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FINITE ELEMENT APPROXIMATION OF THE CAHN–HILLIARD EQUATION WITH DEGENERATE MOBILITY*

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Abstract. We consider a fully practical finite element approximation of the Cahn–Hilliard equation with degenerate mobility

$$\frac{\partial u}{\partial t} = \nabla.(b(u)\, \nabla(-\gamma\Delta u + \Psi'(u))),$$

where $b(\cdot) \geq 0$ is a diffusional mobility and $\Psi(\cdot)$ is a homogeneous free energy. In addition to showing well posedness and stability bounds for our approximation, we prove convergence in one space dimension. Furthermore, an iterative scheme for solving the resulting nonlinear discrete system is analyzed. We also discuss how our approximation has to be modified in order to be applicable to a logarithmic homogeneous free energy. Finally, some numerical experiments are presented.

Key words. fourth order degenerate parabolic equation, Cahn–Hilliard, phase separation, finite elements, convergence analysis

AMS subject classifications. 65M60, 65M12, 35K55, 35K65, 35K35, 82C26

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1. Introduction.

The Cahn–Hilliard equation

$$\frac{\partial u}{\partial t} = \nabla.(b(u)\, \nabla(-\gamma\Delta u + \Psi'(u))), \qquad x \in \Omega,\ t > 0,$$

was introduced to model spinodal decomposition and coarsening phenomena (Ostwald ripening) in binary alloys (cf. [10] and [12]). The quantity u is defined to be the difference of the local concentrations $c_A, c_B \in [0,1]$ of the two components A and B of the alloy and hence u is restricted to lie in the interval $[-1,1]$. The theory of Cahn and Hilliard is based on a Ginzburg–Landau free energy of the form

$$\mathcal{E}(u) := \int_\Omega \left(\tfrac{\gamma}{2}|\nabla u|^2 + \Psi(u)\right) \mathrm{d}x, \qquad \gamma > 0.$$

The first term in the free energy penalizes large gradients and was introduced in the theory of phase transitions to model capillary effects. The second term is the homogeneous free energy, which contains a term describing the entropy of mixing and a term taking into account the interaction between the two components. A mean field model leads to the potential

$$\Psi(u) := \frac{\theta}{2}\left[(1+u)\ln\left[\frac{1+u}{2}\right] + (1-u)\ln\left[\frac{1-u}{2}\right]\right] + F^0(u), \tag{1.1}$$

where θ is the absolute temperature and F^0 is a smooth function on the interval $[-1,1]$. A typical example is $F^0(u) := \frac{\theta_c}{2}(1-u^2)$, giving rise to a double well form of

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Ψ if $\theta < \theta_c$. But there are other reasonable choices of Ψ. If the temperature is below the critical temperature θ_c and the quench is shallow, i.e., $0 \ll \theta < \theta_c$, one could take, e.g.,

$$\Psi(u) := (u^2 - a^2)^2, \qquad a \in \mathbb{R}.$$

This has the advantage of being smooth, but the disadvantage that physically non-admissible values with $|u| > 1$ can be attained during the evolution. For low temperatures, an obstacle potential of the form

$$\Psi(u) := \begin{cases} \frac{1}{2}\left(1 - u^2\right) & \text{if } |u| \le 1, \\ \infty & \text{if } |u| > 1 \end{cases} \tag{1.2}$$

was suggested in [9]. This is formally the limit of the logarithmic potential, (1.1), with $F^0(u) := \frac{1}{2}(1 - u^2)$ in the deep quench limit $\theta \to 0$. The general feature is that below a certain critical temperature precisely two global minima of Ψ exist. As these minima are interpreted as phases, the potential Ψ is said to support two phases. If one minimizes $\mathcal{E}(\cdot)$ subject to the integral constraint $⨍_\Omega u = \bar{u} \in \mathbb{R}$, where $\bar{u}$ lies between the two minima of Ψ, then the minimizer $u_{\min}$, roughly speaking, will give rise to the following structure. The function $u_{\min}$ divides the domain Ω into three sets. On two of these sets $u_{\min}$ will be close to the minima of Ψ, whereas the third will be an interfacial regime of thickness approximately proportional to $\sqrt{\gamma}$ dividing the two phases. Generically the minima are realized as large time limits of the Cahn–Hilliard evolution with constant mobility.

To obtain the Cahn–Hilliard equation one introduces a chemical potential w as the variational derivative of $\mathcal{E}$,

$$w := \frac{\delta \mathcal{E}}{\delta u} = -\gamma \Delta u + \Psi'(u),$$

and defines a flux,

$$\mathcal{J} := -b(u)\nabla w.$$

Here $b(\cdot)$ is the nonnegative diffusional mobility, and in most of the literature on the Cahn–Hilliard equation b was assumed to be constant. But in the original derivation of the equation a u-dependent mobility appeared ([10] and [24]), and in fact with the diffusion in the interfacial region enhanced and hence stronger than in the pure phases. This enhanced interfacial diffusion is, in particular, observed in experiments at low temperatures.

It was suggested by many authors to take a mobility of the form $b(u) := 1 - u^2$; but the main feature a mobility should have is that it is zero in the pure component, i.e., when $u = \pm 1$, and the mobility should be positive for $|u| < 1$. Having defined the flux the Cahn–Hilliard equation now follows from the equation $\frac{\partial u}{\partial t} + \nabla \cdot \mathcal{J} = 0$, which is a consequence of mass conservation. The system is completed by taking initial conditions and the natural and no-flux boundary conditions $\frac{\partial u}{\partial \nu} = \mathcal{J} \cdot \nu = 0$ on $\partial\Omega$, where ν is normal to $\partial\Omega$.

It is the aim of this work to develop an efficient numerical method for the Cahn–Hilliard equation with degenerate mobility. Besides the case in which the homogeneous free energy is smooth we want to be able to handle the cases of a logarithmic free energy and of an obstacle potential. In the following we briefly describe what is known for the Cahn–Hilliard equation with a concentration dependent mobility.

For an overview on the vast literature on the Cahn–Hilliard equation with constant mobility we refer to [17] and [26]. Existence results for the Cahn–Hilliard equation with degenerate mobility were obtained in [27] in one space dimension and in [19] for space dimensions larger than one (see also [22] and [20]). One main feature of these results is the fact that solutions with initial data where $|u_0(\cdot)| \leq 1$ have the property that $|u(\cdot,t)| \leq 1$ for all later times t. This physically reasonable result is true for all potentials Ψ and a degenerate mobility but cannot be guaranteed if one takes $\Psi(u) = (u^2 - a^2)^2$ and a constant mobility. We remark that so far no uniqueness result for the Cahn–Hilliard equation with degenerate mobility is known.

An important result which gave insight into the qualitative behavior of solutions to the Cahn–Hilliard equation with degenerate mobility was established in [11] (see also [21]). They used the technique of formal asymptotic expansions to show that with the scaling $\gamma = \varepsilon^2$, $t \to \varepsilon^2 t$ and in the deep quench limit $\theta \to 0$, one can identify a limit as $\varepsilon \to 0$, which is a geometric motion for the interface known as motion by surface diffusion (cf. [13]). We remark that as $\varepsilon \to 0$ the interface thickness, which is approximately proportional to $\sqrt{\gamma}$, tends to zero and the interfacial region becomes a sharp interface. The limiting motion is an evolution law for hypersurfaces and it reads as

$$V = -\tfrac{\pi^2}{16}\, \Delta_S\, \kappa,$$

where V is the normal velocity, Δ_S is the surface Laplacian, and κ is the mean curvature of the interface. This is a purely local geometric motion for the interface and is in contrast to the Mullins–Sekerka evolution, which is obtained with a constant mobility. In the latter case, two interfaces which are a distance away from each other are coupled through bulk terms. Whereas in the case of motion by surface diffusion, two such interfaces would evolve independently of each other as long as they do not intersect; for example, a collection of spheres which do not intersect each other are stationary. On the level of the Cahn–Hilliard equation with degenerate mobility this property would correspond to a pinning effect (see [23], which reports on pinning effects in spinodal decomposition of polymer mixtures). Also let us mention that the time scale in the asymptotics of [11] is slower than the time scale which was used in the asymptotics for a constant mobility. One should bear in mind these results when studying the numerical simulations presented in section 5.

There are a number of papers on the Cahn–Hilliard equation with constant mobility from the numerical analysis point of view. We refer to [17] for an overview. Most numerical approaches are based on a splitting method, which uses the chemical potential w as an unknown function and hence only requires continuous finite element approximations for $\{u, w\}$ (see [18]). To our knowledge there has been no numerical analysis for the Cahn–Hilliard equation with a degenerate mobility. However, in [4] an error bound is proved for a fully practical piecewise linear finite element approximation of the Cahn–Hilliard equation with a logarithmic free energy and a nondegenerate concentration dependent mobility; see also [3] and [5] for extensions to the multicomponent case and the deep quench limit. Although the numerical approximation in the above papers is well defined for a degenerate mobility, the authors were not able to prove stability bounds and hence convergence of this approximation. The case of a degenerate mobility with its possible lack of uniqueness requires a more delicate approximation.

In what follows we state precisely the problem we wish to approximate numerically and we make some general assumptions. Let Ω be a bounded domain in $\mathbb{R}^d, d \leq 3$, with a Lipschitz boundary $\partial\Omega$. We consider the initial boundary value problem for the Cahn–Hilliard equation:

(P) Find $u(x,t)$ such that

$$\frac{\partial u}{\partial t} = \nabla.(b(u)\, \nabla(-\gamma\Delta u + \Psi'(u))) \qquad \text{in } \Omega_T := \Omega \times (0,T), \tag{1.3a}$$

$$u(x,0) \;=\; u_0(x) \qquad \forall\, x \in \Omega, \tag{1.3b}$$

$$\frac{\partial u}{\partial \nu} \;=\; b(u)\frac{\partial}{\partial \nu}(-\gamma\Delta u + \Psi'(u)) \;=\; 0 \qquad \text{on } \partial\Omega \times (0,T), \tag{1.3c}$$

where ν is normal to $\partial\Omega$ and γ is a positive constant. The diffusional mobility $b \in C([-1,1])$ is assumed to satisfy

$$b(-1) = b(1) = 0 \qquad \text{and} \qquad b(s) > 0 \quad \forall\, s \in (-1,1). \tag{1.4}$$

The free energy $\Psi \in C([-1,1])$ is such that

$$\Psi(s) := \psi_1(s) + \psi_2(s) + \tfrac{\theta_c}{2}(1-s^2), \tag{1.5}$$

where θ_c is a nonnegative constant and $\psi_1 \in C^1((-1,1))$ and $\psi_2 \in C^1([-1,1])$ are convex and concave, respectively. Clearly the third term can be absorbed into $\psi_2(\cdot)$; however, for later purposes we decompose $\Psi(\cdot)$ into this form. Obviously all examples for Ψ given above can be written in the form (1.5). In particular the double obstacle potential, (1.2), corresponds to the case $\psi_1 \equiv \psi_2 \equiv 0$ and $\theta_c = 1$ or $\psi_1 \equiv 0$, $\psi_2(s) = \frac{1-s^2}{2}$ and $\theta_c = 0$. We point out that in the case of a degenerate mobility, the obstacle in the potential (1.2) is not needed to describe the motion in the deep quench limit. In particular, as was shown in [19], the evolution with respect to the potential (1.2) is given by an equation instead of a variational inequality.

In [6] we considered a fully practical finite element approximation of the fourth order nonlinear degenerate parabolic equation (1.3a–c) with $\Psi(\cdot) \equiv 0$ and $b(u) := |u|^p$ for any given $p \in (0,\infty)$. Such problems arise in lubrication approximations of thin viscous films and have been studied extensively in the mathematics literature in recent years. A key feature of this problem is that there is no uniqueness result. In addition to establishing well posedness of our finite element approximation for all $d \le 3$, we proved convergence in one space dimension to solutions using the very weak solution concept introduced in [8] for this problem. This basically states that u is a solution if

$$\int_0^T \langle \tfrac{\partial u}{\partial t}, \eta\rangle \,\mathrm{d}t - \int_{\{|u|>0\}} b(u)\nabla\Delta u \nabla\eta \,\mathrm{d}x\,\mathrm{d}t = 0 \quad \forall\, \eta \in L^2(0,T;H^1(\Omega)).$$

The restriction of convergence to one space dimension is due to the fact that our a priori bounds on the finite element approximation only guarantee in the case of $d = 1$ uniform boundedness and equicontinuity of the approximate solutions, which is necessary to be able to pass to the limit in the discrete problem. For similar reasons, the results of [8] were restricted to one space dimension. In this paper we extend the techniques in [6] to the Cahn–Hilliard equation with degenerate mobility, (1.3a–c).

This paper is organized as follows. In section 2 we formulate a fully practical finite element approximation, $(\mathrm{P}^{h,\Delta t})$, of problem (P) in the case of $\psi_1, \psi_2 \in C^1([-1,1])$. This obviously excludes the choice of Ψ as the logarithmic potential, (1.1). This discretization is based on introducing the chemical potential w and writing the fourth order parabolic equation as a system of equations

$$\tfrac{\partial u}{\partial t} = \nabla.(b(u)\nabla w) \qquad \text{in } \Omega_T, \qquad -\gamma\Delta u + \Psi'(u) = w, \tag{1.6}$$

where the second equation holds on the set $\{ |u| < 1 \}$; and as $b(-1) = b(1) = 0$, see (1.4), then w is only required in this region. Unfortunately, a naive finite element approximation of problem (P) does not a priori guarantee that the discrete solution fulfills $|u| \leq 1$. Therefore we impose the physically reasonable property $|u| \leq 1$ as a constraint. This leads to a variational inequality which has to be solved at each time step. We prove well posedness and stability bounds for our approximation, $(\mathrm{P}^{h,\Delta t})$, of (P) for space dimensions 1, 2, and 3 and show convergence in one space dimension. In section 3 we introduce and prove convergence of an iterative scheme, based on the abstract splitting approach in [25], for solving the nonlinear discrete system arising in $(\mathrm{P}^{h,\Delta t})$ at each time level. In section 4, we introduce a variation of the approximation $(\mathrm{P}^{h,\Delta t})$, studied in section 2, to cope with the choice of a logarithmic free energy. Furthermore, we extend the results of sections 2 and 3 to this case. Finally, in section 5 we report on some numerical experiments.

Notation and auxiliary results. We have adopted the standard notation for Sobolev spaces, denoting the norm of $W^{m,p}(\Omega)$ ($m \in \mathbf{N}$, $p \in [1, \infty]$) by $\| \cdot \|_{m,p}$ and the seminorm by $| \cdot |_{m,p}$. For $p = 2$, $W^{m,2}(\Omega)$ will be denoted by $H^m(\Omega)$ with the associated norm and seminorm written, respectively, as $\| \cdot \|_m$ and $| \cdot |_m$. Throughout, $(\cdot, \cdot)$ denotes the standard L^2 inner product over Ω and $\langle \cdot, \cdot \rangle$ denotes the duality pairing between $\big(H^1(\Omega)\big)'$ and $H^1(\Omega)$.

For later purposes, we recall the following well-known Sobolev interpolation results, e.g., see [1]: Let $p \in [1, \infty]$, $m \geq 1$,

$$r \in \begin{cases} [p, \infty] & \text{if } m - \frac{d}{p} > 0, \\ [p, \infty) & \text{if } m - \frac{d}{p} = 0, \\ [p, -\frac{d}{m-(d/p)}] & \text{if } m - \frac{d}{p} < 0, \end{cases}$$

and $\mu = \frac{d}{m}\left(\frac{1}{p} - \frac{1}{r}\right)$. Then there is a constant C depending only on Ω, p, r, m such that for all $v \in W^{m,p}(\Omega)$ the inequality

$$\|v\|_{0,r} \leq C \|v\|_{0,p}^{1-\mu} \|v\|_{m,p}^{\mu} \tag{1.7}$$

holds. It is convenient to introduce the "inverse Laplacian" operator $\mathcal{G} : \mathcal{F} \to V$ such that

$$(\nabla \mathcal{G} v, \nabla \eta) = \langle v, \eta \rangle \quad \forall\, \eta \in H^1(\Omega), \tag{1.8}$$

where $\mathcal{F} := \left\{ v \in (H^1(\Omega))' : \langle v, 1 \rangle = 0 \right\}$ and $V := \{ v \in H^1(\Omega) : (v, 1) = 0 \}$. The well posedness of $\mathcal{G}$ follows from the Lax–Milgram theorem and the Poincaré inequality

$$|\eta|_{0,p} \leq C(|\eta|_{1,p} + |(\eta, 1)|) \quad \forall\, \eta \in W^{1,p}(\Omega) \quad \text{and} \quad p \in [1, \infty]. \tag{1.9}$$

One can define a norm on $\mathcal{F}$ by

$$\|v\|_{-1} := |\mathcal{G} v|_1 \equiv \langle v, \mathcal{G} v \rangle^{\frac{1}{2}} \quad \forall\, v \in \mathcal{F}. \tag{1.10}$$

We note also for future reference that using a Young's inequality yields for all $\alpha > 0$ that

$$\langle v, \eta \rangle = (\nabla \mathcal{G} v, \nabla \eta) \leq \|v\|_{-1} |\eta|_1 \leq \tfrac{1}{2\alpha} \|v\|_{-1}^2 + \tfrac{\alpha}{2} |\eta|_1^2 \quad \forall\, v \in \mathcal{F},\ \eta \in H^1(\Omega). \tag{1.11}$$

Throughout C denotes a generic constant independent of h and Δt, the mesh and temporal discretization parameters. In addition $C(a_1, \dots, a_I)$ denotes a constant depending on the nonnegative parameters $\{a_i\}_{i=1}^I$, such that for all $C_1 > 0$ there exists a $C_2 > 0$ such that $C(a_1, \dots, a_I) \leq C_2$ if $a_i \leq C_1$ for $i = 1 \to I$.

2. Finite element approximation. We consider the finite element approximation of (P) under the following assumptions on the meshes.

