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STABILITY AND DISCRETIZATION ERROR ANALYSIS FOR THE CAHN–HILLIARD SYSTEM *VIA* RELATIVE ENERGY ESTIMATES

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Abstract. The stability of solutions to the Cahn–Hilliard equation with concentration dependent mobility with respect to perturbations is studied by means of relative energy estimates. As a by-product of this analysis, a weak-strong uniqueness principle is derived on the continuous level under realistic regularity assumptions on strong solutions. The stability estimates are further inherited almost verbatim by appropriate Galerkin approximations in space and time. This allows to derive sharp bounds for the discretization error in terms of certain projection errors and to establish order-optimal *a priori* error estimates for semi- and fully discrete approximation schemes. Numerical tests are presented for illustration of the theoretical results.

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1. Motivation

The Cahn–Hilliard equation is one of the main mathematical models for describing phase separation phenomena, *e.g.*, in binary alloys [12, 13] or spinodal decomposition of binary fluids [8]. In this paper, we study a system with concentration dependent mobility, given by

$$\partial_t \phi = \operatorname{div}(b(\phi)\nabla\mu) \qquad \text{in } \Omega,\ t>0, \tag{1}$$

$$\mu = -\gamma\Delta\phi + f'(\phi) \qquad \text{in } \Omega,\ t>0, \tag{2}$$

and complemented by appropriate initial and boundary conditions. Here ϕ denotes the phase fraction, μ the chemical potential, $b(\phi)$ the concentration dependent mobility, $\gamma > 0$ the interface parameter, and $f(\phi)$ a double well potential whose minima characterize the favorable mixing ratios.

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The second equation (2) defines the chemical potential $\mu = \delta_\phi \mathcal{E}(\phi)$ as the variational derivative of the associated energy functional

$$\mathcal{E}(\phi) = \int_\Omega \frac{\gamma}{2}|\nabla\phi|^2 + f(\phi), \tag{3}$$

which together with (1) encodes the gradient flow structure of the problem and implies the decay of the energy $\mathcal{E}(\phi)$ along weak solutions. This ensures thermodynamic consistency of the model and allows to establish existence of weak solutions by Galerkin approximation, energy estimates, and compactness arguments. On this basis, existence and regularity of weak solutions for the Cahn–Hilliard equation has been established in [18] for constant mobility and polynomial potential. Logarithmic potentials and concentration dependent mobilities were treated in [5, 15]; we refer to [3, 7, 26] for further results concerning the extension to multi-component systems and multiphysical problems. In recent work [11, 34, 37], we considered logarithmic potentials and concentration dependent mobility functions in the context of models for viscoelastic phase separation.

Many theoretical results about the Cahn–Hilliard equation are based on certain approximations in space and/or time and appropriate energy estimates. Finite element approximations of the fourth-order system resulting after elimination of the chemical potential were analyzed in [18]. A mixed finite element approximation for constant mobilities treating ϕ and μ as separate variables was proposed in [21] and further analyzed in [17, 20]. For extensions to logarithmic potentials and degenerate mobilities, we again refer to [5, 15]. In [27, 28], the analysis of finite element approximations has been extended to study the thin-interface limit $\gamma \to 0$. Apart from finite element methods, alternative discretization schemes, like discontinuous Galerkin methods [31, 33, 40] and Fourier-spectral approximations [32] have been investigated. Extensive research has further been devoted to developing stable second order approximations in time; see [38] for an overview and comparison of different approaches. In a recent paper [16], which is probably closest to our investigations, an unconditionally well-posed fully discrete two-step approximation was proposed and a full error analysis was presented yielding order optimal convergence rates. Quantitative convergence results in most works are derived for the case of constant mobility, which allows to apply arguments of linear theory and to cover the terms stemming from the nonlinearity of the chemical potential f by perturbation arguments.

In this paper, we consider problems with *concentration dependent mobility*, and we utilize genuinely nonlinear arguments, namely *relative energy estimates*, to conduct a quantitative stability and error analysis. Related techniques have been used intensively for the study of nonlinear evolution problems and, more recently, also for the convergence analysis of corresponding discretization methods; see [24, 30] for an introduction to the topic and [23, 25, 29, 35] for convergence and asymptotic analysis for fluid flow problems *via* relative energy estimates. For discretization, we here consider conforming finite element approximations of *second order in space and time*, but our arguments, in principle, also apply to higher order approximations and inexact Galerkin approximations.

We here study the case of nonlinear but non-degenerate parameters, *e.g.*, strictly positive mobility $b(\phi)$ and polynomially bounded double well potential $f(\phi)$, for which one can guarantee existence of smooth solutions which is required for the convergence rate analysis. If one assumes the existence of a smooth solution bounded away from the pure states, these conditions could be further relaxed.

The first basic result of this paper is a formal relative energy estimate which allows to deduce quantitative perturbation bounds for sufficiently regular solutions of (1) and (2). As a by-product of this analysis, we also obtain a weak-strong uniqueness principle and thus a rather general argument for uniqueness. Due to the variational character, these stability estimates are inherited almost verbatim by Galerkin approximations in space and Petrov–Galerkin approximation in time, which is our basic approach towards a systematic error analysis. The structure of the relative energy estimates further provides guidelines for the choice of appropriate projection operators required in the error analysis. The discrete relative energy estimates then allow to estimate the discretization error by more or less standard projection error estimates, which finally leads to optimal convergence rates under minimal and less restrictive smoothness requirements than in previous works. This nonlinear convergence rate analysis can be seen as the main contribution of our manuscript.

Compared to previous works, the main novelty of our approach consists of

(a) the development of a genuinely nonlinear stability and error analysis *via* relative energy estimates, which can be extended to more complex systems;
(b) a concise and rather sharp error analysis of a variational discretization method with order optimal convergence rates under minimal regularity assumptions.

