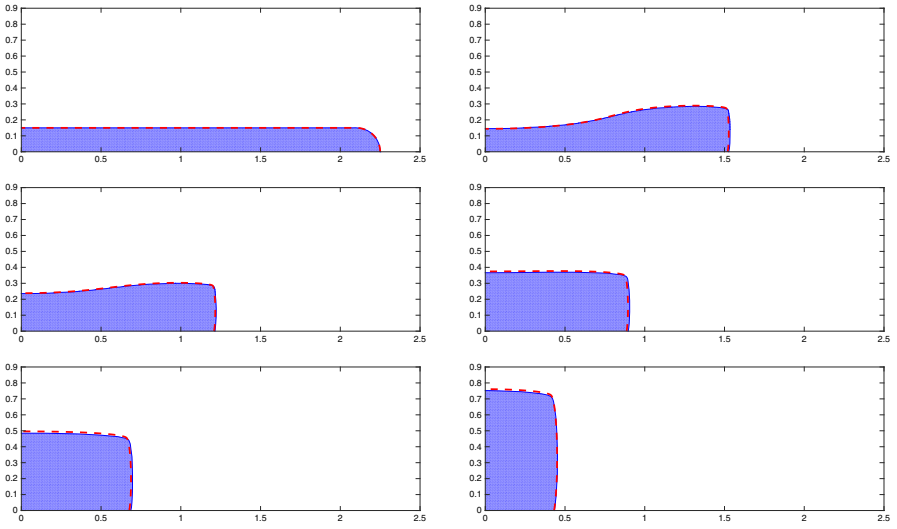

Fig. 8 [Example (b)] Interface profiles at times $t = 0, 0.01, 0.02, 0.03, 0.04, 0.1$ for the DI approximations with $\varepsilon = 1/(64\pi)$, and the red dash line represents the SI approximations (Color figure online)

hand, we consider the computational domain $\Omega = [-\frac{1}{2}, \frac{1}{2}]^3$ and as interfacial parameters consider $\varepsilon = 1/(2^{2+i}\pi)$, for $i = 0, \ldots, 2$, with the corresponding discretization parameters $N_f = 2^{5+i}$, $N_c = 2^{2+i}$, $\Delta t = 10^{-3}/2^{2i}$. In Fig. 11, we show the energy plots of the DI approximations and compare them with the corresponding SI simulation, noting once again an excellent agreement when ε is sufficiently small. We also present a plot of the error in the energy between the DI and SI approximations against

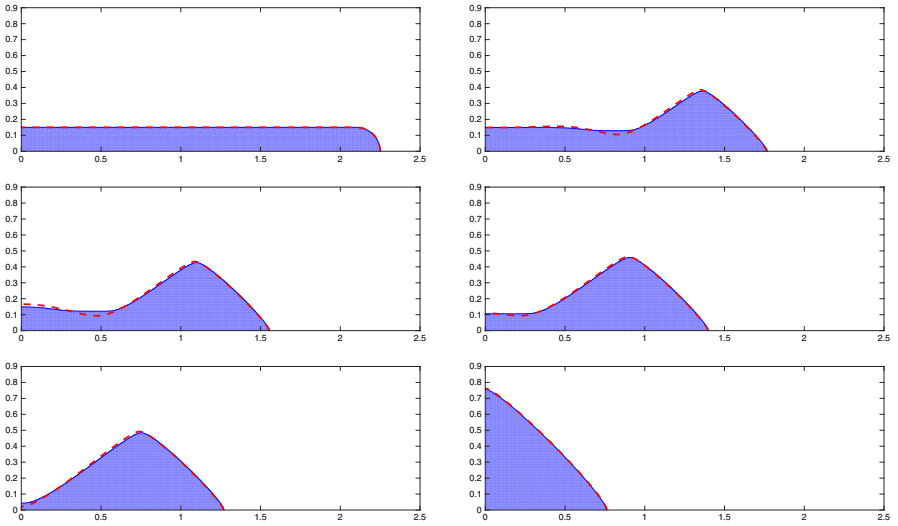

Fig. 9 [Example (c)] Interface profiles at times $t = 0, 0.01, 0.02, 0.03, 0.04, 0.1$ for the DI approximations with $\varepsilon = 1/(64\pi)$, and the red dash line represents the SI approximations (Color figure online)