(A) Let Ω be a polyhedral domain. Let $\{\mathcal{T}^h\}_{h>0}$ be a quasi-uniform family of partitionings of Ω into disjoint open simplices κ with $h_\kappa := \text{diam}(\kappa)$ and $h := \max_{\kappa\in\mathcal{T}^h} h_\kappa$, so that $\overline{\Omega} = \cup_{\kappa\in\mathcal{T}^h}\overline{\kappa}$.

Associated with $\mathcal{T}^h$ is the finite element space

$$S^h := \{\chi \in C(\overline{\Omega}) : \chi\,|_\kappa \text{ is linear } \forall\, \kappa \in \mathcal{T}^h\} \subset H^1(\Omega).$$

We also introduce

$$K^h := \{\chi \in S^h : -1 \le \chi \le 1 \text{ in } \Omega\}.$$

Let J be the set of nodes of $\mathcal{T}^h$ and $\{x_j\}_{j\in J}$ the coordinates of these nodes. Let $\{\chi_j\}_{j\in J}$ be the standard basis functions for S^h; that is, $\chi_j \in K^h$ and $\chi_j(x_i) = \delta_{ij}$ for all $i, j \in J$. We introduce $\pi^h : C(\overline{\Omega}) \to S^h$, the interpolation operator, such that $\pi^h\eta(x_j) = \eta(x_j)$ for all $j \in J$. A discrete semi-inner product on $C(\overline{\Omega})$ is defined by

$$(\eta_1, \eta_2)^h := \int_\Omega \pi^h(\eta_1(x)\,\eta_2(x))\,\mathrm{d}x \equiv \sum_{j\in J}\beta_j\,\eta_1(x_j)\,\eta_2(x_j), \tag{2.1}$$

where $\beta_j := (1, \chi_j)$. The induced seminorm is then $|\cdot|_h := [(\cdot\,,\cdot)^h]^{\frac{1}{2}}$. We introduce the L^2 projection $Q^h : L^2(\Omega) \to S^h$ and the more practical $\hat{Q}^h : L^2(\Omega) \to S^h$ defined by

$$(Q^h\eta, \chi) = (\hat{Q}^h\eta, \chi)^h = (\eta, \chi) \quad \forall\, \chi \in S^h. \tag{2.2}$$

Given N, a positive integer, let $\Delta t := T/N$ denote the time step and $t_n := n\Delta t$, $n = 1 \to N$. Assuming that $\psi_1,\ \psi_2 \in C^1([-1,1])$, we consider the following fully practical finite element approximation of (P):

($\mathrm{P}^{h,\Delta t}$) For $n \ge 1$, find $\{U^n, W^n\} \in K^h \times S^h$ such that

$$\left(\tfrac{U^n - U^{n-1}}{\Delta t}, \chi\right)^h + \big(b(U^{n-1})\nabla W^n, \nabla\chi\big) = 0 \quad \forall\, \chi \in S^h, \tag{2.3a}$$

$$\begin{aligned}\gamma(\nabla U^n, \nabla(\chi - U^n)) &+ (\psi_1'(U^n) - \theta_c U^n, \chi - U^n)^h \\ &\ge (W^n - \psi_2'(U^{n-1}), \chi - U^n)^h \quad \forall\, \chi \in K^h,\end{aligned} \tag{2.3b}$$

where $U^0 \in K^h$ is an approximation of $u_0 \in K := \{\eta \in H^1(\Omega) : -1 \le \eta \le 1$ almost everywhere (a.e.) in $\Omega\}$, e.g., $U^0 \equiv \pi^h u_0$ (if $d = 1$) or $\hat{Q}^h u_0$. As we motivated in the introduction the variational inequality (2.3b) is introduced because we wish to impose the physically reasonable property $|U^n| \le 1$, which is not automatically guaranteed by a straightforward discretization of (P). It follows immediately from (2.3b) that for $n \ge 1$ and for all $j \in J$, either $|U^n(x_j)| = 1$ or $|U^n(x_j)| < 1$ and $\gamma(\nabla U^n, \nabla\chi_j) + (\psi_1'(U^n) - \theta_c U^n, \chi_j)^h = (W^n - \psi_2'(U^{n-1}), \chi_j)^h$.

Hence (2.3b) approximates $-\gamma\Delta u + \Psi'(u) = w$ in the region $|u| < 1$ as required; see (1.6). We note that for a general degenerate mobility $b(\cdot)$ satisfying (1.4), (2.3a) is not fully practical as it assumes that $\int_\kappa b(U^{n-1})\,\mathrm{d}x$ can be calculated exactly. Obviously, one could consider using numerical integration on this term; e.g., replace $(\cdot,\cdot)$ by $(\cdot,\cdot)^h$ in (2.3a). However, for ease of exposition and as the model case $b(s) := 1 - s^2$ can be easily dealt with, we consider (2.3a) in its present form.

Below we recall some well-known results concerning S^h.

$$|\chi|_{m,p_2} \le Ch^{-d(\frac{1}{p_1}-\frac{1}{p_2})}|\chi|_{m,p_1} \quad \forall\, \chi \in S^h, \quad 1 \le p_1 \le p_2 \le \infty, \quad m = 0 \text{ or } 1; \tag{2.4}$$

$$|\chi|_{1,p} \le Ch^{-1}|\chi|_{0,p} \quad \forall\, \chi \in S^h, \quad 1 \le p \le \infty; \tag{2.5}$$

$$\lim_{h\to 0} \|(I-\pi^h)\eta\|_{0,\infty} = 0 \quad \forall\, \eta \in C(\overline{\Omega}); \tag{2.6}$$

$$|(I-Q^h)\eta|_0 + h|(I-Q^h)\eta|_1 \le Ch^m|\eta|_m \quad \forall\, \eta \in H^m(\Omega), \quad m = 1 \text{ or } 2; \tag{2.7}$$

$$|\chi|_0^2 \le |\chi|_h^2 \le (d+2)|\chi|_0^2 \quad \forall\, \chi \in S^h; \tag{2.8}$$

$$|(v^h,\chi)^h - (v^h,\chi)| \le Ch^{1+m}\|v^h\|_m\|\chi\|_1 \quad \forall\, v^h,\chi \in S^h, \quad m = 0 \text{ or } 1; \tag{2.9}$$

and if $d = 1$

$$|(I-\pi^h)\eta|_{m,r} \le Ch^{1-m}|\eta|_{1,r} \quad \forall\, \eta \in W^{1,r}(\Omega), \quad m = 0 \text{ or } 1, \text{ any } r \in [1,\infty]; \tag{2.10}$$

$$\lim_{h\to 0} \|(I-\pi^h)\eta\|_1 = 0 \quad \forall\, \eta \in H^1(\Omega). \tag{2.11}$$

If $d = 1$, then a simple consequence of (2.9) and (2.10) is that

$$\begin{aligned} |(v,\eta)^h - (v,\eta)| &\le |(\pi^h v,\pi^h\eta)^h - (\pi^h v,\pi^h\eta)| + |((I-\pi^h)v,\pi^h\eta)| + |(v,(I-\pi^h)\eta)| \\ &\le C\left[\, |(I-\pi^h)v|_0 + h|v|_0 \,\right] \|\eta\|_1 \qquad \forall\, v \in C(\overline{\Omega}), \quad \forall\, \eta \in H^1(\Omega). \end{aligned} \tag{2.12}$$

Comparing $\hat{Q}^h\eta$ with $Q^h\eta$ and noting (2.9), (2.5), and (2.7) yields that

$$|(I-\hat{Q}^h)\eta|_0 + h|(I-\hat{Q}^h)\eta|_1 \le Ch|\eta|_1 \quad \forall\, \eta \in H^1(\Omega). \tag{2.13}$$

It follows from (2.2) that

$$(\hat{Q}^h\eta)(x_j) \equiv \frac{(\eta,\chi_j)}{(1,\chi_j)} \quad \forall\, j \in J \quad \Longrightarrow \quad \|\hat{Q}^h\eta\|_{0,\infty} \le \|\eta\|_{0,\infty} \quad \forall\, \eta \in L^\infty(\Omega). \tag{2.14}$$

Similarly to (1.8), we introduce the operator $\hat{\mathcal{G}}^h : \mathcal{F}^h \to V^h$ such that

$$(\nabla\hat{\mathcal{G}}^h v,\nabla\chi) = (v,\chi)^h \quad \forall\, \chi \in S^h, \tag{2.15}$$

where $V^h := \{v^h \in S^h : (v^h,1) = 0\}$ and $\mathcal{F}^h := \{v \in C(\overline{\Omega}) : (v,1)^h = 0\}$. Similarly to (1.11), we have for all $\alpha > 0$ that

$$(v,\chi)^h \equiv (\nabla\hat{\mathcal{G}}^h v,\nabla\chi) \le |\hat{\mathcal{G}}^h v|_1|\chi|_1 \le \tfrac{1}{2\alpha}|\hat{\mathcal{G}}^h v|_1^2 + \tfrac{\alpha}{2}|\chi|_1^2 \quad \forall\, v \in \mathcal{F}^h,\ \chi \in S^h. \tag{2.16}$$

We now follow the approach taken in [6]. To establish the existence of a solution $\{U^n,W^n\}_{n=1}^N$ to $(\mathrm{P}^{h,\Delta t})$, we must introduce some notation. In particular we define sets $V^h(U^{n-1})$ in which we seek the update $U^n - U^{n-1}$. Given $q^h \in K^h$ with $⨍\, q^h := \frac{1}{|\Omega|}(q^h,1) \in (-1,1)$, we define a set of passive nodes $J_0(q^h) \subset J$ by

$$j \in J_0(q^h) \Longleftrightarrow (b(q^h),\chi_j) = 0 \Longleftrightarrow b(q^h) \equiv 0 \text{ on } \operatorname{supp}(\chi_j). \tag{2.17}$$

All other nodes we call active nodes and they can be uniquely partitioned so that $J_+(q^h) := J \setminus J_0(q^h) \equiv \bigcup_{m=1}^M I_m(q^h)$, $M \ge 1$, where $I_m(q^h)$, $m = 1 \to M$, are mutually disjoint and maximally connected in the following sense: $I_m(q^h)$ is said to be connected if for all $j,\,k \in I_m(q^h)$, there exist $\{\kappa_\ell\}_{\ell=1}^{L} \subseteq \mathcal{T}^h$, not necessarily distinct, such that

$$\begin{array}{lll} \text{(a)} & x_j \in \overline{\kappa}_1, \quad x_k \in \overline{\kappa}_L, & \\ \text{(b)} & \overline{\kappa}_\ell \cap \overline{\kappa}_{\ell+1} \neq \emptyset, & \ell = 1 \to L-1, \\ \text{(c)} & b(q^h) \not\equiv 0 \text{ on } \kappa_\ell, & \ell = 1 \to L. \end{array} \tag{2.18}$$

$I_m(q^h)$ is said to be maximally connected if there is no other connected subset of $J_+(q^h)$, which contains $I_m(q^h)$. Clearly $J_+(q^h)$ is nonempty, since if $(b(q^h), \chi_j) = 0$ $\forall\ j \in J$ then $b(q^h) \equiv 0$, and since $q^h \in S^h$ it follows that $q^h \equiv 1$ or -1 which contradicts the assumption that $⨍\, q^h \in (-1, 1)$. We then set

$$V^h(q^h) := \{\, v^h \in S^h : v^h(x_j) = 0\ \forall\ j \in J_0(q^h) \text{ and } (v^h, \Xi_m(q^h))^h = 0,\ m = 1 \to M\,\}, \tag{2.19}$$

where for $m = 1 \to M$

$$\Xi_m(q^h) := \sum_{j \in I_m(q^h)} \chi_j. \tag{2.20}$$

The space $V^h(q^h)$ consists of all those $v^h \in S^h$ which are orthogonal, with respect to the $(\cdot,\cdot)^h$ inner product, to χ_j, for all $j \in J_0(q^h)$, and to $\Xi_m(q^h)$, $m = 1 \to M$. We note that for all $q^h \in K^h$, $V^h(q^h) \subseteq V^h$ and that $|q^h| < 1 \Longrightarrow V^h(q^h) \equiv V^h$. Another immediate consequence of the above definitions is that on any $\kappa \in \mathcal{T}^h$ either

$$b(q^h) \equiv 0 \qquad \text{or} \qquad \Xi_{m_\star}(q^h) \equiv 1 \text{ for some } m_\star \text{ and } \Xi_m(q^h) \equiv 0 \text{ for } m \neq m_\star. \tag{2.21}$$

For later reference we state that any $v^h \in S^h$ can be written as

$$v^h \equiv \sum_{j \in J} v^h(x_j)\chi_j \ \equiv\ \overline{v}^h + \sum_{j \in J_0(q^h)} v^h(x_j)\chi_j + \sum_{m=1}^{M} \left[⨍_{\Omega_m(q^h)} v^h \right] \Xi_m(q^h), \tag{2.22a}$$

where $\Omega_m(q^h) := \{\, \cup_{\kappa \in \mathcal{T}^h} \overline{\kappa} : \Xi_m(q^h)(x) = 1\ \forall\ x \in \kappa\,\}$,

$$\begin{aligned} ⨍_{\Omega_m(q^h)} v^h &:= \frac{(v^h, \Xi_m(q^h))^h}{(1, \Xi_m(q^h))}, \quad \text{and} \\ \overline{v}^h &:= \sum_{m=1}^{M} \sum_{j \in I_m(q^h)} \left[v^h(x_j) - ⨍_{\Omega_m(q^h)} v^h \right] \chi_j \in V^h(q^h) \end{aligned} \tag{2.22b}$$

is the projection with respect to the $(\cdot,\cdot)^h$ scalar product of v^h onto $V^h(q^h)$. We remark that $⨍_{\Omega_m(q^h)} v^h$ is not the standard mean value on the set $\Omega_m(q^h)$.

In order to express W^n in terms of U^n and U^{n-1} we introduce for all $q^h \in K^h$ with $⨍\, q^h \in (-1, 1)$ the discrete anisotropic Green's operator $\hat{\mathcal{G}}^h_{q^h} : V^h(q^h) \to V^h(q^h)$ such that

$$(b(q^h)\nabla \hat{\mathcal{G}}^h_{q^h} v^h, \nabla \chi) = (v^h, \chi)^h \qquad \forall\ \chi \in S^h. \tag{2.23}$$

To show the well posedness of $\hat{\mathcal{G}}^h_{q^h}$, we first note that choosing $\chi \equiv \chi_j$, $j \in J_0(q^h)$, in (2.23) leads to both sides vanishing on noting (2.17) and (2.19). Similarly, choosing $\chi \equiv \Xi_m(q^h)$, $m = 1 \to M$, in (2.23) leads to both sides vanishing on noting

(2.21) and (2.19). Therefore for well posedness, it remains to prove uniqueness as $V^h(q^h)$ has finite dimension. If there exist two solutions $Z_i \in V^h(q^h)$, $i = 1, 2$, with $(b(q^h)\nabla Z_i, \nabla\chi) = (v^h, \chi)^h$ for all $\chi \in S^h$, then $Z := Z_1 - Z_2 \in V^h(q^h)$ satisfies, on noting (2.21),

$$b_{\min}(q^h)\sum_{m=1}^{M}\int_{\Omega_m(q^h)} |\nabla Z|^2 \,\mathrm{d}x \leq \sum_{m=1}^{M}\int_{\Omega_m(q^h)} b(q^h)|\nabla Z|^2 \,\mathrm{d}x \equiv \int_\Omega b(q^h)|\nabla Z|^2 \,\mathrm{d}x = 0, \tag{2.24a}$$

where $\Omega(q^h) := \bigcup_{m=1}^{M} \Omega_m(q^h)$ and

$$b_{\min}(q^h) := \min_{\kappa\subset\Omega(q^h)} \frac{1}{|\kappa|}\int_\kappa b(q^h)\,\mathrm{d}x. \tag{2.24b}$$

Hence it follows that Z is constant on each $\Omega_m(q^h)$. However as $Z \in V^h(q^h)$, it follows that $Z \equiv 0$. Thus $\hat{\mathcal{G}}^h_{q^h}$ is well posed.

For later purposes we note from (2.23) and Young's inequality that, similarly to (2.16), for any $\alpha > 0$,

$$|\hat{v}^h|_h^2 \;\leq\; \tfrac{1}{2\alpha}|b(q^h)\nabla\hat{\mathcal{G}}^h_{q^h}\hat{v}^h|_0^2 + \tfrac{\alpha}{2}|\hat{v}^h|_1^2 \quad \forall\, \hat{v}^h \in V^h(q^h). \tag{2.25}$$

THEOREM 2.1. *Let Ω and $\mathcal{T}^h$ be such that assumption* (A) *holds and let $U^0 \in K^h$ with $\fint U^0 \in (-1,1)$. In addition let b and Ψ fulfill the assumptions stated above. Then for all $\Delta t > 0$ there exists a solution $\{U^n, W^n\}_{n=1}^N$ to $(\mathrm{P}^{h,\Delta t})$.*

If $\theta_c^2 b_{\max}\Delta t < 4\gamma$, where $b_{\max} \geq \max_{n=1\to N} b_{\max}^{n-1}$ and $b_{\max}^{n-1} := \|b(U^{n-1})\|_{0,\infty}$, then $\{U^n\}_{n=1}^N$ is unique. Furthermore, the following stability bounds hold:

$$\begin{aligned}\max_{n=1\to N}\|U^n\|_1^2 + (\Delta t)^2\sum_{n=1}^{N}|\tfrac{U^n-U^{n-1}}{\Delta t}|_1^2 + \Delta t\sum_{n=1}^{N}|[b(U^{n-1})]^{\frac12}\nabla W^n|_0^2 \\ +\;\Delta t\sum_{n=1}^{N}[b_{\max}^{n-1}]^{-1}|\hat{\mathcal{G}}^h[\tfrac{U^n-U^{n-1}}{\Delta t}]|_1^2 \;\leq\; C\left[\,|U^0|_1^2+1\right].\end{aligned} \tag{2.26}$$

In addition W^n is unique on $\Omega_m(U^{n-1})$ if $|U^n(x_j)| < 1$ for some $j \in I_m(U^{n-1})$, $m = 1 \to M$, $n = 1 \to N$.