The remainder of the manuscript is organized as follows: In Section 2, we introduce our notation and basic assumptions and recall some results about existence and regularity of solutions. In Section 3, we introduce the relative energy functional and present a formal relative energy estimate which serves as the basis for the following considerations. Furthermore, we will also deduce the weak-strong uniqueness principle in course of the analysis. In Section 4, we study the semi-discretization in space by a mixed finite element method. We will see that the relative energy estimate translates almost verbatim to the semi-discrete setting. This allows us to estimate the difference between the semi-discrete solution and a particular projection of the continuous solution by projection errors and to derive order optimal error convergence rates. In Section 5, we then consider the time discretization by a Petrov–Galerkin approximation, which allows us to extend our arguments almost verbatim to the fully discrete setting. For illustration of our theoretical results, we present some preliminary numerical results in Section 6. Some technical details are provided in the appendix.

2. Notation and preliminary results

Let $L^p(\Omega)$, $W^{k,p}(\Omega)$ be the usual Lebesgue and Sobolev spaces and $\|\cdot\|_{0,p}$, $\|\cdot\|_{k,p}$ the corresponding norms. In the Hilbert space case $p=2$, we write $H^k(\Omega)=W^{k,2}(\Omega)$ and abbreviate $\|\cdot\|_k=\|\cdot\|_{k,2}$. We will sometimes omit the symbol Ω and briefly write L^p for $L^p(\Omega)$, and so on. For ease of presentation, we consider a periodic setting in the following and assume that $\Omega\subset\mathbb{R}^d$ is a hyper cube in dimension $d=2,3$. We then write $H^s_p(\Omega)$, $s\ge 0$, for the space of functions in $H^s(\Omega)$ that can be extended periodically under preservation of class. The corresponding dual spaces are denoted by $H^{-s}_p(\Omega)=H^s_p(\Omega)'$. Note that for $s=0$, we have $H^s_p(\Omega)=H^{-s}_p(\Omega)=L^2_p(\Omega)$, where we identified $L^2(\Omega)$ with its dual space. The norm of the dual spaces are given by

$$\|r\|_{-s}=\sup_{v\in H^s_p(\Omega)}\frac{\langle r,v\rangle}{\|v\|_s}, \tag{4}$$

where $\langle\cdot,\cdot\rangle$ denotes the duality product on $H^{-s}_p(\Omega)\times H^s_p(\Omega)$ for any $s\ge 0$. Note that for functions $u,v\in H^0_p(\Omega)=L^2_p(\Omega)$, we simply have $\langle u,v\rangle=\int_\Omega uv\,\mathrm{d}x$, *i.e.*, for sufficiently regular functions, the duality product can be identified with the scalar product of $L^2(\Omega)$. We further denote by $L^p(a,b;X)$, $W^{k,p}(a,b;X)$, and $H^k(a,b;X)$ the Bochner spaces of appropriately integrable or differentiable functions of time with values in some space X. If $(a,b)=(0,T)$, we also write $L^p(X)$ or $W^{k,p}(X)$ for brevity.

By a periodic weak solution of (1) and (2) on the interval $(0,T)$, we mean a pair

$$\phi\in L^2(0,T;H^3_p(\Omega))\cap H^1(0,T;H^1_p(\Omega)')=:\mathbb{W}(0,T) \tag{5}$$

$$\mu\in L^2(0,T;H^1_p(\Omega))=:\mathbb{Q}(0,T) \tag{6}$$

of functions satisfying the variational identities

$$\langle\partial_t\phi(t),v\rangle+\langle b(\phi(t))\nabla\mu(t),\nabla v\rangle=0, \tag{7}$$

$$\langle\mu(t),w\rangle-\langle\gamma\nabla\phi(t),\nabla w\rangle-\langle f'(\phi(t)),w\rangle=0, \tag{8}$$

for all test functions $v,w\in H^1_p(\Omega)$ and a.a. $0<t<T$. These two identities characterize all sufficiently regular periodic solutions of (1) and (2). The following assumptions on the model parameters will be made:

(A1) $\gamma>0$ is a positive constant;
(A2) $b:\mathbb{R}\to\mathbb{R}_+$ satisfies $b\in C^2(\mathbb{R})$ with $0<b_1\le b(s)\le b_2$, $\|b'\|_\infty\le b_3$, $\|b''\|_\infty\le b_4$;

(A3) $f \in C^4(\mathbb{R})$ such that $f(s), f''(s) \geq -f_1$, for some $f_1 \geq 0$. Furthermore, we assume that f and its derivatives are bounded by $|f^{(k)}(s)| \leq f_2^{(k)} + f_3^{(k)}|s|^{4-k}$ for $0 \leq k \leq 4$ with constants $f_2^{(k)}, f_3^{(k)} \geq 0$.

The growth bounds for f immediately imply that $f(\phi) \in L^1(\Omega)$ for every $\phi \in H^1(\Omega)$. Functions $\phi \in H^1_p(\Omega)$ therefore have bounded energy $\mathcal{E}(\phi) < \infty$.

Remark 1. Here we consider the non-degenerate case with polynomially bounded double well potential $f(\phi)$ and strictly positive mobility function $b(\phi)$. These assumptions allow to prove existence and uniqueness of smooth solutions which is required to establish quantitative convergence rates below. Even in the case of more general potentials and mobilities, we would expect smooth solutions to stay away from the pure states, *i.e.*, from the possible singularities or degeneracies of $f(\cdot)$ and $b(\cdot)$. Validity of the assumptions may then be established by suitable regularization, which is used for the proof of existence in the degenerate case; see *e.g.*, [6, 19].

Under the above assumptions, the existence of periodic weak solutions can be deduced from classical results. For later reference, we make a precise statement.

Lemma 2. *Let (A1)–(A3) hold. Then for any $\phi_0 \in H^1_p(\Omega)$, there exists at least one periodic weak solution (ϕ, μ) of problem (1) and (2) with $\phi(0) = \phi_0$ and satisfying*

$$\int_\Omega \phi(t)\,\mathrm{d}x = \int_\Omega \phi_0\,\mathrm{d}x \qquad \text{and} \qquad \mathcal{E}(\phi(t)) \leq \mathcal{E}(\phi_0) - \int_0^t \mathcal{D}_{\phi(s)}(\mu(s))\,\mathrm{d}s,$$

for a.a. $0 \leq t \leq T$ with $\mathcal{D}_\phi(\mu) = \|b^{1/2}(\phi)\nabla\mu\|_0^2$ the dissipation functional. *If $\phi_0 \in H^k_p(\Omega)$, $1 \leq k \leq 3$ then*

$$\|\phi\|_{L^\infty(H^k_p)} + \|\phi\|_{L^2(H^{k+2}_p)} + \|\partial_t\phi\|_{L^2(H^{k-2}_p)} + \|\mu\|_{L^2(H^k_p)} + \|\mu\|_{L^\infty(H^{k-2}_p)} \leq C_T(\|\phi_0\|_k)$$

with $C_T(\|\phi_0\|_k)$ depending only on the bounds for the coefficients, the domain Ω, the time horizon T, and the bounds for the initial value. In dimension $d = 3$ the estimates $k > 1$ are only valid for sufficiently small T.