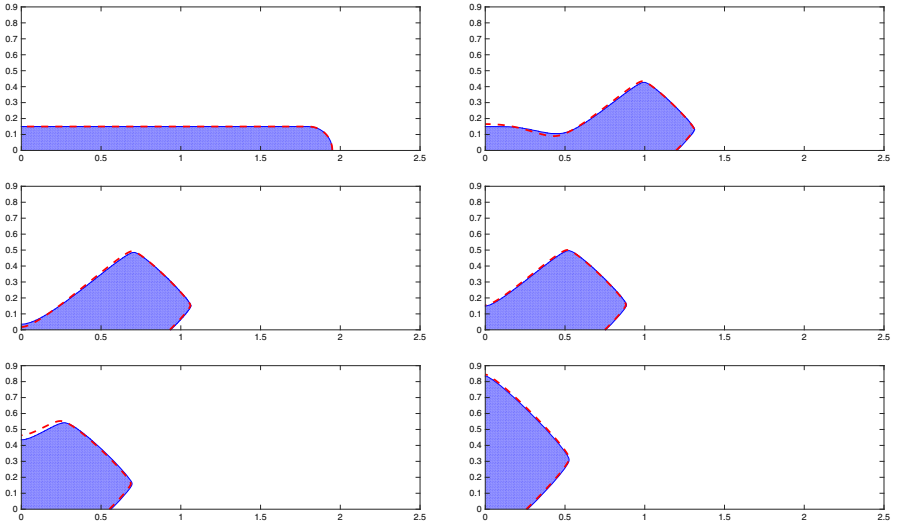

Fig. 10 [Example (d)] Interface profiles at times $t = 0, 0.01, 0.02, 0.03, 0.04, 0.1$ for the DI approximations with $\varepsilon = 1/(64\pi)$, and the red dash line represents the SI approximations (Color figure online)

ε. Note that, the large error for $\varepsilon = 1/(4\pi)$ is due to that DI simulation wrongly predicting a pinch-off.

Moreover, a qualitative comparison between the evolutions of the interface for both approaches is shown in Fig. 12. In particular, at the bottom of Fig. 12, we see that the sharp-interface approximation agrees very well with the zero level set from the DI computation, underlining once more our asymptotic analysis in Sect. 3.

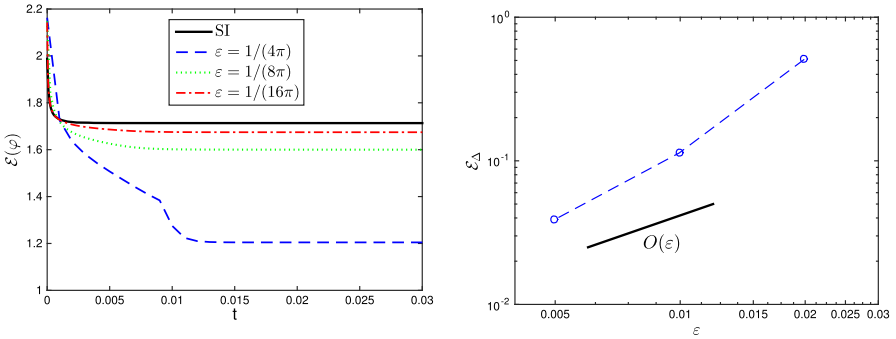

Fig. 11 Left panel: The time history of the energy for the DI and SI approximations for the semisphere experiment in 3d. Right panel: The error $\mathcal{E}_\Delta$ of the energy at the final time between the DI and SI approximations plotted against ε

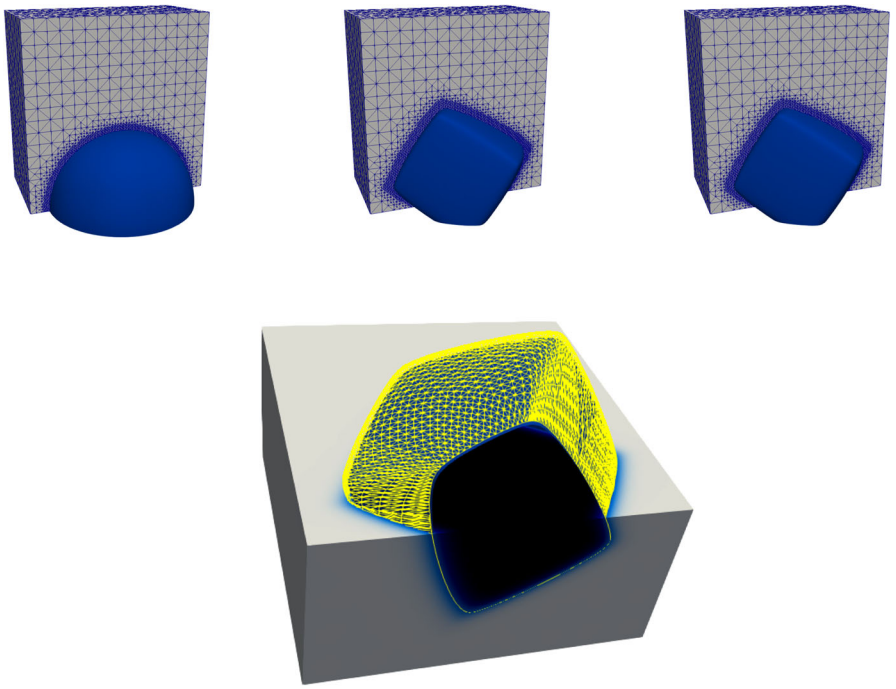

Fig. 12 A visualization of the zero level sets of the DI approximations for $\varepsilon = (16\pi)^{-1}$ at times $t = 0, 0.01, 0.1$, together with a slice through the adaptive mesh. Below a comparison between the DI and the SI computation at time $t = 0.01$

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Data availability The datasets generated during and/or analyzed during the current study are available from the corresponding author on reasonable request.

Declarations

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