Proof. It follows from (2.3a) and (2.23) that for $n \geq 1$, given $U^{n-1} \in K^h$, we seek $U^n \in K^h(U^{n-1})$, where

$$K^h(U^{n-1}) := \{\, \chi \in K^h : \chi - U^{n-1} \in V^h(U^{n-1}) \,\}. \tag{2.27}$$

In addition a solution W^n in (2.3a), (2.3b) can be expressed in terms of U^n as (cf. (2.23) and (2.22a,b))

$$W^n \equiv -\hat{\mathcal{G}}^h_{U^{n-1}}[\tfrac{U^n-U^{n-1}}{\Delta t}] + \sum_{j\in J_0(U^{n-1})}\mu_j^n\chi_j + \sum_{m=1}^{M}\lambda_m^n\Xi_m(U^{n-1}), \tag{2.28}$$

where $\{\mu_j^n\}_{j\in J_0(U^{n-1})}$ and $\{\lambda_m^n\}_{m=1}^M$ are constants. Hence $(\mathrm{P}^{h,\Delta t})$ can be restated as the following: For $n \geq 1$, find $U^n \in K^h(U^{n-1})$ and constant Lagrange multipliers

$\{\mu_j^n\}_{j\in J_0(U^{n-1})}$, $\{\lambda_m^n\}_{m=1}^M$ such that

$$\gamma(\nabla U^n, \nabla(\chi - U^n)) + \left(\hat{\mathcal{G}}^h_{U^{n-1}}[\tfrac{U^n-U^{n-1}}{\Delta t}] + \psi_1'(U^n) - \theta_c U^n, \chi - U^n\right)^h$$
$$\geq \left(\sum_{j\in J_0(U^{n-1})} \mu_j^n \chi_j + \sum_{m=1}^{M} \lambda_m^n \Xi_m(U^{n-1}) - \psi_2'(U^{n-1}), \chi - U^n\right)^h \quad \forall\, \chi \in K^h. \tag{2.29}$$

It follows from (2.29), (2.27), and (2.19) that $U^n \in K^h(U^{n-1})$ is such that

$$\gamma(\nabla U^n, \nabla(\hat{v}^h - U^n)) + (\hat{\mathcal{G}}^h_{U^{n-1}}[\tfrac{U^n-U^{n-1}}{\Delta t}] + \psi_1'(U^n) - \theta_c U^n, \hat{v}^h - U^n)^h$$
$$\geq -(\psi_2'(U^{n-1}), \hat{v}^h - U^n)^h \qquad \forall\, \hat{v}^h \in K^h(U^{n-1}). \tag{2.30}$$

We note that (2.30) is the Euler–Lagrange variational inequality of the minimization problem

$$\min_{\hat{v}^h\in K^h(U^{n-1})} \mathcal{E}^h(\hat{v}^h) := \Big\{\gamma|\hat{v}^h|_1^2 + \tfrac{1}{\Delta t}|[b(U^{n-1})]^{\frac{1}{2}}\nabla\hat{\mathcal{G}}^h_{U^{n-1}}(\hat{v}^h - U^{n-1})|_0^2$$
$$+(2\psi_1(\hat{v}^h) - \theta_c(\hat{v}^h)^2 + 2\psi_2'(U^{n-1})\hat{v}^h, 1)^h\Big\}.$$

As we minimize $\mathcal{E}^h(\cdot)$ on the compact set $K^h(U^{n-1})$, we have existence of a solution to (2.30). Existence of the Lagrange multipliers $\{\mu_j^n\}_{j\in J_0(U^{n-1})}$ and $\{\lambda_m^n\}_{m=1}^M$, for fixed n, follows from standard optimization theory; e.g., see [15]. Therefore, on noting (2.28), we have existence of a solution $\{U^n, W^n\}_{n=1}^N$ to ($\mathrm{P}^{h,\Delta t}$).

For fixed $n \geq 1$, if (2.29) has two solutions $\{\, U^{n,i}, \{\mu_j^{n,i}\}_{j\in J_0(U^{n-1})}, \{\lambda_m^{n,i}\}_{m=1}^M \,\}$, $i = 1, 2$, then it follows from (2.30), the convexity of $\psi_1(\cdot)$, and (2.25) that $\overline{U}^n := U^{n,1} - U^{n,2} \in V^h(U^{n-1})$ satisfies

$$\begin{aligned}
&\gamma|\overline{U}^n|_1^2 + \tfrac{1}{\Delta t}|[b(U^{n-1})]^{\frac{1}{2}}\nabla\hat{\mathcal{G}}^h_{U^{n-1}}\overline{U}^n|_0^2 \\
&\leq \gamma|\overline{U}^n|_1^2 + \tfrac{1}{\Delta t}|[b(U^{n-1})]^{\frac{1}{2}}\nabla\hat{\mathcal{G}}^h_{U^{n-1}}\overline{U}^n|_0^2 + (\psi_1'(U^{n,1}) - \psi_1'(U^{n,2}), \overline{U}^n) \\
&\leq \theta_c|\overline{U}^n|_h^2 \leq \tfrac{1}{\Delta t}|[b(U^{n-1})]^{\frac{1}{2}}\nabla\hat{\mathcal{G}}^h_{U^{n-1}}\overline{U}^n|_0^2 + \tfrac{\theta_c^2 b_{\max}^{n-1}\Delta t}{4}|\overline{U}^n|_1^2.
\end{aligned}$$

Therefore the uniqueness of U^n follows from (1.9) and $⨍ U^n = ⨍ U^0$ under the stated restriction on Δt. If $|U^n(x_j)| < 1$ for some $j \in I_m(U^{n-1})$, then $(1 - (U^n(x_j))^2)$ $\Xi_m(U^{n-1}(x_j)) > 0$ and choosing $\chi \equiv U^n \pm \delta\,\pi^h[(1 - (U^n)^2)\,\Xi_m(U^{n-1})] \not\equiv 0$ in (2.29) for $\delta > 0$ sufficiently small yields uniqueness of the Lagrange multiplier λ_m^n. Hence the desired uniqueness result on W^n follows from noting (2.28).

We now prove the stability bound (2.26). For fixed $n \geq 1$ choosing $\chi \equiv W^n$ in (2.3a), $\chi \equiv U^{n-1}$ in (2.3b), and combining yields that

$$\begin{aligned}
&\tfrac{\gamma}{2}|U^n|_1^2 + \tfrac{\gamma}{2}|U^n - U^{n-1}|_1^2 - \tfrac{\gamma}{2}|U^{n-1}|_1^2 + (\Psi(U^n), 1)^h - (\Psi(U^{n-1}), 1)^h \\
&\quad -\tfrac{\theta_c}{2}|U^n - U^{n-1}|_h^2 + \Delta t|[b(U^{n-1})]^{\frac{1}{2}}\nabla W^n|_0^2 \\
&\leq \gamma(\nabla U^n, \nabla(U^n - U^{n-1})) + (\psi_1'(U^n) + \psi_2'(U^{n-1}), U^n - U^{n-1})^h \\
&\quad +\Delta t|[b(U^{n-1})]^{\frac{1}{2}}\nabla W^n|_0^2 - \theta_c(U^n, U^n - U^{n-1})^h \leq 0,
\end{aligned} \tag{2.31}$$

where we have noted the identity

$$2s(s - r) = s^2 - r^2 + (s - r)^2 \qquad \forall\, r, s \in \mathbb{R}, \tag{2.32}$$

and the convexity and concavity of ψ_1 and ψ_2, respectively. Choosing $\chi \equiv \Delta t(U^n - U^{n-1})$ in (2.3a) and applying a Young's inequality, similarly to (2.25), with $\alpha = \frac{3\gamma}{2\theta_c}$ and noting the stated restriction on Δt, it follows from (2.31) that

$$\begin{aligned} &\tfrac{\gamma}{2}|U^n|_1^2 + \tfrac{\gamma}{8}|U^n - U^{n-1}|_1^2 - \tfrac{\gamma}{2}|U^{n-1}|_1^2 \\ &+(\Psi(U^n),1)^h - (\Psi(U^{n-1}),1)^h + \tfrac{2}{3}\Delta t|[b(U^{n-1})]^{\frac{1}{2}}\nabla W^n|_0^2 \le 0. \end{aligned} \tag{2.33}$$

Summing from $n = 1 \to m$, for $m = 1 \to N$, and noting the properties of ψ_i $(i = 1, 2)$, (1.9), and $⨍\, U^n = ⨍\, U^0$ yields the first three bounds in (2.26). Choosing $\chi \equiv \hat{\mathcal{G}}^h(\frac{U^n - U^{n-1}}{\Delta t})$ in (2.3a) and noting (2.15) yields for $n \ge 1$ that

$$\begin{aligned} |\hat{\mathcal{G}}^h[\tfrac{U^n-U^{n-1}}{\Delta t}]|_1^2 = (\tfrac{U^n-U^{n-1}}{\Delta t}, \hat{\mathcal{G}}^h[\tfrac{U^n-U^{n-1}}{\Delta t}])^h \;=\; -(b(U^{n-1})\nabla W^n, \nabla\hat{\mathcal{G}}^h[\tfrac{U^n-U^{n-1}}{\Delta t}]) \\ \le |[b(U^{n-1})]\nabla W^n|_0^2 \;\le\; b_{\max}^{n-1}|[b(U^{n-1})]^{\frac{1}{2}}\nabla W^n|_0^2. \end{aligned} \tag{2.34}$$

Summing (2.34) from $n = 1 \to N$ and noting the third bound in (2.26) yields the desired fourth bound in (2.26). □

Remark. (i) Given a convex function $\psi_1 \in C([-,1,1])$, a concave function $\psi \in C([-1,1])$ and $\alpha \in \mathbb{R}^+$, the free energy $\Psi(s) := \psi_1(s) + \psi(s) + \frac{\alpha}{2}(1-s^2)$ can be written in the form (1.5) with either (a) $\psi_2(\cdot) \equiv \psi(\cdot)$ and $\theta_c = \alpha$ or (b) $\psi_2(\cdot) \equiv \psi(\cdot) + \frac{\alpha}{2}(1-s^2)$ and $\theta_c = 0$. We see from Theorem 2.1 that a time step restriction is required for the well posedness of $(\mathrm{P}^{h,\Delta t})$ in case (a) but not in case (b).

(ii) As can be seen from (2.33) the finite element approximation has the property that $\frac{\gamma}{2}|U|_1^2 + (\Psi(U),1)^h$ is a Lyapunov function for the discrete evolution.

Let

$$U(t) := \tfrac{t-t_{n-1}}{\Delta t}U^n + \tfrac{t_n - t}{\Delta t}U^{n-1}, \qquad t \in [t_{n-1}, t_n], \quad n \ge 1, \tag{2.35a}$$

and

$$U^+(t) := U^n, \qquad U^-(t) := U^{n-1}, \qquad t \in (t_{n-1}, t_n], \quad n \ge 1. \tag{2.35b}$$

We note for future reference that

$$U - U^{\pm} = (t - t_n^{\pm})\tfrac{\partial U}{\partial t}, \qquad t \in (t_{n-1}, t_n), \quad n \ge 1, \tag{2.36}$$

where $t_n^+ := t_n$ and $t_n^- := t_{n-1}$. Using the above notation and introducing analogous notation for W, (2.3a,b) can be restated as the following.

Find $\{U,\ W\} \in H^1(0,T;K^h) \times L^2(0,T;S^h)$ such that

$$\int_0^T \Big[\big(\tfrac{\partial U}{\partial t}, \chi\big)^h + \big(b(U^-)\nabla W^+, \nabla\chi\big) \Big]\, \mathrm{d}t = 0 \quad \forall\, \chi \in L^2(0,T;S^h), \tag{2.37a}$$

$$\begin{aligned} &\int_0^T \big[\, \gamma(\nabla U^+, \nabla(\chi - U^+)) + (\psi_1'(U^+) + \psi_2'(U^-) - \theta_c U^+, \chi - U^+)^h \,\big]\, \mathrm{d}t \\ &\qquad \ge \int_0^T (W^+, \chi - U^+)^h\, \mathrm{d}t \qquad \forall\, \chi \in L^2(0,T;K^h). \end{aligned} \tag{2.37b}$$

THEOREM 2.2. *Let $d = 1$ and $u_0 \in K$ with $⨍\, u_0 \in (-1,1)$. Let $\{\mathcal{T}^h, U^0, \Delta t\}_{h>0}$ be such that*

(i) *$U^0 \in K^h$ and $U^0 \to u_0$ in $H^1(\Omega)$ as $h \to 0$,*

(ii) *Ω and $\{\mathcal{T}^h\}_{h>0}$ fulfill assumption* (A),

(iii) $\Delta t \to 0$ *as* $h \to 0$.

Then there exists a subsequence of $\{U, W\}_h$ *and a function* $u \in L^\infty(0,T;K) \cap H^1(0,T;(H^1(\Omega))') \cap C^{\frac{1}{2},\frac{1}{8}}_{x,t}(\overline{\Omega}_T)$ *and a* $w \in L^2_{loc}(\{|u|<1\})$ *with* $\frac{\partial w}{\partial x} \in L^2_{loc}(\{|u|<1\})$ *such that as* $h \to 0$,

$$U,\ U^\pm \to u \qquad \textit{uniformly on } \overline{\Omega}_T, \tag{2.38}$$

$$U,\ U^\pm \to u \qquad \textit{weakly in } L^2(0,T;H^1(\Omega)), \tag{2.39}$$

$$W^+ \to w, \quad \frac{\partial W^+}{\partial x} \to \frac{\partial w}{\partial x} \qquad \textit{weakly in } L^2_{loc}(\{|u|<1\}), \tag{2.40}$$

where $\{|u|<1\} := \{(x,t) \in \Omega_T \,:\, -1 < u(x,t) < 1\}$.

Furthermore, u *and* w *fulfill* $u(\cdot,0) = u_0(\cdot)$ *and*

$$\int_0^T \langle \tfrac{\partial u}{\partial t}, \eta \rangle \,\mathrm{d}t + \int_{\{|u|<1\}} b(u) \frac{\partial w}{\partial x}\frac{\partial \eta}{\partial x}\,\mathrm{d}x\,\mathrm{d}t = 0 \quad \forall\, \eta \in L^2(0,T;H^1(\Omega)), \tag{2.41a}$$

$$w = -\gamma \frac{\partial^2 u}{\partial x^2} + \Psi'(u) \qquad \textit{on the set} \qquad \{|u|<1\}. \tag{2.41b}$$

Proof. Without loss of generality we assume that $\theta_c^2 \|b\|_{0,\infty} \Delta t < 4\gamma$ and that h is sufficiently small. We note that the assumption (i) implies that $⨍\, U^0 \in (-1,1)$ for h sufficiently small. Hence the definition (2.35a,b), the first three bounds in (2.26), (2.10), and (1.9) together with the fact that $V^h(q^h) \subseteq V^h$ imply

$$\|U\|^2_{L^\infty(0,T;H^1(\Omega))} + \Delta t\, \|U\|^2_{H^1(0,T;H^1(\Omega))} + \left\| [b(U^-)]^{\frac{1}{2}} \frac{\partial W^+}{\partial x} \right\|^2_{L^2(\Omega_T)} \le C. \tag{2.42}$$

Furthermore, we deduce from (2.36) and (2.42) that

$$\|U - U^\pm\|^2_{L^2(0,T;H^1(\Omega))} \le (\Delta t)^2 \|\tfrac{\partial U}{\partial t}\|^2_{L^2(0,T;H^1(\Omega))} \le C\,\Delta t. \tag{2.43}$$

In the next step we show that the discrete solutions U are uniformly Hölder continuous. The first bound in (2.42) gives via a standard imbedding result

$$|U(y_2,t) - U(y_1,t)| \;\le\; C\,|y_2 - y_1|^{\frac{1}{2}} \qquad \forall\, y_1,\, y_2 \in \overline{\Omega}, \quad \forall\, t \ge 0. \tag{2.44}$$

In addition it follows from (1.7), (2.8), (2.16), (2.42), and (2.26) that

$$\begin{aligned}
\|U(\cdot,t_b) - U(\cdot,t_a)\|_{0,\infty} \;&\le\; C\, \|U(\cdot,t_b) - U(\cdot,t_a)\|_0^{\frac{1}{2}}\; \|U(\cdot,t_b) - U(\cdot,t_a)\|_1^{\frac{1}{2}} \\
&\le C\, |\hat{\mathcal{G}}^h\,(U(\cdot,t_b) - U(\cdot,t_a))\,|_1^{\frac{1}{4}}\; \|U(\cdot,t_b) - U(\cdot,t_a)\|_1^{\frac{3}{4}} \\
&\le C \left| \hat{\mathcal{G}}^h \left[\int_{t_a}^{t_b} \frac{\partial U}{\partial t}(\cdot,t)\,\mathrm{d}t \right] \right|_1^{\frac{1}{4}} \left(2\, \|U\|_{L^\infty(0,T;H^1(\Omega))} \right)^{\frac{3}{4}} \\
&\le C \left| \int_{t_a}^{t_b} \hat{\mathcal{G}}^h \frac{\partial U}{\partial t}(\cdot,t)\,\mathrm{d}t \right|_1^{\frac{1}{4}} \;\le\; C(t_b - t_a)^{\frac{1}{8}} \left(\int_{t_a}^{t_b} \left| \hat{\mathcal{G}}^h \frac{\partial U}{\partial t} \right|_1^2 \mathrm{d}t \right)^{\frac{1}{8}} \\
&\le C(t_b - t_a)^{\frac{1}{8}} \qquad \forall\, t_b \ge t_a \ge 0.
\end{aligned} \tag{2.45}$$

An immediate consequence of (2.45) is that

$$\|U - U^\pm\|_{L^\infty(\Omega_T)} \le C(\Delta t)^{\frac{1}{8}}. \tag{2.46}$$

Now (2.42), (2.44), and (2.45) imply that the $C^{\frac{1}{2},\frac{1}{8}}_{x,t}(\overline{\Omega}_T)$ norm of U is bounded independently of h, Δt, and T. Hence, under the stated assumptions on Δt, every sequence