Proof. Existence of weak solutions and the *a priori* bounds for $k = 1$ and any time $T > 0$ in dimension $d = 2, 3$ follow from standard arguments; see [4, 6] for similar results under even more general assumptions on the problem data. Conservation of mass and dissipation of energy follow from the variational identities (7) and (8) by formally testing with $(v, w) = (1, 0)$ and $(v, w) = (\mu, \partial_t\phi)$, respectively. Improved regularity and the bounds with $k > 1$, which require a restriction on the maximal time T in dimension $d = 3$, can be obtained by a boot-strap argument and regularity results for the Poisson problem; details are given in Appendix C [8]. ☐

Remark 3. From the estimates of Lemma 2 and the embedding theorem for Bochner spaces, see *e.g.*, Chapter 25 of [39], one can see that weak solutions (ϕ, μ) are continuous functions of time, *e.g.*, $\phi_0 \in H^3_p(\Omega)$, we have

$$(\phi, \mu) \in C([0, T]; H^3_p(\Omega) \times H^1_p(\Omega)), \tag{9}$$

and hence ϕ is uniformly bounded on $\Omega \times (0, T)$. This will be used in Section 4 below.

3. A stability estimate and uniqueness

As a first step of our analysis, we study the stability of periodic weak solutions (ϕ, μ) of the system (1) and (2) with respect to perturbations. Let $(\hat\phi, \hat\mu)$ be a pair of sufficiently regular functions. Then

$$\langle \partial_t\hat\phi(t), v\rangle + \langle b(\phi(t))\nabla\hat\mu(t), \nabla v\rangle =: \langle \hat r_1(t), v\rangle, \tag{10}$$

$$\langle \hat\mu(t), w\rangle - \langle \gamma\nabla\hat\phi(t), \nabla w\rangle - \langle f'(\hat\phi(t)), w\rangle =: \langle \hat r_2(t), w\rangle, \tag{11}$$

for all $v, w \in H^1_p(\Omega)$ and a.a. $0 < t < T$, defines two residual functionals $\hat r_1(t), \hat r_2(t)$. The functions $(\hat\phi, \hat\mu)$ can be understood as solutions of the perturbed variational problem (10) and (11) for given right-hand sides $\hat r_1, \hat r_2$.

Remark 4. Note that a term $b(\phi)$ appears in (10) which explicitly depends on the solution ϕ of (1) and (2). Equation (10) therefore includes some sort of linearization around ϕ which greatly simplifies the proofs.

3.1. Stability *via* relative energy

To measure the difference between a solution (ϕ, μ) of (7) and (8) and a solution $(\hat{\phi}, \hat{\mu})$ of the perturbed problem (10) and (11), we utilize a regularized *relative energy* functional

$$\mathcal{E}_\alpha(\phi|\hat{\phi}) := \mathcal{E}(\phi) - \mathcal{E}(\hat{\phi}) - \langle \mathcal{E}'(\hat{\phi}), \phi - \hat{\phi}\rangle + \tfrac{\alpha}{2}\|\phi - \hat{\phi}\|^2 \tag{12}$$

with regularization parameter

(A4) $\alpha = \gamma + f_1$,

where $-f_1$ is the constant in the lower bound for f'' from assumption (A3). This implies that the regularized energy functional $\mathcal{E}_\alpha(\phi) = \mathcal{E}(\phi) + \frac{\alpha}{2}\|\phi\|_0^2$ becomes strictly convex such that $\mathcal{E}_\alpha(\phi|\hat{\phi})$ amounts to the associated Bregman divergence [9]. Moreover, the norm distance of two functions can be bounded by the relative energy.

Lemma 5. *Let (A1)–(A4) hold. Then*

$$\frac{\gamma}{2}\|\phi - \hat{\phi}\|_1^2 \leq \mathcal{E}_\alpha(\phi|\hat{\phi}) \leq \Gamma(1 + \|\phi\|_1^2 + \|\hat{\phi}\|_1^2)\|\phi - \hat{\phi}\|_1^2, \tag{13}$$

for all functions $\phi, \hat{\phi} \in H_p^1(\Omega)$ with uniform constant $\Gamma = \Gamma(f_2^{(2)}, f_3^{(2)}, \Omega)$.

Proof. For $g(x) = |x|^2$, one has $g(x|\hat{x}) = g(x) - g(\hat{x}) - \langle g'(\hat{x}), (x - \hat{x})\rangle = |x - \hat{x}|^2$ which allows to handle the quadratic contributions. It thus suffices to consider the nonlinear terms in $\mathcal{E}_\alpha(\phi|\hat{\phi})$. The lower bound then follows directly from noting that

$$\int_\Omega f(\phi|\hat{\phi})\,\mathrm{d}x \geq -\frac{f_1}{2}\|\phi - \hat{\phi}\|_0^2$$

and the particular choice of α. For the upper bound, we use the growth bounds for f, which shows that

$$\begin{aligned}
\int_\Omega f(\phi|\hat{\phi})\,\mathrm{d}x &= \int_\Omega \int_0^1 f''(s\phi + (1-s)\hat{\phi})\,\mathrm{d}s\,(\phi - \hat{\phi})^2\,\mathrm{d}x \\
&\leq \int_\Omega (f_2^{(2)} + f_3^{(2)}(|\phi|^2 + |\hat{\phi}|^2))|\phi - \hat{\phi}|^2\,\mathrm{d}x \\
&\leq f_2^{(2)}\|\phi - \hat{\phi}\|_0^2 + f_3^{(2)}(\|\phi\|_{0,4}^2 + \|\hat{\phi}\|_{0,4}^2)\|\phi - \hat{\phi}\|_{0,4}^2.
\end{aligned}$$

In the last step, we simply used Hölder's inequality, and by embedding of H^1 into L^4, we may estimate $\|\phi\|_{0,4} \leq C(\Omega)\|\phi\|_1$, which yields the required upper bound. $\square$

Using the specific problem structure and basic manipulation, we can now derive the following stability estimate which will be the basis for our further considerations.