$\{U\}_h$ is uniformly bounded and equicontinuous on $\overline{\Omega}_T$ for any $T > 0$. Therefore by the Arzelà–Ascoli theorem there exists a subsequence such that

$$U \to u \in C^{\frac{1}{2},\frac{1}{8}}_{x,t}(\overline{\Omega}_T) \qquad \text{uniformly on } \overline{\Omega}_T \text{ as } h \to 0 \tag{2.47}$$

and $|u| \leq 1$. Moreover (2.42) implies that this same subsequence is such that

$$U \to u \qquad \text{weakly in } L^2(0,T;H^1(\Omega)) \text{ as } h \to 0. \tag{2.48}$$

For any $\eta \in H^1(0,T;H^1(\Omega))$ we choose $\chi \equiv \pi^h\eta$ in (2.37a) and now analyze the subsequent terms. First, we have that

$$\begin{aligned}&\int_0^T \left(\tfrac{\partial U}{\partial t}, \pi^h\eta\right)^h \mathrm{d}t \\ &= -\int_0^T \left(U, \tfrac{\partial(\pi^h\eta)}{\partial t}\right)^h \mathrm{d}t + \left(U(\cdot,T), \pi^h\eta(\cdot,T)\right)^h - \left(U(\cdot,0), \pi^h\eta(\cdot,0)\right)^h .\end{aligned} \tag{2.49}$$

Next we conclude using the regularity of η, (2.12), and (2.47) that

$$\int_0^T \left(U, \tfrac{\partial(\pi^h\eta)}{\partial t}\right)^h \mathrm{d}t \to \int_0^T \left(u, \tfrac{\partial\eta}{\partial t}\right) \mathrm{d}t \qquad \text{as } h \to 0 \quad \text{for all } \eta \text{ as above.} \tag{2.50}$$

In view of (2.42) we deduce that

$$\begin{aligned}&\left| \int_{\Omega_T} b(U^-)\tfrac{\partial W^+}{\partial x}\tfrac{\partial}{\partial x}(I-\pi^h)\eta \,\mathrm{d}x\,\mathrm{d}t \right| \\ &\leq \|[b(U^-)]^{\frac{1}{2}}\|_{L^\infty(\Omega_T)} \, \|[b(U^-)]^{\frac{1}{2}}\tfrac{\partial W^+}{\partial x}\|_{L^2(\Omega_T)} \, \|(I-\pi^h)\eta\|_{L^2(0,T;H^1(\Omega))} \\ &\leq C\|(I-\pi^h)\eta\|_{L^2(0,T;H^1(\Omega))}.\end{aligned} \tag{2.51}$$

We now show the compactness of $\{W^+\}_h$ on compact subsets of $\{|u| < 1\}$. For any $\delta > 0$, we set

$$D^+_\delta := \{\, (x,t) \in \overline{\Omega}_T : |u(x,t)| < 1-\delta \,\} \quad \text{and} \quad D^+_\delta(t) := \{\, x \in \overline{\Omega} : |u(x,t)| < 1-\delta \,\}. \tag{2.52}$$

For a fixed $\delta > 0$, it follows from (2.47) and (2.46) that there exists an $h_0(\delta) \in \mathbb{R}^+$ such that for all $h \leq h_0(\delta)$

$$\begin{aligned} 1-2\delta \leq |U^\pm(x,t)| \leq 1 \qquad &\forall\ (x,t) \notin D^+_\delta \\ \text{and} \qquad |U^\pm(x,t)| \leq 1 - \tfrac{1}{8}\delta \quad &\forall\ (x,t) \in D^+_{\frac{\delta}{4}}.\end{aligned} \tag{2.53}$$

On noting (2.53) and (2.42) we have that

$$\begin{aligned}&\left| \int_{\Omega_T\setminus D^+_\delta} b(U^-)\tfrac{\partial W^+}{\partial x}\tfrac{\partial \eta}{\partial x}\,\mathrm{d}x\,\mathrm{d}t \right| \\ &\leq \|[b(U^-)]^{\frac{1}{2}}\|_{L^\infty(\Omega_T\setminus D^+_\delta)} \, \|[b(U^-)]^{\frac{1}{2}}\tfrac{\partial W^+}{\partial x}\|_{L^2(\Omega_T)} \, \|\eta\|_{L^2(0,T;H^1(\Omega))} \\ &\leq C[B_{\max}(2\delta)]^{\frac{1}{2}} \, \|\eta\|_{L^2(0,T;H^1(\Omega))} \qquad \forall\ \eta \in L^2(0,T;H^1(\Omega)), \quad \forall\ h \leq h_0(\delta),\end{aligned} \tag{2.54}$$

and

$$B_{\min}(\tfrac{\delta}{8}) \int_{D^+_{\frac{\delta}{2}}} |\tfrac{\partial W^+}{\partial x}|^2 \,\mathrm{d}x\,\mathrm{d}t \;\leq\; \int_{D^+_{\frac{\delta}{2}}} b(U^-)|\tfrac{\partial W^+}{\partial x}|^2 \,\mathrm{d}x\,\mathrm{d}t \;\leq\; C \qquad \forall\, h \leq h_0(\delta), \tag{2.55}$$

where

$$B_{\max}(\delta) := \max_{1-\delta \leq |z| \leq 1} b(z) \quad \text{and} \quad B_{\min}(\delta) := \min_{|z| \leq 1-\delta} b(z).$$

In what follows we want to relate W^+ to U^+ and U^- on the sets D^+_δ. From (2.53) we have that for all $h \leq h_0(\delta)$ and for almost every (a.e.) $t \in (0,T)$

$$\chi(\cdot,t) \equiv U^+(\cdot,t) \pm \tfrac{1}{8}\delta \frac{\eta^h(\cdot,t)}{\|\eta^h(\cdot,t)\|_{0,\infty}} \in K^h \qquad \forall\, \eta^h \in L^2(0,T;S^h) \quad \text{with } \mathrm{supp}(\eta^h) \subset D^+_{\frac{\delta}{4}}. \tag{2.56}$$

Choosing such χ in (2.37b) yields for all $h \leq h_0(\delta)$ that

$$\int_0^T \Big[\, \gamma(\tfrac{\partial U^+}{\partial x}, \tfrac{\partial \eta^h}{\partial x}) + (\psi_1'(U^+) + \psi_2'(U^-) - \theta_c U^+, \eta^h)^h \,\Big]\, \mathrm{d}t = \int_0^T (W^+, \eta^h)^h \,\mathrm{d}t \qquad \forall\, \eta^h \in L^2(0,T;S^h) \quad \text{with } \mathrm{supp}(\eta^h) \subset D^+_{\frac{\delta}{4}}. \tag{2.57}$$

Next we derive a bound of W^+ locally on the set $\{|u| < 1\}$. For any $t \in [0,T]$, we choose a cut-off function $\theta_\delta(\cdot,t) \in C_0^\infty(D^+_{\frac{\delta}{2}}(t))$ such that

$$\theta_\delta(\cdot,t) \equiv 1 \quad \text{on } D^+_\delta(t), \qquad 0 \leq \theta_\delta(\cdot,t) \leq 1, \qquad |\tfrac{\partial}{\partial x}\theta_\delta(\cdot,t)| \leq C\delta^{-2}. \tag{2.58}$$

This last property can be achieved since for y_1, $y_2 \in \overline{\Omega}$ such that $|u(y_1,t)| \geq 1 - \frac{1}{2}\delta$ and $|u(y_2,t)| \leq 1-\delta$ we have from (2.47) that $\frac{1}{2}\delta \leq |u(y_2,t) - u(y_1,t)| \leq C|y_2 - y_1|^{\frac{1}{2}}$. It follows from (2.14) and (2.58) that there exists an $h_1(\delta) \leq h_0(\delta)$ such that

$$\mathrm{supp}(\hat{Q}^h(\theta_\delta^2\, W^+)) \subset D^+_{\frac{\delta}{4}} \quad \forall\, h \leq h_1(\delta). \tag{2.59}$$

It follows from (2.2), (2.59), (2.57), (2.13), the continuity properties of ψ_i $(i = 1,2)$, $|U| \leq 1$, and (2.58) that for all $h \leq h_1(\delta)$

$$\begin{aligned}
&\int_{\Omega_T} \theta_\delta^2\, (W^+)^2 \,\mathrm{d}x\,\mathrm{d}t = \int_0^T (W^+, \hat{Q}^h(\theta_\delta^2\, W^+))^h \,\mathrm{d}t \\
&= \int_0^T \Big[\gamma(\tfrac{\partial U^+}{\partial x}, \tfrac{\partial}{\partial x}(\hat{Q}^h(\theta_\delta^2\, W^+))) + (\psi_1'(U^+) + \psi_2'(U^-) - \theta_c U^+, \hat{Q}^h(\theta_\delta^2\, W^+))^h\Big]\, \mathrm{d}t \\
&\leq C\|U^+\|_{L^2(0,T;H^1(\Omega))}\, \|\tfrac{\partial}{\partial x}(\theta_\delta^2\, W^+)\|_{L^2(\Omega_T)} + C\|\theta_\delta W^+\|_{L^2(\Omega_T)} \\
&\leq C(\delta^{-1})\, (\|U^+\|_{L^2(0,T;H^1(\Omega))} + 1) \left[\, \|\tfrac{\partial W^+}{\partial x}\|_{L^2(D^+_{\frac{\delta}{2}})} + \|\theta_\delta\, W^+\|_{L^2(\Omega_T)} \right].
\end{aligned} \tag{2.60}$$

Applying Young's inequality then gives

$$\int_{\Omega_T} \theta_\delta^2\, (W^+)^2 \,\mathrm{d}x\,\mathrm{d}t \leq C(\delta^{-1}) \left[1 + \|U^+\|^2_{L^2(0,T;H^1(\Omega))} + \|\tfrac{\partial W^+}{\partial x}\|^2_{L^2(D^+_{\frac{\delta}{2}})} \right]. \tag{2.61}$$

Therefore combining (2.55), (2.61), and (2.42) we have that

$$\|W^+\|_{L^2(0,T;H^1(D_\delta^+(t)))} \le C(\delta^{-1})[B_{\min}(\tfrac{\delta}{8})]^{-1} \le C(\delta^{-1}) \qquad \forall\, h \le h_1(\delta). \tag{2.62}$$

The last estimate implies the existence of a subsequence and a $w \in L^2(0,T;H^1(D_\delta^+(t)))$ such that

$$W^+ \to w, \quad \tfrac{\partial W^+}{\partial x} \to \tfrac{\partial w}{\partial x} \qquad \text{weakly in } L^2(D_\delta^+) \text{ as } h \to 0. \tag{2.63}$$

Next noting the uniform continuity of b, (2.55), and (2.38) we conclude that

$$\begin{aligned}
&\left| \int_{D_\delta^+} [b(U^-) - b(u)] \tfrac{\partial W^+}{\partial x} \tfrac{\partial \eta}{\partial x} \,\mathrm{d}x\,\mathrm{d}t \right| \\
&\le \|b(u) - b(U^-)\|_{L^\infty(\Omega_T)} \, \|\tfrac{\partial W^+}{\partial x}\|_{L^2(D_\delta^+)} \, \|\eta\|_{L^2(0,T;H^1(\Omega))} \\
&\le \frac{C}{[B_{\min}(\frac{\delta}{8})]^{\frac12}} \, \|b(u) - b(U^-)\|_{L^\infty(\Omega_T)} \, \|\eta\|_{L^2(0,T;H^1(\Omega))}
\end{aligned} \tag{2.64}$$

will converge to 0 as $h \to 0$.

Combining (2.51), (2.64), and (2.63) and noting (2.11), (2.47), and (2.46) yields that

$$\int_{D_\delta^+} b(U^-) \tfrac{\partial W^+}{\partial x} \tfrac{\partial}{\partial x}(\pi^h \eta) \,\mathrm{d}x\,\mathrm{d}t \to \int_{D_\delta^+} b(u) \tfrac{\partial w}{\partial x} \tfrac{\partial \eta}{\partial x} \,\mathrm{d}x\,\mathrm{d}t \quad \text{as } h \to 0 \qquad \forall\, \eta \in L^2(0,T;H^1(\Omega)). \tag{2.65}$$

Moreover, by (2.11), (2.48), and (2.43) we have that

$$\int_0^T (\tfrac{\partial U^+}{\partial x}, \tfrac{\partial}{\partial x}(\pi^h \eta)) \,\mathrm{d}t \to \int_0^T (\tfrac{\partial u}{\partial x}, \tfrac{\partial \eta}{\partial x}) \,\mathrm{d}t \quad \text{as } h \to 0 \quad \forall\, \eta \in L^2(0,T;H^1(\Omega)). \tag{2.66}$$

Using (2.1), (2.10), and (2.62) we deduce that

$$\begin{aligned}
\left| \int_0^T \left[(W^+, \pi^h \eta)^h - (W^+, \eta) \right] \mathrm{d}t \right| &\equiv \left| \int_{\Omega_T} (I - \pi^h)(W^+ \eta) \,\mathrm{d}x\,\mathrm{d}t \right| \\
&\le Ch \int_{\Omega_T} |\tfrac{\partial}{\partial x}(W^+ \eta)| \,\mathrm{d}x\,\mathrm{d}t \\
&\le Ch \, \|W^+\|_{L^2(0,T;H^1(D_\delta^+(t)))} \, \|\eta\|_{L^2(0,T;H^1(\Omega))} \\
&\le C(\delta^{-1}) \, h \, \|\eta\|_{L^2(0,T;H^1(\Omega))} \\
&\qquad \forall\, \eta \in L^2(0,T;H^1(\Omega)) \text{ with } \mathrm{supp}(\eta) \subset D_\delta^+.
\end{aligned} \tag{2.67}$$

Noting that $\psi_1 \in C^1([-1,1])$ and using (2.1), (2.10), (2.38), (2.12), and (2.6) yields that

$$\begin{aligned}
&\left| \int_0^T \left[(\psi_1'(U^+), \pi^h \eta)^h - (\psi_1'(u), \eta) \right] \mathrm{d}t \right| \\
&\le \int_0^T \left| (\psi_1'(U^+) - \psi_1'(u), \pi^h \eta)^h \right| \mathrm{d}t + \int_0^T \left| (\psi_1'(u), \pi^h \eta)^h - (\psi_1'(u), \eta) \right| \mathrm{d}t \\
&\qquad \to 0 \qquad \text{as } h \to 0 \qquad \forall\, \eta \in L^2(0,T;H^1(\Omega)).
\end{aligned} \tag{2.68}$$

Using a similar argument for the remaining terms and combining (2.67), (2.63), and (2.68) implies that

$$\int_0^T (W^+ - \psi_1'(U^+) - \psi_2'(U^-) + \theta_c U^+, \pi^h \eta)^h \, \mathrm{d}t \to \int_0^T (w - \Psi'(u), \eta) \, \mathrm{d}t$$

$$\text{as } h \to 0 \qquad \forall\, \eta \in L^2(0,T;H^1(\Omega)) \quad \text{with } \mathrm{supp}(\eta) \subset D_\delta^+. \tag{2.69}$$

Combining (2.66) and (2.69) and noting (2.57) yields that

$$\int_{D_\delta^+} \left[\gamma \tfrac{\partial u}{\partial x} \tfrac{\partial \eta}{\partial x} + (\Psi'(u) - w)\, \eta \right] \mathrm{d}x \, \mathrm{d}t = 0$$

$$\forall\, \eta \in L^2(0,T;H^1(\Omega)) \text{ with } \mathrm{supp}(\eta) \subset D_\delta^+. \tag{2.70}$$

This uniquely defines w in terms of u on the set D_δ^+. Repeating (2.65) for all $\delta > 0$ and noting (2.54), $B_{\max}(\delta) \to 0$ as $\delta \to 0$ and (2.11) yield that

$$\int_{\Omega_T} b(U^-) \tfrac{\partial W^+}{\partial x} \tfrac{\partial}{\partial x}(\pi^h \eta) \, \mathrm{d}x \, \mathrm{d}t \to \int_{D_0^+} b(u) \tfrac{\partial w}{\partial x} \tfrac{\partial \eta}{\partial x} \, \mathrm{d}x \, \mathrm{d}t \quad \text{as } h \to 0$$

$$\forall\, \eta \in L^2(0,T;H^1(\Omega)). \tag{2.71}$$

Combining (2.37a), (2.49), (2.50), (2.71) and arguing similarly as in (2.68) by using (2.38), (2.12), (2.6), and assumption (i) we conclude that for all $\eta \in H^1(0,T;H^1(\Omega))$

$$(u(\cdot,T), \eta(\cdot,T)) - (u_0(\cdot), \eta(\cdot,0)) - \int_0^T (u, \tfrac{\partial \eta}{\partial t}) \, \mathrm{d}t + \int_{D_0^+} b(u) \tfrac{\partial w}{\partial x} \tfrac{\partial \eta}{\partial x} \, \mathrm{d}x \, \mathrm{d}t = 0. \tag{2.72}$$

The fact that $\left\{ b(U^-) \frac{\partial W^+}{\partial x} \right\}_{h>0}$ is uniformly bounded in $L^2(\Omega_T)$ implies that $b(u) \frac{\partial w}{\partial x} \in L^2(D_0^+)$ and hence we conclude from (2.72) that $u \in H^1(0,T;(H^1(\Omega))')$. Therefore combining the above results, repeating (2.70) for all $\delta > 0$ yields that $u \in L^\infty(0,T;H^1(\Omega)) \cap H^1(0,T;(H^1(\Omega))') \cap C_{x,t}^{\frac{1}{2},\frac{1}{8}}(\overline{\Omega}_T)$ and $w \in L^2_{loc}(D_0^+)$, with $\frac{\partial w}{\partial x} \in L^2_{loc}(D_0^+)$, are such that $u(\cdot,0) = u_0(\cdot)$ and

$$\int_0^T \left\langle \tfrac{\partial u}{\partial t}, \eta \right\rangle \mathrm{d}t + \int_{D_0^+} b(u) \tfrac{\partial w}{\partial x} \tfrac{\partial \eta}{\partial x} \, \mathrm{d}x \, \mathrm{d}t = 0 \quad \forall\, \eta \in L^2(0,T;H^1(\Omega)), \tag{2.73a}$$

$$\int_{D_0^+} \left[\gamma \tfrac{\partial u}{\partial x} \tfrac{\partial \eta}{\partial x} + (\Psi'(u) - w)\, \eta \right] \mathrm{d}x \, \mathrm{d}t = 0$$

$$\forall\, \eta \in L^2(0,T;H^1(\Omega)) \text{ with } \mathrm{supp}(\eta) \subset D_0^+. \tag{2.73b}$$

Hence we have established the desired result (2.41a,b). □

Remark. Theorem 2.2 also establishes existence of a solution to problem (P) and yields the result of [27], where existence is proved in one space dimension, (see also [19]). In addition we note that we assumed only continuity of the mobility b. All other existence results for degenerate parabolic equations of fourth order in the literature require at least Hölder regularity for b.

3. Solution of the discrete variational inequality. We now consider an algorithm for solving the variational inequality at each time level in $(\mathrm{P}^{h,\Delta t})$. This is based on the general splitting algorithm of [25]; see also [16] and [2] where this algorithm has been applied to solve $(\mathrm{P}^{h,\Delta t})$ with constant mobility.

For n fixed, multiplying (2.3b) by $\mu > 0$, a "relaxation" parameter, adding $(U^n, \chi - U^n)^h$ to both sides, and rearranging on noting (2.3a) and (2.29), it follows that $\{U^n, W^n\} \in K^h \times S^h$ satisfy

$$(U^n + \mu\psi_1'(U^n), \chi - U^n)^h \geq (Z^n, \chi - U^n)^h \quad \forall\, \chi \in K^h, \tag{3.1a}$$

$$\left(\frac{U^n - U^{n-1}}{\Delta t}, \chi\right)^h + b^{n-1}(\nabla W^n, \nabla\chi) = ([b^{n-1} - b(U^{n-1})]\nabla W^n, \nabla\chi) \quad \forall\, \chi \in S^h, \tag{3.1b}$$

where $Z^n \in S^h$ is such that

$$(Z^n, \chi)^h := (U^n, \chi)^h - \mu\left[\gamma(\nabla U^n, \nabla\chi) + (\psi_2'(U^{n-1}) - \theta_c U^n - W^n, \chi)^h\right] \quad \forall\, \chi \in S^h \tag{3.1c}$$

and b^{n-1} is chosen such that $b^{n-1} \in [b_{\max}^{n-1}, b_{\max}]$ with $b_{\max}^{n-1}$ and $b_{\max}$ as defined in Theorem 2.1. We introduce $X^n \in S^h$ such that

$$(X^n, \chi)^h := (U^n, \chi)^h + \mu\left[\gamma(\nabla U^n, \nabla\chi) + (\psi_2'(U^{n-1}) - \theta_c U^n - W^n, \chi)^h\right] \quad \forall\, \chi \in S^h \tag{3.1d}$$

and note that $X^n = 2U^n - Z^n$. We use this as a basis for constructing our iterative procedure: For $n \geq 1$ set $\{U^{n,0}, W^{n,0}\} \equiv \{U^{n-1}, W^{n-1}\} \in K^h \times S^h$, where $W^0 \in S^h$ is arbitrary if $n = 1$.

For $k \geq 0$ we define $Z^{n,k} \in S^h$ such that for all $\chi \in S^h$

$$(Z^{n,k}, \chi)^h = (U^{n,k}, \chi)^h - \mu\left[\gamma(\nabla U^{n,k}, \nabla\chi) + (\psi_2'(U^{n-1}) - \theta_c U^{n,k} - W^{n,k}, \chi)^h\right]. \tag{3.2a}$$

Then find $U^{n,k+\frac{1}{2}} \in K^h$ such that

$$\begin{aligned} U^{n,k+\frac{1}{2}}(x_j) &= U^{n-1}(x_j) \quad \text{if } j \in J_0(U^{n-1}),\\ (U^{n,k+\frac{1}{2}}(x_j) + \mu\psi_1'(U^{n,k+\frac{1}{2}}(x_j)) - Z^{n,k}(x_j))&(r - U^{n,k+\frac{1}{2}}(x_j)) \geq 0\\ &\forall\, r \in [-1, 1] \quad \text{if } j \in J_+(U^{n-1}), \end{aligned} \tag{3.2b}$$

and find $\{U^{n,k+1}, W^{n,k+1}\} \in S^h \times S^h$ such that

$$\left(\frac{U^{n,k+1} - U^{n-1}}{\Delta t}, \chi\right)^h + b^{n-1}(\nabla W^{n,k+1}, \nabla\chi) = ([b^{n-1} - b(U^{n-1})]\nabla W^{n,k}, \nabla\chi) \quad \forall\, \chi \in S^h, \tag{3.2c}$$

$$\begin{aligned} (U^{n,k+1}, \chi)^h + \mu\left[\gamma(\nabla U^{n,k+1}, \nabla\chi) + (\psi_2'(U^{n-1}) - \theta_c U^{n,k+1} - W^{n,k+1}, \chi)^h\right]&\\ = (X^{n,k+1}, \chi)^h \quad \forall\, \chi \in S^h&, \end{aligned} \tag{3.2d}$$

where $X^{n,k+1} := 2U^{n,k+\frac{1}{2}} - Z^{n,k}$. For $j \in J_+(U^{n-1})$ existence and uniqueness of $U^{n,k+\frac{1}{2}}(x_j)$ in the variational inequality (3.2b) follows from the monotonicity of $\psi_1'(\cdot)$.

It remains to show that (3.2c) and (3.2d) possess a unique solution $\{U^{n,k+1}, W^{n,k+1}\} \in S^h \times S^h$. Let $A^{n,k} \in V^h$ be such that

$$(A^{n,k}, \chi)^h = (b(U^{n-1})\nabla W^{n,k}, \nabla\chi) \quad \forall\, \chi \in S^h. \tag{3.3}$$

It then follows from (3.2c), (2.15), and (3.2d) with $\chi \equiv 1$ that

$$\begin{aligned} W^{n,k+1} &= (I - ⨍\,)W^{n,k} - [b^{n-1}]^{-1}\hat{\mathcal{G}}^h(\tfrac{U^{n,k+1}-U^{n-1}}{\Delta t} + A^{n,k}) \\ &\quad + ⨍\,(\tfrac{1}{\mu}(U^{n,k+1} - X^{n,k+1}) + \pi^h\psi_2'(U^{n-1}) - \theta_c U^{n,k+1}). \end{aligned} \tag{3.4}$$

Therefore (3.2c,d) may be written equivalently as follows: find $U^{n,k+1} \in S^h_m := \{v^h \in S^h : ⨍\, v^h = ⨍\, U^0\}$ such that

$$\begin{aligned} &(U^{n,k+1}, (I - ⨍\,)\chi)^h \\ &\quad +\mu\Big[\gamma(\nabla U^{n,k+1}, \nabla\chi) + \Big([b^{n-1}]^{-1}\hat{\mathcal{G}}^h\Big[\tfrac{U^{n,k+1}-U^{n-1}}{\Delta t}\Big] - \theta_c(I - ⨍\,)U^{n,k+1}, \chi\Big)^h\Big] \\ &= (X^{n,k+1} + \mu(W^{n,k} - \psi_2'(U^{n-1}) - [b^{n-1}]^{-1}\hat{\mathcal{G}}^h A^{n,k}), (I - ⨍\,)\chi)^h \quad \forall\, \chi \in S^h. \end{aligned} \tag{3.5}$$

Existence of $U^{n,k+1} \in S^h_m$ satisfying (3.5) follows, noting (2.16) and the time step restriction $\theta_c^2 b^{n-1}\Delta t < 4\gamma$, since this is the Euler–Lagrange equation of the minimization problem

$$\begin{aligned} &\min_{\chi \in S^h_m} \Big\{|\chi|_h^2 + \mu\Big[\gamma|\chi|_1^2 + \tfrac{1}{b^{n-1}\Delta t}|\nabla\hat{\mathcal{G}}^h(\chi - U^{n-1})|_0^2 - \theta_c|\chi|_h^2\Big] \\ &-2(X^{n,k+1} + \mu(W^{n,k} - \psi_2'(U^{n-1}) - [b^{n-1}]^{-1}\hat{\mathcal{G}}^h A^{n,k}), \chi)^h\Big\}. \end{aligned}$$

Uniqueness of $U^{n,k+1}$ follows in a similar way to that of U^n. Finally, $W^{n,k+1}$ is uniquely defined by (3.4). Hence the iterative procedure (3.2a–d) is well defined.

THEOREM 3.1. *Let $3\theta_c^2 b^{n-1}\Delta t < 4\gamma$. Then for all $\mu \in \mathbb{R}^+$ and $\{U^{n,0}, W^{n,0}\} \in S^h \times S^h$ the sequence $\{U^{n,k}, W^{n,k}\}_{k\geq 0}$ generated by the algorithm* (3.2a–d) *satisfies*

$$U^{n,k} \to U^n \quad \text{and} \quad \int_\Omega b(U^{n-1})|\nabla(W^{n,k+1} - W^n)|^2\,\mathrm{d}x \to 0 \quad \text{as} \quad k \to \infty. \tag{3.6}$$

In addition, if $\psi_1'(\cdot)$ is strictly monotone then $U^{n,k+\frac{1}{2}} \to U^n$ as $k \to \infty$.

Proof. It follows from (3.1c), (3.1d), (3.2a), (3.2d), and by the definition of $X^{n,k+1}$ that for $k \geq 0$

$$U^n = \tfrac{1}{2}(X^n + Z^n), \quad U^{n,k} = \tfrac{1}{2}(X^{n,k} + Z^{n,k}), \quad U^{n,k+\frac{1}{2}} = \tfrac{1}{2}(X^{n,k+1} + Z^{n,k}). \tag{3.7}$$

As $U^{n,k+1}, U^n \in S^h_m$, it follows from (3.2d), (3.1d), and (3.7) that

$$\begin{aligned} &\gamma|U^{n,k+1} - U^n|_1^2 - \theta_c|U^{n,k+1} - U^n|_h^2 - (W^{n,k+1} - W^n, U^{n,k+1} - U^n)^h \\ &= \tfrac{1}{4\mu}(X^{n,k+1} - X^n - Z^{n,k+1} + Z^n, X^{n,k+1} - X^n + Z^{n,k+1} - Z^n)^h \\ &= \tfrac{1}{4\mu}(|X^{n,k+1} - X^n|_h^2 - |Z^{n,k+1} - Z^n|_h^2). \end{aligned} \tag{3.8}$$

Choosing $\chi \equiv U^{n,k+\frac{1}{2}}$ in (3.1a) and for $j \in J_+(U^{n-1})$ choosing $\chi \equiv U^n(x_j)$ in (3.2b), multiplying by β_j on recalling (2.1), and summing over j yields, on noting that $U^n(x_j) = U^{n,k+\frac{1}{2}}(x_j)$ for $j \in J_0(U^{n-1})$,

$$|U^{n,k+\frac{1}{2}} - U^n|_h^2 + \mu(\psi_1'(U^{n,k+\frac{1}{2}}) - \psi_1'(U^n), U^{n,k+\frac{1}{2}} - U^n)^h \leq (Z^{n,k} - Z^n, U^{n,k+\frac{1}{2}} - U^n)^h. \tag{3.9}$$

Combining (3.9) and (3.7) yields that

$$4\mu(\psi_1'(U^{n,k+\frac{1}{2}}) - \psi_1'(U^n), U^{n,k+\frac{1}{2}} - U^n)^h + |X^{n,k+1} - X^n|_h^2 \le |Z^{n,k} - Z^n|_h^2. \tag{3.10}$$

Using (3.2c), (3.1b), and (2.32) it follows that

$$\begin{aligned}
&-(W^{n,k+1} - W^n, U^{n,k+1} - U^n)^h \\
&= -(W^{n,k+1} - W^n, U^{n,k+1} - U^{n-1})^h - (W^{n,k+1} - W^n, U^{n-1} - U^n)^h \\
&= \Delta t |[b(U^{n-1})]^{\frac{1}{2}} \nabla (W^{n,k+1} - W^n)|_0^2 \\
&\quad + \Delta t([b^{n-1} - b(U^{n-1})] \nabla (W^{n,k+1} - W^{n,k}), \nabla (W^{n,k+1} - W^n)) \\
&= \Delta t |[b(U^{n-1})]^{\frac{1}{2}} \nabla (W^{n,k+1} - W^n)|_0^2 + \tfrac{\Delta t}{2}\Big[|[b^{n-1} - b(U^{n-1})]^{\frac{1}{2}} \nabla (W^{n,k+1} - W^n)|_0^2 \\
&\quad - |[b^{n-1} - b(U^{n-1})]^{\frac{1}{2}} \nabla (W^{n,k} - W^n)|_0^2 + |[b^{n-1} - b(U^{n-1})]^{\frac{1}{2}} \nabla (W^{n,k+1} - W^{n,k})|_0^2 \Big].
\end{aligned} \tag{3.11}$$

Similarly to (3.11) and using Young's inequality we have that for any $\delta \in (0,1)$

$$\begin{aligned}
&\theta_c |U^{n,k+1} - U^n|_h^2 = \theta_c (U^{n,k+1} - U^{n-1}, U^{n,k+1} - U^n)^h + \theta_c (U^{n-1} - U^n, U^{n,k+1} - U^n)^h \\
&= -\theta_c \Delta t (b(U^{n-1}) \nabla (W^{n,k+1} - W^n), \nabla (U^{n,k+1} - U^n)) \\
&\quad - \theta_c \Delta t ([b^{n-1} - b(U^{n-1})] \nabla (W^{n,k+1} - W^{n,k}), \nabla (U^{n,k+1} - U^n)) \\
&\le \tfrac{\theta_c^2 b^{n-1} \Delta t}{4} \left(2 + \tfrac{1}{1-\delta}\right) |U^{n,k+1} - U^n|_1^2 + \tfrac{\Delta t}{2} |[b^{n-1} - b(U^{n-1})]^{\frac{1}{2}} \nabla (W^{n,k+1} - W^{n,k})|_0^2 \\
&\quad + (1-\delta) \Delta t |[b(U^{n-1})]^{\frac{1}{2}} \nabla (W^{n,k+1} - W^n)|_0^2.
\end{aligned} \tag{3.12}$$

Combining (3.8), (3.10), (3.11), (3.12), and rearranging yields that

$$\begin{aligned}
&\left(\gamma - \tfrac{\theta_c^2 b^{n-1} \Delta t}{4} \left(2 + \tfrac{1}{1-\delta}\right)\right) |U^{n,k+1} - U^n|_1^2 \\
&\quad + \tfrac{1}{4\mu} |Z^{n,k+1} - Z^n|_h^2 + \tfrac{\Delta t}{2} |[b^{n-1} - b(U^{n-1})]^{\frac{1}{2}} \nabla (W^{n,k+1} - W^n)|_0^2 \\
&\quad + \delta \Delta t |[b(U^{n-1})]^{\frac{1}{2}} \nabla (W^{n,k+1} - W^n)|_0^2 + (\psi_1'(U^{n,k+\frac{1}{2}}) - \psi_1'(U^n), U^{n,k+\frac{1}{2}} - U^n)^h \\
&\le \tfrac{1}{4\mu} |Z^{n,k} - Z^n|_h^2 + \tfrac{\Delta t}{2} |[b^{n-1} - b(U^{n-1})]^{\frac{1}{2}} \nabla (W^{n,k} - W^n)|_0^2.
\end{aligned} \tag{3.13}$$

Therefore noting the monotonicity of $\psi_1'(\cdot)$ and the restriction on Δt we have that for δ sufficiently small $\{\frac{1}{4\mu}|Z^{n,k} - Z^n|_h^2 + \frac{\Delta t}{2}|[b^{n-1} - b(U^{n-1})]^{\frac{1}{2}} \nabla (W^{n,k} - W^n)|_0^2\}_{k \ge 0}$ is a decreasing sequence which is bounded below and so has a limit. Therefore the desired results (3.6) follow from this and (3.13). ∎

Remark. We see from (3.2a–d) and (3.5) that at each iteration one needs to solve only (i) a fixed linear system with constant coefficients and (ii) a nonlinear equation at each mesh point. On a uniform mesh (i) can be solved efficiently using a discrete cosine transform; see [9, section 5], where a similar problem is solved.

4. Logarithmic free energy. In this section we modify our approximation ($\mathrm{P}^{h,\Delta t}$) and the results in the previous two sections to cope with the logarithmic free energy, that is

$$\psi_1(s) := \tfrac{\theta}{2}\left[(1+s)\ln[\tfrac{1+s}{2}] + (1-s)\ln[\tfrac{1-s}{2}]\right] . \tag{4.1}$$

Here we have the additional difficulty that $\Psi'(\cdot)$ (see (1.5)) is not uniformly bounded on $(-1,1)$ with $\psi_1'(\pm 1) = \pm\infty$.

Our modified approximation is the following.