Theorem 6. *Let (A1)–(A4) hold and $(\phi, \mu) \in \mathbb{W}(0,T) \times \mathbb{Q}(0,T)$ denote a periodic weak solution of (1) and (2). Furthermore, let $\hat{\phi} \in \mathbb{W}(0,T) \cap W^{1,1}(0,T; L^2(\Omega))$ and $\hat{\mu} \in \mathbb{Q}(0,T)$ be given and $(\hat{r}_1, \hat{r}_2)$ be defined by (10) and (11). Then*

$$\mathcal{E}_\alpha(\phi(t)|\hat{\phi}(t)) + \int_0^t \mathcal{D}_{\phi(s)}(\mu(s)|\hat{\mu}(s))\,\mathrm{d}s \leq e^{c(t)}\mathcal{E}_\alpha(\phi(0)|\hat{\phi}(0)) + Ce^{c(t)}\int_0^t \|\hat{r}_1(s)\|_{-1}^2 + \|\hat{r}_2(s)\|_1^2\,\mathrm{d}s \tag{14}$$

with relative dissipation functional $\mathcal{D}_\phi(\mu|\hat\mu) = \frac{1}{2}\|b^{1/2}(\phi)\nabla(\mu-\hat\mu)\|_0^2$, *parameter* $c(t) = c_0 t + c_1\int_0^t \|\partial_t\hat\phi(s)\|_0\,\mathrm{d}s$, *and constants* c_0, c_1, C *depending only on the domain* Ω *and the uniform bounds for the functions* (ϕ,μ) *and* $(\hat\phi,\hat\mu)$ *in* $L^\infty(H^1)\times L^2(H^1)$.

Proof. For ease of presentation, we assume for the moment that (ϕ,μ) and $(\hat\phi,\hat\mu)$ are sufficiently regular, such that all computations in the following are justified. The general case can then be deduced by a density argument; details are given in the appendix. Formal differentiation of the relative energy with respect to time yields

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}_\alpha(\phi|\hat\phi) &= \langle\mathcal{E}'_\alpha(\phi),\partial_t\phi\rangle - \langle\mathcal{E}'_\alpha(\hat\phi),\partial_t\hat\phi\rangle - \langle\mathcal{E}'_\alpha(\hat\phi),\partial_t\phi-\partial_t\hat\phi\rangle - \langle\mathcal{E}''_\alpha(\hat\phi)\partial_t\hat\phi,\phi-\hat\phi\rangle\\ &= \langle\mathcal{E}'_\alpha(\phi)-\mathcal{E}'_\alpha(\hat\phi),\partial_t\phi-\partial_t\hat\phi\rangle + \langle\mathcal{E}'_\alpha(\phi)-\mathcal{E}'_\alpha(\hat\phi)-\mathcal{E}''_\alpha(\hat\phi)(\phi-\hat\phi),\partial_t\hat\phi\rangle.\end{aligned}$$

From the definition of the relative energy $\mathcal{E}_\alpha$ and using the variational identities (7), (8) and (10), (11), which are satisfied by the functions (ϕ,μ) and $(\hat\phi,\hat\mu)$, we get

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}_\alpha(\phi|\hat\phi) &= \gamma\langle\nabla\phi-\nabla\hat\phi,\nabla\partial_t\phi-\nabla\partial_t\hat\phi\rangle + \langle f'(\phi)-f'(\hat\phi),\partial_t\phi-\partial_t\hat\phi\rangle\\ &\quad+\alpha\langle\phi-\hat\phi,\partial_t\phi-\partial_t\hat\phi\rangle + \langle f'(\phi)-f'(\hat\phi)-f''(\hat\phi)(\phi-\hat\phi),\partial_t\hat\phi\rangle\\ &= \langle\mu-\hat\mu+\hat r_2,\partial_t\phi-\partial_t\hat\phi\rangle + \alpha\langle\phi-\hat\phi,\partial_t\phi-\partial_t\hat\phi\rangle + \langle f'(\phi)-f'(\hat\phi)-f''(\hat\phi)(\phi-\hat\phi),\partial_t\hat\phi\rangle\\ &= -\langle b(\phi)\nabla(\mu-\hat\mu),\nabla(\mu-\hat\mu+\hat r_2)\rangle - \langle r_1,\mu-\hat\mu+\hat r_2\rangle - \alpha\langle b(\phi)\nabla(\mu-\hat\mu),\nabla(\phi-\hat\phi)\rangle - \alpha\langle r_1,\phi-\hat\phi\rangle\\ &\quad+\langle f'(\phi)-f'(\hat\phi)-f''(\hat\phi)(\phi-\hat\phi),\partial_t\hat\phi\rangle\\ &= \text{(i)} + \text{(ii)} + \text{(iii)} + \text{(iv)} + \text{(v)}.\end{aligned}$$

We can now estimate the individual terms separately. Before we proceed, let us note that by the energy bounds for weak solutions (ϕ,μ), Lemma 2, and by the assumptions on $\hat\phi$ in the statement of Theorem 6, we know that

$$\|\phi\|_{L^\infty(H^1)} \le C(\|\phi_0\|_1) \quad\text{and}\quad \|\hat\phi\|_{L^\infty(H^1)}, \|\partial_t\hat\phi\|_{L^1(L^2)} \le \hat C. \tag{15}$$