$(\widetilde{\mathrm{P}}^{h,\Delta t})$ For $n \geq 1$, find $\{U^n, W^n\} \in S^h \times S^h$ such that

$$\left(\tfrac{U^n - U^{n-1}}{\Delta t}, \chi\right)^h + \left(b(U^{n-1})\nabla W^n, \nabla \chi\right) = 0 \quad \forall\, \chi \in S^h, \tag{4.2a}$$

$$\gamma(\nabla U^n, \nabla \chi) + (\psi_1'(U^n) - \theta_c U^n, \chi)^h = (W^n - \psi_2'(U^{n-1}), \chi)^h \quad \forall\, \chi \in \widetilde{V}^h(U^{n-1}), \tag{4.2b}$$

where $U^0 \in K^h$ is an approximation of u_0 and for $q^h \in K^h$ we define

$$\widetilde{V}^h(q^h) := \left\{v^h \in S^h : v^h(x_j) = 0 \quad \forall\, j \in J_0(q^h)\right\}. \tag{4.3}$$

Clearly (4.2b) implies that $|U^n(x_j)| < 1$ for all $j \in J_+(U^{n-1})$. Moreover, we will show that $(\widetilde{\mathrm{P}}^{h,\Delta t})$ has the property that $\|U^0\|_{0,\infty} < 1$ implies $\|U^n\|_{0,\infty} < 1$ for all $n \geq 1$. We prove well posedness of this approximation via the regularization

$$\psi_{1,\varepsilon}(s) := \begin{cases} \frac{\theta}{2}(1+s)\ln\left[\frac{1+s}{2}\right] + \frac{\theta}{4\varepsilon}(1-s)^2 + \frac{\theta}{2}(1-s)\ln\left[\frac{\varepsilon}{2}\right] - \frac{\theta\varepsilon}{4} & \text{if } s \geq 1-\varepsilon, \\ \psi_1(s) & \text{if } |s| \leq 1-\varepsilon, \\ \frac{\theta}{2}(1-s)\ln\left[\frac{1-s}{2}\right] + \frac{\theta}{4\varepsilon}(1+s)^2 + \frac{\theta}{2}(1+s)\ln\left[\frac{\varepsilon}{2}\right] - \frac{\theta\varepsilon}{4} & \text{if } s \leq -1+\varepsilon. \end{cases} \tag{4.4}$$

Let us emphasize that we introduce $\psi_{1,\varepsilon}$ only to prove well posedness of problem $(\widetilde{\mathrm{P}}^{h,\Delta t})$. In practice we solve $(\widetilde{\mathrm{P}}^{h,\Delta t})$ directly. We note that $\psi_{1,\varepsilon}(s) \leq \psi_1(s)$ for all $|s| \leq 1$ and define $\Psi_{1,\varepsilon}(s) := \psi_{1,\varepsilon}(s) + \frac{\theta_c}{2}(1-s^2)$ for all $s \in \mathbb{R}$. The monotone function

$$\psi_{1,\varepsilon}'(s) = \begin{cases} \frac{\theta}{2}\left(1 + \ln(1+s)\right) - \frac{\theta}{2\varepsilon}(1-s) - \frac{\theta}{2}\ln\varepsilon & \text{if } s \geq 1-\varepsilon, \\ \psi_1'(s) & \text{if } |s| \leq 1-\varepsilon, \\ -\frac{\theta}{2}\left(1 + \ln(1-s)\right) + \frac{\theta}{2\varepsilon}(1+s) + \frac{\theta}{2}\ln\varepsilon & \text{if } s \leq -1+\varepsilon, \end{cases} \tag{4.5}$$

and the function $\Psi_{1,\varepsilon}'$ satisfy the following properties:

- For all $r, s \in \mathbb{R}$, on noting (2.32),

$$\begin{aligned} \Psi_{1,\varepsilon}'(s)(r-s) = \psi_{1,\varepsilon}'(s)(r-s) - \theta_c s(r-s) &\leq \psi_{1,\varepsilon}(r) - \psi_{1,\varepsilon}(s) + \theta_c s(s-r) \\ &= \Psi_{1,\varepsilon}(r) - \Psi_{1,\varepsilon}(s) + \tfrac{\theta_c}{2}(r-s)^2. \end{aligned} \tag{4.6}$$

- For $\varepsilon \leq 1$ and for all $r, s \in \mathbb{R}$,

$$\begin{aligned} (\psi_{1,\varepsilon}'(r) - \psi_{1,\varepsilon}'(s))^2 &\leq \|\psi_{1,\varepsilon}''\|_{0,\infty}(\psi_{1,\varepsilon}'(r) - \psi_{1,\varepsilon}'(s))(r-s) \\ &\leq \tfrac{\theta}{\varepsilon}(\psi_{1,\varepsilon}'(r) - \psi_{1,\varepsilon}'(s))(r-s). \end{aligned} \tag{4.7}$$

It is a simple matter to show that $\Psi_{1,\varepsilon}$ is bounded below for ε sufficiently small; e.g., if $\varepsilon \leq \varepsilon_0 := \theta/(8\theta_c)$, then

$$\Psi_{1,\varepsilon}(s) \geq \tfrac{\theta}{8\varepsilon}\left([s-1]_+^2 + [-1-s]_+^2\right) - \theta_c \geq -\theta_c \qquad \forall\, s \in \mathbb{R}, \tag{4.8}$$

where $[\cdot]_+ := \max\{\cdot, 0\}$; see [4] for details. In addition we introduce the concave preserving extension $\widetilde{\psi}_2 \in C^1(\mathbb{R})$ of $\psi_2 \in C^1([-1,1])$,

$$\widetilde{\psi}_2(s) := \begin{cases} \psi_2(1) + (s-1)\psi_2'(1) & \text{if } s \geq 1, \\ \psi_2(s) & \text{if } |s| \leq 1, \\ \psi_2(-1) + (s+1)\psi_2'(-1) & \text{if } s \leq -1, \end{cases} \tag{4.9}$$

and then define

$$\Psi_\varepsilon(s) := \Psi_{1,\varepsilon}(s) + \widetilde{\psi}_2(s) \qquad \forall\ s \in \mathbb{R}. \tag{4.10}$$

It follows immediately from (4.8) and (4.9) that Ψ_ε is bounded below; e.g., if $\varepsilon \le \varepsilon_0$ then

$$\Psi_\varepsilon(s) \ge \tfrac{\theta}{16\varepsilon}\left([s-1]_+^2 + [-1-s]_+^2\right) - C \ge -C \qquad \forall\ s \in \mathbb{R}. \tag{4.11}$$

Finally, we need a further restriction on the mesh in order to prove well posedness of $(\widetilde{\mathrm{P}}^{h,\Delta t})$. We modify our assumption (A) to

($\tilde{\mathrm{A}}$) In addition to the assumption (A), we assume for all $h > 0$ that $\mathcal{T}^h$ is an acute partitioning; that is, for (i) $d = 2$, the angle of any triangle does not exceed $\frac{\pi}{2}$, and (ii) $d = 3$, the angle between any two faces of the same tetrahedron does not exceed $\frac{\pi}{2}$.

This acuteness assumption yields that

$$\int_\kappa \nabla\chi_i \cdot \nabla\chi_j \,\mathrm{d}x \le 0, \quad i \ne j, \quad \forall\ \kappa \in \mathcal{T}^h. \tag{4.12}$$

In addition it follows from (4.7) and $(\widetilde{\mathrm{A}})$ that for all $\varepsilon \le 1$ and for all $\kappa \in \mathcal{T}^h$

$$\begin{aligned}\int_\kappa |\nabla\pi^h[\psi'_{1,\varepsilon}(\chi)]|^2 \,\mathrm{d}x &\le \psi''_{1,\varepsilon}(\sup_{x\in\kappa}|\chi(x)|)\int_\kappa \nabla\chi\cdot\nabla\pi^h[\psi'_{1,\varepsilon}(\chi)]\,\mathrm{d}x \\ &\le \tfrac{\theta}{\varepsilon}\int_\kappa \nabla\chi\cdot\nabla\pi^h[\psi'_{1,\varepsilon}(\chi)]\,\mathrm{d}x \qquad \forall\ \chi\in S^h;\end{aligned} \tag{4.13}$$

see, e.g., [14].

THEOREM 4.1. *Let Ω and $\mathcal{T}^h$ be such that assumption $(\widetilde{\mathrm{A}})$ holds and let $U^0 \in K^h$ with $⨍\, U^0 \in (-1,1)$. Then for all $\Delta t > 0$ such that $\theta_c^2 b_{\max}\Delta t < 4\gamma$, there exists a solution $\{U^n, W^n\}_{n=1}^N$ to $(\widetilde{\mathrm{P}}^{h,\Delta t})$. Moreover, $\{U^n\}_{n=1}^N$ is unique and the stability bounds* (2.26) *hold. In addition W^n is unique on $\Omega(U^{n-1})$, $n = 1 \to N$.*

Proof. Given $U^{n-1} \in K^h$ with $|U^{n-1}|_1 \le C$, we prove existence of $\{U^n, W^n\}$ solving (4.2a–b) by introducing a regularized version, as follows.

Find $\{U^n_\varepsilon, W^n_\varepsilon\} \in S^h \times S^h$ such that

$$\left(\tfrac{U^n_\varepsilon - U^{n-1}}{\Delta t}, \chi\right)^h + \left(b(U^{n-1})\nabla W^n_\varepsilon, \nabla\chi\right) = 0 \quad \forall\ \chi \in S^h, \tag{4.14a}$$

$$\gamma(\nabla U^n_\varepsilon, \nabla\chi) + (\Psi'_{1,\varepsilon}(U^n_\varepsilon), \chi)^h = (W^n_\varepsilon - \psi'_2(U^{n-1}), \chi)^h \quad \forall\ \chi \in \widetilde{V}^h(U^{n-1}). \tag{4.14b}$$

Similarly to (2.28) we have that

$$W^n_\varepsilon \equiv -\hat{\mathcal{G}}^h_{U^{n-1}}\left[\tfrac{U^n_\varepsilon - U^{n-1}}{\Delta t}\right] + \sum_{j\in J_0(U^{n-1})} \mu^n_{j,\varepsilon}\chi_j + \sum_{m=1}^M \lambda^n_{m,\varepsilon}\Xi_m(U^{n-1}). \tag{4.15}$$

Existence of $\{U^n_\varepsilon, W^n_\varepsilon\}$, uniqueness of U^n_ε, and uniqueness of W^n_ε on $\Omega_m(U^{n-1})$, $m = 1 \to M$, follows as for $\{U^n, W^n\}$ in the proof of Theorem 2.1 under the stated time step restriction. Similarly to (2.33), on noting the convexity of $\psi_{1,\varepsilon}$, the concavity of $\widetilde{\psi}_2$, and the assumptions on U^{n-1}, we have that $U^n_\varepsilon - U^{n-1} \in \widetilde{V}^h(U^{n-1})$ is such that

$$\begin{aligned}&\tfrac{\gamma}{2}|U^n_\varepsilon|_1^2 + \tfrac{\gamma}{8}|U^n_\varepsilon - U^{n-1}|_1^2 + (\Psi_\varepsilon(U^n_\varepsilon), 1)^h + \tfrac{2}{3}\Delta t|[b(U^{n-1})]^{\frac12}\nabla W^n_\varepsilon|_0^2 \\ &\qquad \le (\Psi_\varepsilon(U^{n-1}), 1)^h + \tfrac{\gamma}{2}|U^{n-1}|_1^2 \le C.\end{aligned} \tag{4.16}$$

From (4.16) and (4.11) we deduce that

$$|[U_\varepsilon^n - 1]_+|_h^2 + |[-U_\varepsilon^n - 1]_+|_h^2 \le C\varepsilon. \tag{4.17}$$

Hence it follows from (4.17), (2.8), and (2.4) that

$$\|[U_\varepsilon^n - 1]_+\|_{0,\infty} + \|[-U_\varepsilon^n - 1]_+\|_{0,\infty} \ \le \ Ch^{-\frac{d}{2}}\varepsilon^{\frac{1}{2}} \tag{4.18a}$$

and from (4.4) and (4.18a) that

$$\|\psi_{1,\varepsilon}(U_\varepsilon^n)\|_{0,\infty} \ \le \ \max\{\,1,\, \psi_{1,\varepsilon}(\|U_\varepsilon^n\|_{0,\infty})\,\} \ \le \ C(h^{-1}). \tag{4.18b}$$

The next part of the proof is now concerned with establishing an ε independent bound on $|\Psi'_{1,\varepsilon}(U_\varepsilon^n)\Xi_m(U^{n-1})|_h$. Due to the logarithmic term in Ψ_1 this then implies that the $\varepsilon \to 0$ limits of subsequences of U_ε^n are less than one in magnitude on the set $J_+(U^{n-1})$. Using a Poincaré type inequality on $\Omega_m(U^{n-1})$ it follows similarly to (2.24a) by noting (2.22b) and (4.16) that

$$\begin{aligned} &|[(I - ⨍_{\Omega_m(U^{n-1})})W_\varepsilon^n]\,\Xi_m(U^{n-1})|_h^2 \\ &\quad\le C(h^{-1})\int_{\Omega_m(U^{n-1})} |\nabla W_\varepsilon^n|^2 \,\mathrm{d}x \\ &\quad\le C(h^{-1})\,[b_{\min}(U^{n-1})]^{-1}\int_{\Omega_m(U^{n-1})} b(U^{n-1})|\nabla W_\varepsilon^n|^2 \,\mathrm{d}x \\ &\quad\le C(h^{-1})\,[b_{\min}(U^{n-1})]^{-1}(\Delta t)^{-1}. \end{aligned} \tag{4.19}$$

We now bound $⨍_{\Omega_m(U^{n-1})} W_\varepsilon^n$. Choosing $\chi \equiv \Xi_m(U^{n-1})$ in (4.14b) yields that

$$(W_\varepsilon^n, \Xi_m(U^{n-1}))^h = (\Psi'_{1,\varepsilon}(U_\varepsilon^n), \Xi_m(U^{n-1}))^h + \tau_{\varepsilon,m}, \tag{4.20}$$

where $\tau_{\varepsilon,m} := \gamma(\nabla U_\varepsilon^n, \nabla[\Xi_m(U^{n-1})]) + (\psi_2'(U^{n-1}), \Xi_m(U^{n-1}))^h$. It is convenient to introduce the set $\Upsilon_m(U^{n-1}) := \operatorname{supp}\{\Xi_m(U^{n-1})\} \setminus \Omega_m(U^{n-1})$, and noting (4.16) we have that

$$\begin{aligned} |(\nabla U_\varepsilon^n, \nabla[\Xi_m(U^{n-1})])| &= \left| \int_{\Upsilon_m(U^{n-1})} \nabla U_\varepsilon^n \cdot \nabla[\Xi_m(U^{n-1})]\,\mathrm{d}x \right| \\ &\le |\Upsilon_m(U^{n-1})|^{\frac{1}{2}}\,\|\nabla[\Xi_m(U^{n-1})]\|_{0,\infty}\,|U_\varepsilon^n|_1 \le Ch^{-1}. \end{aligned} \tag{4.21}$$

Noting that $U^{n-1} \in K^h$, $\psi_2' \in C([-1,1])$, and (4.21), it follows that

$$|\tau_{\varepsilon,m}| \le C[1 + h^{-1}]. \tag{4.22}$$

Similarly to (4.21), we have on noting (2.4), (1.9), and (4.16) that

$$\begin{aligned} &(\nabla U_\varepsilon^n, \nabla[\pi^h([(I - ⨍_{\Omega_m(U^{n-1})})U_\varepsilon^n]\,\Xi_m(U^{n-1}))]) \\ &= \int_{\Omega_m(U^{n-1})} |\nabla U_\varepsilon^n|^2 \,\mathrm{d}x + \int_{\Upsilon_m(U^{n-1})} \nabla U_\varepsilon^n \cdot \nabla[\pi^h([(I - ⨍_{\Omega_m(U^{n-1})})U_\varepsilon^n]\,\Xi_m(U^{n-1}))]\,\mathrm{d}x \\ &\le |U_\varepsilon^n|_1^2 + C|U_\varepsilon^n|_1 |\Upsilon_m(U^{n-1})|^{\frac{1}{2}} \|\nabla[\Xi_m(U^{n-1})]\|_{0,\infty}\,\|U_\varepsilon^n\|_{0,\infty} \\ &\le C[1 + h^{-1}]\|U_\varepsilon^n\|_1^2 \le C(h^{-1}). \end{aligned} \tag{4.23}$$

Now choosing $\chi \equiv \pi^h([(I - \fint_{\Omega_m(U^{n-1})})U_\varepsilon^n]\,\Xi_m(U^{n-1}))$ in (4.14b) it follows on noting (4.6), $\psi_2 \in C^1([-1,1])$, $U^{n-1} \in K^h$, (4.23), (4.17), the remark after (4.4), (4.8), and (4.19) that for all $\lambda \in [-1,1]$

$$\begin{aligned}
&(\Psi'_{1,\varepsilon}(U_\varepsilon^n)\,\Xi_m(U^{n-1}), \lambda - \fint_{\Omega_m(U^{n-1})} U_\varepsilon^n)^h \\
&= (\Psi'_{1,\varepsilon}(U_\varepsilon^n)\,\Xi_m(U^{n-1}), \lambda - U_\varepsilon^n)^h \\
&\quad + (W_\varepsilon^n - \psi_2'(U^{n-1}), [(I - \fint_{\Omega_m(U^{n-1})})U_\varepsilon^n]\,\Xi_m(U^{n-1}))^h \\
&\quad - \gamma(\nabla U_\varepsilon^n, \nabla[\pi^h([(I - \fint_{\Omega_m(U^{n-1})})U_\varepsilon^n]\,\Xi_m(U^{n-1}))]) \\
&\le (\Psi_{1,\varepsilon}(\lambda) - \Psi_{1,\varepsilon}(U_\varepsilon^n), \Xi_m(U^{n-1}))^h + \tfrac{\theta_c}{2}|U_\varepsilon^n - \lambda|_h^2 \\
&\quad + |[(I - \fint_{\Omega_m(U^{n-1})})W_\varepsilon^n]\,\Xi_m(U^{n-1})|_h^2 + C[\,1 + |U_\varepsilon^n|_h^2 + C(h^{-1})\,] \\
&\le C([b_{\min}(U^{n-1})]^{-1}, h^{-1}, (\Delta t)^{-1}).
\end{aligned} \tag{4.24}$$

Here and below we have used the notation $C(a_1, \ldots, a_I)$ defined at the end of section 1. Hence choosing $\lambda = \pm 1$ in (4.24) and noting that $\fint_{\Omega_m(U^{n-1})} U_\varepsilon^n = \fint_{\Omega_m(U^{n-1})} U^{n-1} \in (-1,1)$, we deduce that

$$|(\Psi'_{1,\varepsilon}(U_\varepsilon^n), \Xi_m(U^{n-1}))^h| \le C([b_{\min}(U^{n-1})]^{-1}, h^{-1}, (\Delta t)^{-1}). \tag{4.25}$$

We note that the constant on the right-hand side depends on $\fint_{\Omega_m(U^{n-1})} U^{n-1}$ but is independent of ε. Furthermore, combining (4.20), (4.25), and (4.22) it follows that

$$|(W_\varepsilon^n, \Xi_m(U^{n-1}))^h| \le C([b_{\min}(U^{n-1})]^{-1}, h^{-1}, (\Delta t)^{-1}). \tag{4.26}$$

Hence combining (4.19) and (4.26) yields that

$$|W_\varepsilon^n\,\Xi_m(U^{n-1})|_h \le C([b_{\min}(U^{n-1})]^{-1}, h^{-1}, (\Delta t)^{-1}). \tag{4.27}$$

Choosing $\chi \equiv \pi^h[\Psi'_{1,\varepsilon}(U_\varepsilon^n)\,\Xi_m(U^{n-1})] \in \widetilde{V}^h(U^{n-1})$ in (4.14b) and rearranging yields that

$$\begin{aligned}
&\gamma \int_{\Omega_m(U^{n-1})} \nabla U_\varepsilon^n \cdot \nabla \pi^h[\psi'_{1,\varepsilon}(U_\varepsilon^n)]\,\mathrm{d}x + |\Psi'_{1,\varepsilon}(U_\varepsilon^n)\,\Xi_m(U^{n-1})|_h^2 \\
&= -\gamma \int_{\Upsilon_m(U^{n-1})} \nabla U_\varepsilon^n \cdot \nabla \pi^h[\psi'_{1,\varepsilon}(U_\varepsilon^n)\,\Xi_m(U^{n-1})]\,\mathrm{d}x + \gamma\,\theta_c(\nabla U_\varepsilon^n, \nabla \pi^h[U_\varepsilon^n\,\Xi_m(U^{n-1})]) \\
&\quad + (W_\varepsilon^n - \psi_2'(U^{n-1}), \Psi'_{1,\varepsilon}(U_\varepsilon^n)\,\Xi_m(U^{n-1}))^h.
\end{aligned} \tag{4.28}$$

We now estimate the terms on the right-hand side of (4.28). For any simplex $\kappa \subset \Upsilon_m(U^{n-1})$ with vertices $\{\widetilde{x}_j\}_{j=1}^{d+1} \subset \{x_j\}_{j\in J}$ and corresponding basis functions $\{\widetilde{\chi}_j\}_{j=1}^{d+1} \subset \{\chi_j\}_{j\in J}$, we have on noting (4.12), (4.6), and (4.18b) that

$$\begin{aligned}
&-\int_\kappa \nabla U_\varepsilon^n . \nabla \pi^h[\psi'_{1,\varepsilon}(U_\varepsilon^n)\,\Xi_m(U^{n-1})]\,\mathrm{d}x \\
&= -\sum_{i,j=1}^{d+1} U_\varepsilon^n(\widetilde{x}_i)\,\psi'_{1,\varepsilon}(U_\varepsilon^n(\widetilde{x}_j))\,\Xi_m(U^{n-1})(\widetilde{x}_j) \int_\kappa \nabla\widetilde{\chi}_i \cdot \nabla\widetilde{\chi}_j\,\mathrm{d}x \\
&= -\sum_{i,j=1}^{d+1} [U_\varepsilon^n(\widetilde{x}_i) - U_\varepsilon^n(\widetilde{x}_j)]\,\psi'_{1,\varepsilon}(U_\varepsilon^n(\widetilde{x}_j))\,\Xi_m(U^{n-1})(\widetilde{x}_j) \int_\kappa \nabla\widetilde{\chi}_i \cdot \nabla\widetilde{\chi}_j\,\mathrm{d}x
\end{aligned}$$

$$\leq - \sum_{i,j=1}^{d+1} [\psi_{1,\varepsilon}(U^n_\varepsilon(\widetilde{x}_i)) - \psi_{1,\varepsilon}(U^n_\varepsilon(\widetilde{x}_j))]\, \Xi_m(U^{n-1})(\widetilde{x}_j) \int_\kappa \nabla\widetilde{\chi}_i \cdot \nabla\widetilde{\chi}_j \,\mathrm{d}x$$

$$\leq C(h^{-1}). \tag{4.29}$$

Hence, by summing (4.29) over all $\kappa \subset \Upsilon_m(U^{n-1})$, we deduce that

$$- \int_{\Upsilon_m(U^{n-1})} \nabla U^n_\varepsilon \cdot \nabla \pi^h [\psi'_{1,\varepsilon}(U^n_\varepsilon)\, \Xi_m(U^{n-1})] \,\mathrm{d}x \leq C(h^{-1}). \tag{4.30}$$

Similarly to (4.23), we have that

$$(\nabla U^n_\varepsilon, \nabla \pi^h [U^n_\varepsilon\, \Xi_m(U^{n-1})]) \leq C(h^{-1}). \tag{4.31}$$

It follows from (4.28), on noting (4.13), (4.30), (4.31), a Young's inequality, (4.27), $U^{n-1} \in K^h$, and $\psi'_2 \in C([-1,1])$, that

$$|\Psi'_{1,\varepsilon}(U^n_\varepsilon)\, \Xi_m(U^{n-1})|_h \;\leq\; C([b_{\min}(U^{n-1})]^{-1}, h^{-1}, (\Delta t)^{-1}). \tag{4.32}$$

It follows from (4.16), the fact that $(U^n_\varepsilon, 1)^h = (U^{n-1}, 1)^h$, (1.9), and (4.17) that there exists $U^n \in K^h$ and a subsequence $\{U^n_{\varepsilon'}\}$ such that $U^n_{\varepsilon'} \to U^n$ as $\varepsilon' \to 0$. As $U^n_\varepsilon - U^{n-1} \in \widetilde{V}^h(U^{n-1})$, it follows that $U^n - U^{n-1} \in \widetilde{V}^h(U^{n-1})$. It follows from (4.32) and the above that there exists $\phi^n \in S^h$ and a subsequence $\{U^n_{\varepsilon'}\}$ such that $\pi^h[\Psi'_{1,\varepsilon'}(U^n_{\varepsilon'})] \to \phi^n - \theta_c U^n$ on $\Omega(U^{n-1})$ as $\varepsilon' \to 0$. Since $\Psi'_{1,\varepsilon'}(U^n_{\varepsilon'}(x_j))$ is uniformly bounded in ε, noting (4.7) and using that for all $s \in \mathbb{R}$ $[\psi'_{1,\varepsilon}]^{-1}(s) \to [\psi'_1]^{-1}(s)$ as $\varepsilon \to 0$, we have that $U^n(x_j) = [\psi'_1]^{-1}(\phi^n(x_j))$ and therefore $\phi^n(x_j) = \psi'_1(U^n(x_j))$ for all $j \in J_+(U^{n-1})$. Hence we have that

$$|\Psi'_1(U^n)\, \Xi_m(U^{n-1})|^2_h \leq C([b_{\min}(U^{n-1})]^{-1}, h^{-1}, (\Delta t)^{-1}), \tag{4.33}$$

which immediately implies that $|U^n(x_j)| < 1$ for all $j \in J_+(U^{n-1})$. Finally, it follows from (4.27) that there exists $W^n \in S^h$ and a subsequence $\{W^n_{\varepsilon'}\}$ such that $W^n_{\varepsilon'} \to W^n$ on $\Omega(U^{n-1})$ as $\varepsilon' \to 0$. Hence we may pass to the limit $\varepsilon' \to 0$ in (4.14a,b), on noting (2.21), to prove existence of a solution $\{U^n, W^n\}_{n=1}^N$ to $(\widetilde{\mathrm{P}}^{h,\Delta t})$.

The uniqueness result follows as in Theorem 2.1 on noting that $|U^n(x_j)| < 1$ for all $j \in J_+(U^{n-1})$. The stability bounds (2.26) follow as in Theorem 2.1 by choosing $\chi \equiv W^n \in S^h$ in (4.2a) and $\chi \equiv U^n - U^{n-1} \in \widetilde{V}^h(U^{n-1})$ in (4.2b). ∎

Adopting the notation (2.35a,b) for the solution $\{U^n, W^n\}_{n=1}^N$ of $(\widetilde{\mathrm{P}}^{h,\Delta t})$, we have the analogue of Theorem 2.2.

THEOREM 4.2. *Let the assumptions of Theorem* 2.2 *hold with* (A) *replaced by* $(\widetilde{\mathrm{A}})$, *and now in particular with* ψ_1 *assumed to be of the logarithmic form* (4.1). *Then there exists a subsequence of solutions* $\{U, W\}_h$ *of problem* $(\widetilde{\mathrm{P}}^{h,\Delta t})$ *and a function* $u \in L^\infty(0,T;K) \cap H^1(0,T;(H^1(\Omega))') \cap C^{\frac{1}{2},\frac{1}{8}}_{x,t}(\overline{\Omega}_T)$ *and a* $w \in L^2_{loc}(\{|u| < 1\})$ *with* $\frac{\partial w}{\partial x} \in L^2_{loc}(\{|u| < 1\})$ *such that as* $h \to 0$, (2.38)–(2.40) *and* (2.41a,b) *hold.*

Proof. The proof is the same as that of Theorem 2.2 with the following minor changes. We mention only the modifications caused by the presence of the logarithmic free energy which implies that Ψ' becomes unbounded. Clearly the inequality, the test function $\chi - U^+$, and K^h in (2.37b) are replaced by equality, χ, and $\widetilde{V}^h$, respectively. Although (2.56) is redundant, (2.57) still holds on noting the above and (2.53). It follows from (2.59) and (2.53) that $C\|\theta_\delta W^+\|_{L^2(\Omega_T)}$ on the right-hand side of the first inequality in (2.60) is replaced by $C(\delta^{-1})\|\theta_\delta W^+\|_{L^2(\Omega_T)}$ with the final bound of (2.60) remaining the same. Clearly (2.68) remains true for all $\eta \in L^2(0,T;H^1(\Omega))$ with $\mathrm{supp}(\eta) \subset D_\delta^+$ on noting the technique used in (2.67). Hence (2.70) remains true. ∎

Finally, we modify the iterative algorithm in section 3 to solve the nonlinear algebraic system for $\{U^n, W^n\}$ arising in $(\widetilde{\mathrm{P}}^{h,\Delta t})$. We have that $\{U^n, W^n\} \in S^h \times S^h$ satisfy

$$(4.34)\qquad \begin{aligned} (U^n + \mu\psi_1'(U^n), \chi)^h &= (Z^n, \chi)^h \quad \forall\, \chi \in \widetilde{V}^h(U^{n-1}),\\ U^n(x_j) &= U^{n-1}(x_j) \quad \forall\, j \in J_0(U^{n-1}) \end{aligned}$$

in place of (3.1a) with (3.1b–d) remaining the same. Hence we modify our iterative procedure (3.2a–d) by replacing (3.2b) by the following: Find $U^{n,k+\frac{1}{2}} \in S^h$ such that

$$(4.35)\qquad \begin{aligned} U^{n,k+\frac{1}{2}}(x_j) &= U^{n-1}(x_j) \quad \text{if } j \in J_0(U^{n-1}),\\ U^{n,k+\frac{1}{2}}(x_j) + \mu\psi_1'(U^{n,k+\frac{1}{2}}(x_j)) &= Z^{n,k}(x_j) \quad \text{if } j \in J_+(U^{n-1}) \end{aligned}$$

and keeping (3.2a,c,d) the same. For $j \in J_+(U^{n-1})$ existence and uniqueness of $U^{n,k+\frac{1}{2}}(x_j)$ follows from the monotonicity of $\psi_1'(\cdot)$. Hence this modified iterative procedure is well defined.

THEOREM 4.3. *Let $3\theta_c^2 b^{n-1}\Delta t < 4\gamma$. Then for all $\mu \in \mathbb{R}^+$ and $\{U^{n,0}, W^{n,0}\} \in S^h \times S^h$ the sequence $\{U^{n,k}, W^{n,k}\}_{k\ge 0}$ generated by the modified algorithm,* (3.2a–d) *with* (3.2b) *replaced by* (4.35)*, satisfies*

$$(4.36)\qquad U^{n,k},\ U^{n,k+\frac{1}{2}} \to U^n \quad \text{and} \quad \int_\Omega b(U^{n-1})|\nabla(W^{n,k+1} - W^n)|^2\,\mathrm{d}x \to 0 \quad \text{as} \quad k \to \infty.$$

Proof. The proof is just a simple modification of the proof of Theorem 3.1 to take into account the changes (4.34) and (4.35) to (3.1a) and (3.2b), respectively. We introduce the following modification of the discrete semi-inner product, (2.1):

$$(4.37)\qquad (\eta_1, \eta_2)^h_{J_+(U^{n-1})} := \sum_{j \in J_+(U^{n-1})} \beta_j\, \eta_1(x_j)\, \eta_2(x_j) \qquad \forall\, \eta_1, \eta_2 \in C(\Omega(U^{n-1})).$$

The only changes to the proof of Theorem 3.1 are the following: $(\cdot\,,\cdot)^h$ on the left-hand sides of (3.9), (3.10), and (3.13) is replaced by $(\cdot\,,\cdot)^h_{J_+(U^{n-1})}$. The right-hand side of (3.9) remains the same as $U^{n,k+\frac{1}{2}}(x_j) = U^{n-1}(x_j) = U^n(x_j)$ for all $j \in J_0(U^{n-1})$. Hence we obtain the desired convergence (4.36). ∎

5. Numerical experiments. In this section we report on some numerical results with the intention of demonstrating the practicability of our method as well as showing that in the case of a degenerate mobility a quite different qualitative behavior is observed when compared to results obtained with constant mobility.

In order to avoid numerical difficulties we introduced approximative analogues of the sets $I_m(q^h)$ denoted by $\hat{I}_m(q^h)$, which were defined by replacing (c) in (2.18) by (ĉ) $b(q^h) > tol_1 := 10^{-6}$ at a vertex of κ_l, $l = 1 \to L$. In addition, for each n we adopted the following stopping criterion for (3.2a–d): If $\|U^{n,k_\star} - U^{n,k_\star-1}\|_{0,\infty} < tol$ with $tol = 10^{-7}$ then we set $\{U^n, W^n\} \equiv \{\overline{U}^{n,k_\star}, W^{n,k_\star}\}$, where $\overline{U}^{n,k_\star} \in K^h$ was defined by

$$\overline{U}_j^{n,k_\star} := \begin{cases} \max\{-1, \min\{U_j^{n,k_\star}, 1\}\} & \text{if } j \in \hat{J}_+(U^{n-1}) := \cup_{m=1}^M \hat{I}_m(U^{n-1}), \\ U_j^{n-1} & \text{if } j \in \hat{J}_0(U^{n-1}) := J \setminus \hat{J}_+(U^{n-1}), \end{cases} \tag{5.1}$$

if ψ_1' was not strictly monotone and $\{U^n, W^n\} \equiv \{U^{n,k_\star-\frac{1}{2}}, W^{n,k_\star}\}$ otherwise. Finally, we chose, from experimental evidence, the "relaxation" parameter $\mu \propto h$ in (3.2a–d) in order to improve its convergence.

All computations were performed in double precision on a Sparc 20. The program was written in Fortran 77 using the NAG subroutine C06HBF for calculating the discrete cosine transform used in solving (3.5).

5.1. One space dimension. The computations were performed on a uniform partitioning of $\Omega = (0,1)$ with mesh points $x_j = (j-1)h$, $j = 1 \to \#J$, where $h = 1/(\#J-1)$. We note that the integral on the right-hand side of (3.3) can be evaluated exactly using Simpson's rule if $b(\cdot)$ is quadratic.

Experiment 1. One characteristic feature of the discretizations $(\mathrm{P}^{h,\Delta t})$ and $(\widetilde{\mathrm{P}}^{h,\Delta t})$ is that

$$U^{n-1}(x_{j-1}) = U^{n-1}(x_j) = U^{n-1}(x_{j+1}) = \pm 1 \Longrightarrow j \in J_0(U^{n-1}) \text{ and } U^n(x_j) = \pm 1, \tag{5.2}$$

so that the free boundaries $\partial\{|U^n| = 1\}$ can advance at most one mesh point locally from one time level to the next. This implies that over a time interval of length T the free boundary can advance by at most a distance of $\frac{h}{\Delta t}T$. To be able to track a free boundary which moves with a finite but a priori unknown speed, one needs to choose Δt and h such that $\frac{h}{\Delta t} \to \infty$. For a nonuniform mesh the above requirement on h and Δt has to be replaced by $\frac{\min_{\kappa \in \mathcal{T}^h} h_\kappa}{\Delta t} \to \infty$. If we choose the time step too large, e.g., if $\frac{h}{\Delta t} \to 0$, we obtain the existence of a solution in the limit as $h, \Delta t \to 0$ which would not spread at all for all initial data $u_0 \in K$. Similar results hold for the degenerate equation

$$u_t + (u^p u_{xxx})_x = 0 \quad \text{in } \Omega_T, \qquad u_x = u^p u_{xxx} = 0 \quad \text{on } \partial\Omega \times (0,T);$$

(cf. Lemma 5.1 in [7] and [6]).