Using Hölder's and Young's inequalities, we can then bound

$$\text{(i)} = -\|b^{1/2}(\phi)\nabla(\mu-\hat\mu)\|_0^2 + \langle b(\phi)\nabla(\mu-\hat\mu),\nabla\hat r_2\rangle \le -(2-2\delta)\mathcal{D}_\phi(\mu|\hat\mu) + C(\delta,b_2)\|\hat r_2\|_1^2,$$

with $\delta>0$ arbitrary, constant $C(\delta,b_2) = b_2/(4\delta)$, and b_2 denoting the upper bound for the function b in assumption (A2). By definition of the dual norm, a Poincaré inequality, and the bounds for the coefficients, the second term can be estimated by

$$\begin{aligned}\text{(ii)} &\le \|\hat r_1\|_{-1}(\|\mu-\hat\mu\|_1 + \|\hat r_2\|_1)\\ &\le \|\hat r_1\|_{-1}(C(\Omega)|\langle\mu-\hat\mu,1\rangle| + C(\Omega,b_1)\|b^{1/2}(\phi)\nabla(\mu-\hat\mu)\|_0 + \|\hat r_2\|_1)\\ &\le C(\Omega,b_1,\delta)\|\hat r_1\|_{-1}^2 + |\langle\mu-\hat\mu,1\rangle|^2 + 2\delta\,D_\phi(\mu|\hat\mu) + \|\hat r_2\|_1^2.\end{aligned}$$

In the last step, we utilized Young's inequality to separate the factors with the same parameter $\delta>0$ as before. For the second term on the right-hand side, we can use the identities (8) and (11) with $w=1$, which leads to

$$|\langle\mu-\hat\mu,1\rangle| = |\langle f'(\phi)-f'(\hat\phi)+\hat r_2,1\rangle| \le \|\hat r_2\|_{0,1} + \|f'(\phi)-f'(\hat\phi)\|_{0,1}.$$

From the bounds for the potential f in assumption (A3), we can further deduce that

$$|f'(\phi)-f'(\hat\phi)| = |\int_0^1 f''(\hat\phi+s(\phi-\hat\phi))\,\mathrm{d}s(\phi-\hat\phi)| \le (f_2^{(2)} + f_3^{(2)}(|\phi|+|\hat\phi|)^2)|\phi-\hat\phi|.$$

An application of Hölder's inequality, the norm estimates for the continuous embedding of $H^1(\Omega)$ into $L^p(\Omega)$, and the uniform bounds for ϕ, $\hat\phi$ in (15), then lead to

$$\begin{aligned}\|f'(\phi)-f'(\hat\phi)\|_{0,1} &\le C(\Omega)(f_2^{(2)}+2f_3^{(2)}(\|\phi\|_{0,6}^2+\|\hat\phi\|_{0,6}^2))\|\phi-\hat\phi\|_{0,6}\\ &\le C(\Omega,f_2^{(2)},f_3^{(2)},\|\phi_0\|_1,\|\hat\phi\|_{L^\infty(H^1)})\|\phi-\hat\phi\|_1.\end{aligned}$$

Using $\|\hat r_2\|_{0,1}\le C(\Omega)\|\hat r_2\|_1$ and the lower bound (13) for the relative energy, we get

$$\text{(ii)}\le 2\delta\,\mathcal{D}_\phi(\mu|\hat\mu)+C(\Omega,b_1,\delta)\|r_1\|_{-1}^2+C(\Omega)\|\hat r_2\|_1^2+C(\Omega,f_2^{(2)},f_3^{(2)},\|\phi_0\|_1,\|\hat\phi\|_{L^\infty(H^1)},\gamma)\,\mathcal{E}_\alpha(\phi|\hat\phi).$$

Condition (13) further allows us to estimate

$$\text{(iii)}+\text{(iv)}\le 2\delta\,\mathcal{D}_\phi(\mu|\bar\mu)+C(\delta,b_2,\alpha,\gamma)\mathcal{E}_\alpha(\phi|\hat\phi)+C(\alpha)\|r_1\|_{-1}^2.$$

From the bounds in assumption (A3), we can deduce that

$$|f'(\phi)-f'(\hat\phi)-f''(\hat\phi)(\phi-\hat\phi)|\le (f_2^{(3)}+f_3^{(3)}(|\phi|+|\hat\phi|))|\phi-\hat\phi|^2.$$

Using Hölders inequality, embedding estimates, and the uniform bounds in (15), we can further bound the fifth term in the above estimate by

$$\begin{aligned}\text{(v)}&\le\|\partial_t\hat\phi\|_0\|f'(\phi)-f'(\hat\phi)-f''(\hat\phi)(\phi-\hat\phi)\|_0\le\|\partial_t\hat\phi\|_0(f_2^{(3)}+f_3^{(3)}(\|\phi\|_{0,6}+\|\hat\phi\|_{0,6}))\|\phi-\hat\phi\|_{0,6}^2\\ &\le C(\Omega,f_2^{(3)},f_3^{(3)},\|\phi_0\|_1,\|\hat\phi\|_{L^\infty(H^1)},\gamma)\|\partial_t\hat\phi\|_0\,\mathcal{E}_\alpha(\phi|\hat\phi).\end{aligned}$$

By combination of the individual estimates and choosing $\delta=1/6$, we finally obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}_\alpha(\phi|\hat\phi)\le-\mathcal{D}_\phi(\mu|\hat\mu)+(c_0+c_1\|\partial_t\hat\phi\|_0)\mathcal{E}_\alpha(\phi|\hat\phi)+C_2\|\hat r_1\|_{-1}^2+C_3\|\hat r_2\|_1^2,$$

with constants c_0,c_1, C_2, C_3 depending only on the bounds for the coefficients, the domain, and the bounds for $\|\phi_0\|_1$ and $\|\hat\phi\|_{L^\infty(H^1)}$. An application of Gronwall's inequality (A.1) with $v(t)=\mathcal{E}_\alpha(\phi(t)|\hat\phi(t))$, $g(t)=-\mathcal{D}_{\phi(t)}+C_2\|\hat r_1(t)\|_{-1}+C_3\|\hat r_2(t)\|_1$, and $\lambda(t)=c_0+c_1\|\partial_t\hat\phi(t)\|_0$, which is integrable since $\partial_t\hat\phi\in L^1(L^2)$, then leads to the stability estimate of the theorem with $c=c_0T+c_1\hat C$ and $C=\max\{C_2,C_3\}$. □

Remark 7. The lower bound (13) for the relative energy, and the estimate

$$\frac{b_1}{2}\|\nabla\mu-\nabla\hat\mu\|_0^2\le\mathcal{D}_\phi(\mu|\hat\mu), \tag{16}$$

for the relative dissipation immediately lead to the bounds

$$\|\phi-\hat\phi\|_{L^\infty(H^1)}^2+\|\mu-\hat\mu\|_{L^2(H^1)}^2\le C_1\mathcal{E}_\alpha(\phi(0)|\hat\phi(0))+C_2(\|\hat r_1\|_{L^2(H_p^{-1})}^2+\|\hat r_2\|_{L^2(H^1)}^2)$$

for the error. With similar arguments as used for the estimate of the term (ii), we can also bound the full norm $\|\mu-\hat\mu\|_{L^2(H_p^1)}$. The stability estimate thus provides perturbation bounds in the natural norms for the problem.

3.2. A weak-strong uniqueness principle

As a direct consequence of Theorem 6, one can see that sufficiently regular weak solutions of (1) and (2) depend stably on perturbations in the problem parameters and the initial data. Another consequence of Theorem 6 is the following weak-strong uniqueness principle.

Theorem 8. *Let $(\hat{\phi}, \hat{\mu})$ be a periodic weak solution of (1) and (2) with regularity $\hat{\phi} \in W^{1,1}(0,T;L^2(\Omega))$ and $\hat{\mu} \in L^2(0,T;W_p^{1,3}(\Omega))$. Then no other weak solution (ϕ,μ) with the same initial value $\phi(0) = \hat{\phi}(0)$ exists.*

Proof. Let (ϕ,μ) be a weak solution with the same initial values $\phi(0) = \hat{\phi}(0)$. Then $(\hat{\phi},\hat{\mu})$ can be seen to solve (10) and (11) with residuals

$$\langle \hat{r}_1, v\rangle = \langle (b(\phi) - b(\hat{\phi}))\nabla\hat{\mu}, \nabla v\rangle \quad \text{and} \quad \hat{r}_2 = 0,$$

and the first residual can be further estimated by

$$\begin{aligned}\int_0^t \|\hat{r}_1(s)\|_{-1}^2 \,\mathrm{d}s &\le \int_0^t \|(b(\phi(s)) - b(\hat{\phi}(s)))\nabla\hat{\mu}(s)\|_0^2 \,\mathrm{d}s \le C(b_3)\int_0^t \|\phi(s) - \hat{\phi}(s)\|_{0,6}^2 \|\nabla\hat{\mu}(s)\|_{0,3}^2 \,\mathrm{d}s \\ &\le C(b_3,\gamma,\Omega)\int_0^t \|\nabla\hat{\mu}(s)\|_{0,3}^2 \mathcal{E}(\phi(s)|\hat{\phi}(s)) \,\mathrm{d}s.\end{aligned}$$

By assumption on the initial values, we have $\mathcal{E}_\alpha(\phi(0)|\hat{\phi}(0)) = 0$, and the estimate of Theorem 6 thus leads to

$$\mathcal{E}_\alpha(\phi(t)|\hat{\phi}(t)) + \int_0^t \mathcal{D}_{\phi(s)}(\mu(s)|\hat{\mu}(s)) \,\mathrm{d}s \le C(T)\int_0^t \|\nabla\hat{\mu}(s)\|_{0,3}^2 \mathcal{E}(\phi(s)|\hat{\phi}(s)) \,\mathrm{d}s.$$

Since $\|\nabla\hat{\mu}(t)\|_{0,3}^2 \in L^1(0,T)$, we can use the Gronwall inequality (A.1) to see that $\mathcal{E}_\alpha(\phi(t)|\hat{\phi}(t)) \le 0$ for $0 \le t \le T$, which together with Lemma 5 yields the claim. □

Remark 9. Note that for regular initial values, *e.g.*, $\hat{\phi}(0) = \phi_0 \in H_p^2(\Omega)$, the existence of a weak solution $(\hat{\phi},\hat{\mu})$ with the required regularity follows from Lemma 2. In that case, we therefore obtain a unique weak solution.

4. Galerkin semi-discretization

We now turn to the systematic discretization in space, for which we consider a Galerkin approximation of the variational principle (7) and (8) with *second order* conforming finite elements. As will become clear from our analysis, higher order and non-conforming approximations could be treated with similar arguments.

Let $\mathcal{T}_h$ be geometrically conforming partition of $\Omega \subset \mathbb{R}^d$, $d = 2, 3$ into triangles or tetrahedra [14, 22]. We denote by ρ_K and h_K the inner-circle radius and diameter of the element $K \in \mathcal{T}_h$ and call $h = \max_{K\in\mathcal{T}_h} h_K$ the global mesh size. We assume that $\mathcal{T}_h$ is quasi-uniform, *i.e.*, there exists a constant $\sigma > 0$ such that $\sigma h \le \rho_N \le h_N \le h$ for all $K \in \mathcal{T}_h$, and that $\mathcal{T}_h$ is periodic in the sense that it can be extended periodically to periodic extensions of the domain Ω. We then denote by

$$\mathcal{V}_h := \{v \in H_p^1(\Omega) : v|_K \in P_2(K) \quad \forall K \in \mathcal{T}_h\},$$

the space of continuous periodic piecewise quadratic polynomials over the mesh $\mathcal{T}_h$. We further introduce the approximation spaces

$$\mathbb{W}_h(0,T) := H^1(0,T;\mathcal{V}_h) \quad \text{and} \quad \mathbb{Q}_h(0,T) := L^2(0,T;\mathcal{V}_h).$$

The semi-discrete approximation for (7) and (8) now reads as follows.

Problem 10. *Let $\phi_{0,h} \in \mathcal{V}_h$ be given. Find $(\phi_h,\mu_h) \in \mathbb{W}_h(0,T)\times\mathbb{Q}_h(0,T)$ such that $\phi_h(0) = \phi_{0,h}$ and such that for all $v_h, w_h \in \mathcal{V}_h$ and all $0 \le t \le T$, there holds*

$$\langle \partial_t\phi_h(t), v_h\rangle + \langle b(\phi_h(t))\nabla\mu_h(t), \nabla v_h\rangle = 0, \tag{17}$$

$$\langle \mu_h(t), w_h\rangle - \langle \gamma\nabla\phi_h(t), \nabla w_h\rangle - \langle f'(\phi_h(t)), w_h\rangle = 0. \tag{18}$$

Before we turn to a detailed stability and error analysis, let us briefly summarize some basic properties of this discretization strategy.