As data we took $\gamma = 0.01$, $\psi_1 \equiv \psi_2 \equiv 0$, and $\theta_c = 1$, i.e., the deep quench limit, $b(u) := 1 - u^2$, and

$$u_0(x) = \begin{cases} \cos\left(\frac{x-\frac{1}{2}}{\sqrt{\gamma}}\right) - 1 & \text{if } |x - \frac{1}{2}| \le \frac{\pi\sqrt{\gamma}}{2}, \\ -1 & \text{otherwise.} \end{cases}$$

We note that $u_0 \notin C^1([0,1])$ may be considered to be a stationary solution of (P) on noting (2.41a,b), since $-\gamma\frac{\partial^2 u_0}{\partial x^2} - u_0 = 1$ for $|u_0| < 1$. We performed two separate sets of experiments, one with $\Delta t = 40.96h^2$ and $h = 2^{-6-l}$, the other with $\Delta t = 0.08h^{\frac{1}{2}}$ and $h = 2^{-6-2l}$, both for $l = 0$, 1, 2, 3, and 4. In both cases we took $b_{\max} = b^{n-1} = 1$. Note that the time step restriction of Theorem 3.1, and hence Theorem 2.1, holds. We see in Figure 5.1 when $\Delta t = 40.96h^2$ that our numerical solution in the limit $h \to 0$ appears to spread to the stationary $C^1([0,1])$ solution:

$$\begin{cases} \frac{1}{\pi}\left[1 + \cos\left(\frac{x-\frac{1}{2}}{\sqrt{\gamma}}\right)\right] - 1 & \text{if } |x - \frac{1}{2}| \le \pi\sqrt{\gamma}, \\ -1 & \text{otherwise.} \end{cases}$$

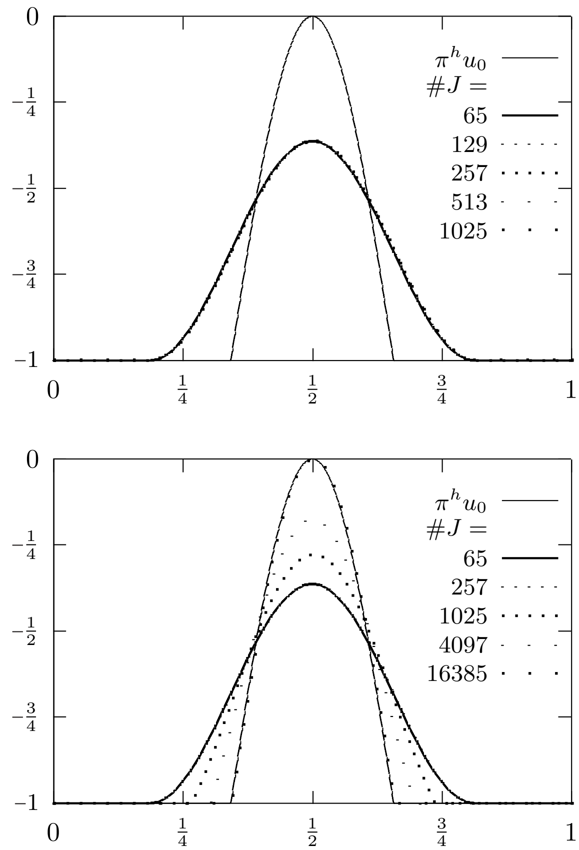

FIG. 5.1. *$U(x, 0.2)$ plotted against x with $\Delta t = 40.96h^2$ and $\Delta t = 0.08h^{\frac{1}{2}}$ for several values of h.*

In contrast, when $\Delta t = 0.08h^{\frac{1}{2}}$ the solutions with $\#J = 65$ and 256 are more or less identical to the above. However, for h sufficiently small the region $\partial\{|u(\cdot, t)| = 1\}$ cannot advance sufficiently fast to capture the apparent former solution. It certainly appears that the limit $h \to 0$ yields that u_0 is a stationary solution. This numerical experiment also appears to indicate that as posed (P) does not have a unique solution. In this context we refer to [19], where existence of a solution is proved with the property that $u \in L^2(0, T; H^2(\Omega))$ for arbitrary initial data $u_0 \in H^1(\Omega)$. Since $u_0 \notin H^2(\Omega)$ this means that u_0 as initial data would lead to a nonstationary solution. We conjecture that we compute the solutions constructed in [19] if we take our time step small enough.

Experiment 2. In the second experiment we took $\psi_2 \equiv 0$ and $\theta_c = 1$ as in the previous experiment, but we varied ψ_1. For the initial data we took

$$u_0(x) = \begin{cases} 1 & \text{if } 0 \le x \le \frac{1}{3} - \frac{1}{20}, \\ 20(\frac{1}{3} - x) & \text{if } |x - \frac{1}{3}| \le \frac{1}{20}, \\ -20|x - \frac{41}{50}| & \text{if } |x - \frac{41}{50}| \le \frac{1}{20}, \\ -1 & \text{otherwise,} \end{cases}$$

with $\gamma = 10^{-3}$, $h = 0.005$, and $\Delta t = 10h^2$.

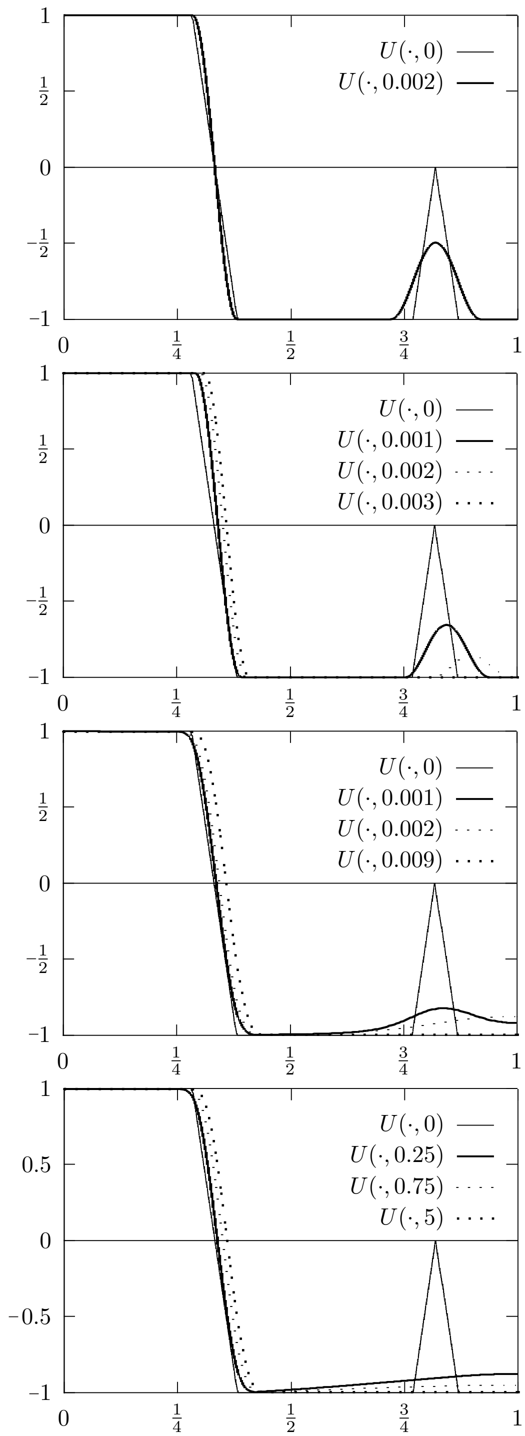

FIG. 5.2. *$U(x,t)$ plotted against x at different times, where Ψ is given by* (1.2) *and* (1.1) *with $\theta = 0.3$ for constant and degenerate mobility.*

In Figure 5.2 the graphs are arranged as follows: the first two rows are for Ψ as given in the previous experiment (the deep quench limit (1.2)), and the last two rows are for $\psi_1(u) = \frac{3}{20}\left[(1+u)\ln\left[\frac{1+u}{2}\right] + (1-u)\ln\left[\frac{1-u}{2}\right]\right]$; the second and third rows are for $b(u) \equiv 1$ (constant mobility) and the first and fourth are for $b(u) := 1 - u^2$ (degenerate mobility). In all cases we took $b_{\max} = b^{n-1} = 1$ and note that the time step restriction of Theorem 3.1, and hence Theorem 2.1, holds. We make the following remarks:

- The algorithm (3.2a–d) with $b_{\max} \equiv b \equiv 1$ is precisely that described in [2] to solve ($\mathrm{P}^{h,\Delta t}$) for n fixed and constant mobility.
- To ensure that our computations were not dependent on h we repeated the experiment with $h = 0.0025$ and obtained graphically indistinguishable pictures.
- For constant mobility, regardless of which Ψ we take the second "bump" gets drawn out to the left rather quickly. This is due to the fact that the mobility is positive in the pure phases, i.e., at points where u is close to the minima of Ψ.
- With $b(u) := 1 - u^2$ and Ψ given by the double obstacle potential (1.2) the second "bump" does not lose "mass." However for the logarithmic Ψ, we observe diffusion through the bulk although the time scale is greatly increased; see [11]. As in the case of the constant mobility the final profile is given by one transition layer. We remark that the minima for the logarithmic potential Ψ are less than one in magnitude. For θ converging to zero the minima converge to ± 1. This implies that the diffusion through the bulk becomes smaller and smaller at low temperatures. Also we note that $|U| < 1$ in the last two rows of Figure 5.2 (the case of the logarithmic potential).

5.2. Two space dimensions.

Experiment 3. We performed two numerical experiments in two spatial dimensions with $\Omega = (0,1) \times (0,1)$. In the first experiment we took degenerate mobility, $b(u) := 1 - u^2$. In the second experiment we took exactly the same data, but now with constant mobility, $b(u) \equiv 1$.

We took a uniform mesh consisting of squares e of length $h = 1/256$, each of which was then subdivided into two triangles by its northeast diagonal. We used the following discrete semi-inner product on $C(\overline{\Omega})$,

$$(\chi_1, \chi_2)^h_\star := \int_\Omega \Pi^h(\chi_1(x)\chi_2(x))\,\mathrm{d}x, \tag{5.3}$$

in place of (2.1). Here Π^h is the piecewise continuous bilinear interpolant on Ω which is affine linear for x_1 (or x_2) fixed and interpolates at the vertices on each square e. Using (5.3) instead of (2.1) only changes the algorithm at the corners of the square Ω and has the advantage that one can then solve (3.5) using "the discrete cosine transform"; see [9]. We note that similarly to (2.8), the induced norm from (5.3) on S^h is equivalent to the standard L^2 norm. Therefore it is easy to adapt the proofs to show that Theorems 2.1, 3.1, and 4.1 in this paper remain true with this choice of discrete semi-inner product.

We took Ψ to be the deep quench limit (1.2) with the splitting $\psi_1(u) \equiv 0$, $\psi_2(u) := \frac{1}{2}(1-u^2)$, and $\theta_c = 0$ (this allows us to take an arbitrarily large time step), $\gamma = 3.2 \times 10^{-4}$, $\Delta t = 1.6 \times 10^{-3}$ and we relaxed our stopping criterion to be $tol = 10^{-6}$. Once again we took $b^{n-1} = 1$.

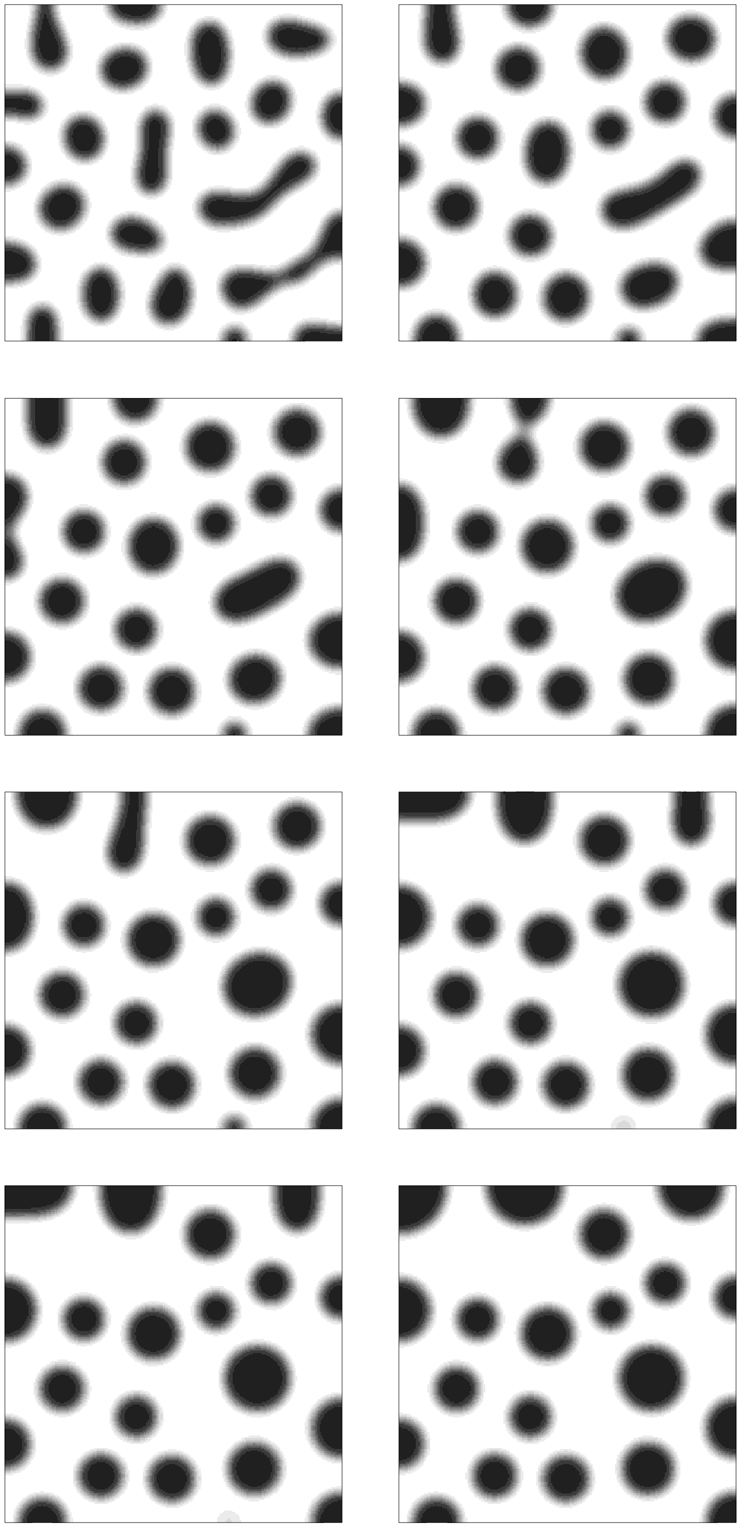

FIG. 5.3. *$U(\cdot, t)$ plotted for $t = 0.04$, 0.08, 0.12, 0.20, 0.24, 0.44, 0.48, and 2.76 when $b(u) := 1 - u^2$ and Ψ is given by* (1.2).

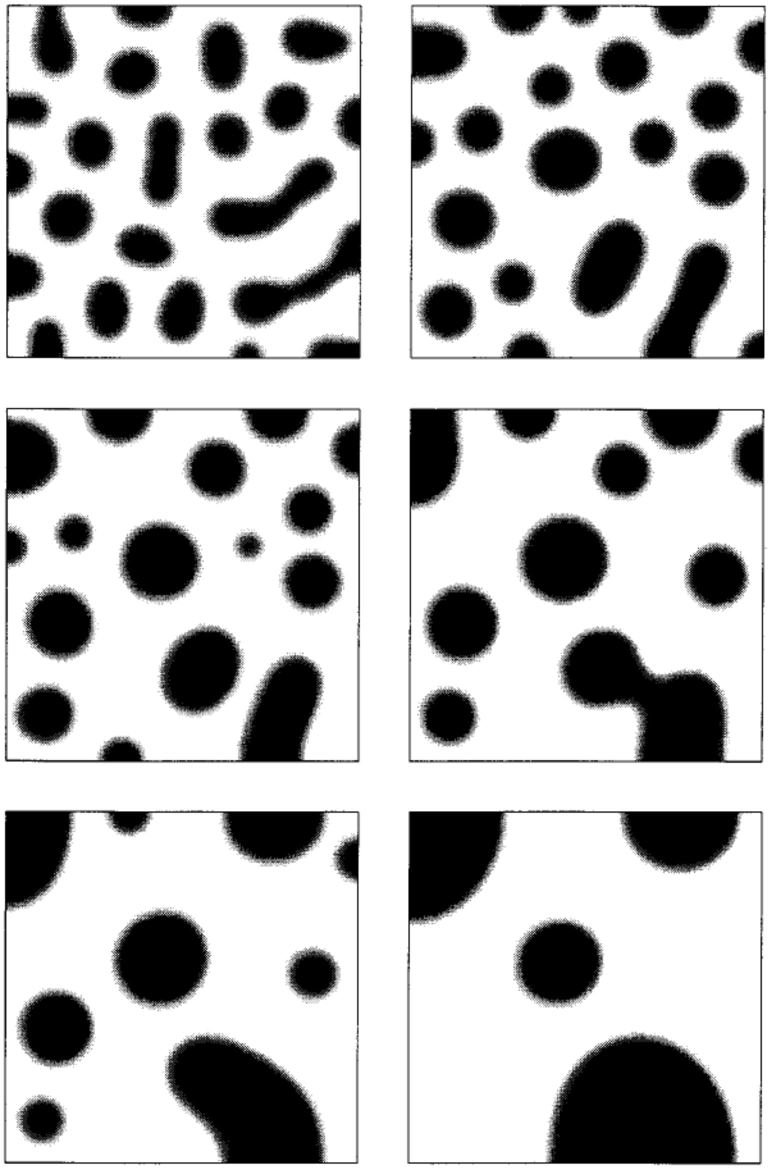

FIG. 5.4. *$U(\cdot, t)$ plotted for $t = 0$, 0.04, 0.08, 0.16, 0.24, and 0.64 when $b(u) \equiv 1$ and Ψ is given by* (1.2).

For the above choices of b, $A^{n,k}$ satisfying (3.3) can be evaluated exactly by sampling at the midpoints of the sides over each triangle κ. The initial data were taken to be $U^0 = -0.4 \pm \delta^h$, where $\delta^h \in S^h$ with $\|\delta^h\|_{0,\infty} \leq 0.05$. In Figures 5.3 and 5.4 we plot a grey scale grid plot of $U(\cdot, t)$ at several times. The pictures are arranged in a matrix format with time increasing to the right in rows then down columns. The grey scale ranges from -0.9 to 0.9 in steps of 0.2 with pure black/white representing values larger/smaller than $0.9/-0.9$. We note that there are approximately 10 mesh points across each interface. The final numerical solution plotted in Figure 5.3 is a stationary numerical solution, that is, the stopping criterion for the iterative procedure is satisfied in a single step from one time level to the next. However, the final picture in Figure 5.4 is not stationary.

In Figure 5.3, the case of degenerate mobility, after the early stages there is very little interaction of regions which do not intersect and the evolution takes place locally where the local mass is preserved. The final frame yields a numerical stationary solution consisting of many circles which do not intersect; this corresponds to a pinning effect reported in [23] for spinodal decomposition of polymer mixtures. In Figure 5.4, the case of constant mobility, we start with $U^0(\cdot) \equiv U(\cdot, 0.04)$ from the first experiment. In contrast, there is evolution and growth of regions which do not intersect (see Figure 5.4); moreover, circles which coexist are not stationary since there is a coupling through bulk terms.

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