Lemma 11. *Let (A1)–(A3) hold. Then for any initial value $\phi_{0,h} \in \mathcal{V}_h$, Problem 10 has a unique solution (ϕ_h, μ_h). Moreover, for all $0 \le t \le T$, one has $\int_\Omega \phi_h(t)\,\mathrm{d}x = \int_\Omega \phi_{0,h}\,\mathrm{d}x$ and $\mathcal{E}(\phi_h(t)) + \int_0^t \mathcal{D}_{\phi_h}(\mu_h)\,\mathrm{d}s = \mathcal{E}(\phi_{0,h})$.*

Proof. Using our assumptions (A1)–(A3), the existence of a unique discrete solution $(\phi_h, \mu_h) \in C^1(0,T;\mathcal{V}_h) \times C^0(0,T;\mathcal{V}_h)$ can be deduced from the Picard-Lindelöf theorem. Conservation of mass and dissipation of energy then follow with similar arguments as on the continuous level, *i.e.*, by testing the equations (17) and (18) with $(v_h, w_h) = (1, 0)$ and $(v_h, w_h) = (\mu_h, \partial_t \phi_h)$, respectively. $\square$

4.1. Semi-discrete stability estimate

With similar arguments as on the continuous level, we now establish stability of the semi-discrete solution with respect to perturbations. For a given pair of functions $(\hat\phi_h, \hat\mu_h) \in \mathbb{W}_h(0,T) \times \mathbb{Q}_h(0,T)$, we define semi-discrete residuals $(\hat r_{1,h}, \hat r_{2,h}) \in L^2(0,T;\mathcal{V}_h \times \mathcal{V}_h)$ by the variational identities

$$\langle \partial_t \hat\phi_h(t), v_h\rangle + \langle b(\phi_h(t))\nabla\hat\mu_h(t), \nabla v_h\rangle =: \langle \hat r_{1,h}(t), v_h\rangle, \tag{19}$$

$$\langle \hat\mu_h(t), w_h\rangle - \langle \gamma\nabla\hat\phi_h(t), \nabla w_h\rangle - \langle f'(\hat\phi_h(t)), w_h\rangle =: \langle \hat r_{2,h}(t), w_h\rangle, \tag{20}$$

for all $v_h, w_h \in \mathcal{V}_h$ and $0 \le t \le T$. The functions $(\hat\phi_h, \hat\mu_h)$ can again be understood as solutions of a perturbed semi-discrete problem. With almost identical arguments as used in the proof of Theorem 6, we now obtain the following stability estimate.

Lemma 12. *Let (A1)–(A4) hold and $(\phi_h, \mu_h) \in \mathbb{W}_h(0,T) \times \mathbb{Q}_h(0,T)$ be a solution of Problem 10. Further, let $(\hat\phi_h, \hat\mu_h) \in \mathbb{W}_h(0,T) \times \mathbb{Q}_h(0,T)$ be given and $(\hat r_{1,h}, \hat r_{2,h})$ denote the corresponding residuals defined by (19) and (20). Then the estimate*

$$\begin{aligned}\mathcal{E}_\alpha(\phi_h(t)|\hat\phi_h(t)) &+ \int_0^t \mathcal{D}_{\phi_h(s)}(\mu_h(s)|\hat\mu_h(s))\,\mathrm{d}s \\ &\le e^{c(t)}\mathcal{E}_\alpha(\phi_h(0)|\hat\phi_h(0)) + Ce^{c(t)}\int_0^t \|\hat r_{1,h}(s)\|_{-1,h}^2 + \|\hat r_{2,h}(s)\|_1^2\,\mathrm{d}s\end{aligned} \tag{21}$$

holds for a.a $0 \le t \le T$ with $c(t) = c_0 t + c_1\int_0^t \|\partial_t\hat\phi_h\|_0\,\mathrm{d}s$ and c_0, c_1, C depending on the uniform $L^\infty(H^1) \times L^2(H^1)$ bounds for (ϕ_h, μ_h) and $(\hat\phi_h, \hat\mu_h)$, respectively, and

$$\|\hat r\|_{-1,h} = \sup_{v_h \in \mathcal{V}_h} \frac{(\hat r, v_h)}{\|v_h\|_1} \le \|\hat r\|_{-1} \tag{22}$$

denoting the discrete-dual norm.

The assertion follows with the very same arguments as used in the proof of Theorem 6; details are left to the reader. Lemma 12 allows to investigate the stability of the semi-discrete solution (ϕ_h, μ_h) with respect to perturbations in the problem data. By choosing $(\hat\phi_h, \hat\mu_h)$ as a particular discrete approximation for the solution (ϕ, μ) of (1) and (2), we will be able to derive quantitative error estimates for the semi-discrete approximation.

4.2. Auxiliary results

We start by introducing some projection operators and recall the corresponding error estimates. Let $\pi_h^0 : H_p^1(\Omega) \to \mathcal{V}_h$ denote the L^2-orthogonal projection which is characterized by

$$\langle \pi_h^0 u - u, v_h\rangle = 0 \qquad \forall v_h \in \mathcal{V}_h. \tag{23}$$

By definition, π_h^0 is a contraction in $L^2(\Omega)$ and on quasi-uniform meshes

$$\|u - \pi_h^0 u\|_s \leq Ch^{r-s}\|u\|_r \tag{24}$$

for all $-1 \leq s \leq r$ and $0 \leq r \leq 3$; see [10]. We further make use of the H^1-elliptic projection $\pi_h^1 : H_p^1(\Omega) \to \mathcal{V}_h$, which is characterized by the variational problem

$$\langle \nabla(\pi_h^1 u - u), \nabla v_h \rangle + \langle \pi_h^1 u - u, v_h \rangle = 0 \qquad \forall v_h \in \mathcal{V}_h. \tag{25}$$

By standard finite element error analysis and duality arguments, one can show that

$$\|u - \pi_h^1 u\|_s \leq Ch^{r-s}\|u\|_r, \tag{26}$$

for all $-1 \leq s \leq r$ and $1 \leq r \leq 3$; see again [10] for details. Since we assumed quasi-uniformity of the simplicial mesh $\mathcal{T}_h$, we can further use inverse inequalities

$$\|v_h\|_1 \leq c_{inv} h^{-1}\|v_h\|_0 \quad \text{and} \quad \|v_h\|_{0,p} \leq c_{inv} h^{d/p-d/q}\|v_h\|_{0,q} \tag{27}$$

which hold for all functions $v_h \in \mathcal{V}_h$ and all $1 \leq q \leq p \leq \infty$ in dimension d. By combining the previous estimates, one can further see that

$$\|\pi_h^1 u\|_{0,\infty} \leq C\|u\|_2 \tag{28}$$

in dimension $d \leq 3$. Let us note that all estimates also hold in dimension one, *i.e.*, for piecewise polynomial approximations in time.

4.3. Projection error estimates

Let (ϕ, μ) be a periodic weak solution of the system (1) and (2). We then define $\hat{\phi}_h(t) = \pi_h^1 \phi(t) \in \mathcal{V}_h$, $0 \leq t \leq T$, as the H^1-elliptic projection, and $\hat{\mu}_h(t) \in \mathcal{V}_h$ by solving the elliptic variational problems

$$\langle \hat{\mu}_h(t) - \mu(t), w_h \rangle = \gamma \langle \nabla \hat{\phi}_h(t) - \nabla \phi(t), \nabla w_h \rangle + \langle f'(\hat{\phi}_h(t)) - f'(\phi(t)), w_h \rangle \tag{29}$$

for all $w_h \in \mathcal{V}_h$ and all $0 \leq t \leq T$. This problem is linear in $\hat{\mu}_h$ and finite-dimensional, hence existence of a unique solution follows directly. For this choice of approximations $(\hat{\phi}_h, \hat{\mu}_h)$, we have the following error estimates.

Lemma 13. *Let (A1)–(A3) hold, (ϕ, μ) be a periodic weak solution of (1) and (2) with regular initial value $\phi(0) \in H_p^3(\Omega)$, and let $\hat{\phi}_h$, $\hat{\mu}_h$ be defined as above. Then*

$$\begin{aligned}
\|\phi(t) - \hat{\phi}_h(t)\|_1 &\leq Ch^2\|\phi(t)\|_3, \\
\|\partial_t \phi(t) - \partial_t \hat{\phi}_h(t)\|_{-1,h} &\leq Ch^2\|\partial_t \phi(t)\|_1, \\
\|\mu(t) - \hat{\mu}_h(t)\|_1 &\leq C' h^2(\|\mu(t)\|_3 + \|\phi(t)\|_3),
\end{aligned}$$

for a.a. $0 \leq t \leq T$ with $C = C(\Omega, \sigma)$ and $C' = C'(\Omega, \sigma, \gamma, f_2^{(2)}, f_3^{(2)}, C_T(\|\phi_0\|_3))$.

Proof. The estimates for $\phi - \hat{\phi}_h$ and $\partial_t \phi - \partial_t \hat{\phi}_h$ follow directly from (26). We then use the triangle inequality to split the error in the chemical potential into

$$\|\hat{\mu}_h - \mu\|_1 \leq \|\hat{\mu}_h - \pi_h^0 \mu\|_1 + \|\pi_h^0 \mu - \mu\|_1.$$

With the help of (24) the last term can be estimated by $\|\pi_h^0 \mu - \mu\|_1 \leq Ch^2\|\mu\|_3$. By the inverse inequalities (27), the discrete error can be bounded by

$$\|\hat{\mu}_h - \pi_h^0 \mu\|_1 \leq C_\sigma h^{-1}\|\hat{\mu}_h - \pi_h^0 \mu\|_0,$$

and for the error in the L^2-norm, we can deduce from (23) that

$$\|\hat\mu_h - \pi_h^0\mu\|_0^2 = (\hat\mu_h - \pi_h^0\mu, \hat\mu_h - \pi_h^0\mu) = (\hat\mu_h - \mu, \hat\mu_h - \pi_h^0\mu),$$

since $w_h = \hat\mu_h - \pi_h^0\mu \in \mathcal{V}_h$. We can then use (29) with this test function w_h, to get

$$\begin{aligned}(\hat\mu_h - \hat\mu, w_h) &= \gamma(\nabla(\hat\phi_h - \phi), \nabla w_h) + (f'(\hat\phi_h) - f'(\phi), w_h)\\ &= \gamma(\phi - \hat\phi_h, w_h) + (f'(\hat\phi_h) - f'(\phi), w_h),\end{aligned}$$

where we used the particular choice of $\hat\phi_h = \pi_h^1\phi$ and (25), to replace the gradient term in the second step. Proceeding with standard arguments, we then obtain

$$\begin{aligned}(\hat\mu_h - \hat\mu, w_h) &\le \gamma\|\phi - \hat\phi_h\|_0\|w_h\|_0 + \|f'(\hat\phi_h) - f'(\phi)\|_0\|w_h\|_0\\ &\le C(f_2^{(2)}, f_3^{(2)}, C_T, \Omega)\|\hat\phi_h - \phi\|_0\|w_h\|_0.\end{aligned}$$

For the nonlinear term, we here used the mean value theorem and the polynomial bounds for f'' as well as $\|\phi\|_{0,\infty} + \|\hat\phi_h\|_{0,\infty} \le C\|\phi\|_2$. In summary, we thus obtain

$$\|\hat\mu_h - \mu\|_1 \le Ch^2(\|\mu\|_3 + \|\phi\|_3),$$

with constant C independent of the mesh size and uniform for all $0 \le t \le T$. □

4.4. Error estimates

Using that (ϕ, μ) solves (7) and (8) and by the definition of $(\hat\phi_h, \hat\mu_h)$, one can see that (19) and (20) is satisfied with residuals $\hat r_{2,h} = 0$ and

$$\langle \hat r_{1,h}, v_h\rangle = \langle \partial_t\hat\phi_h - \partial_t\phi, v_h\rangle + \langle b(\phi_h)\nabla(\hat\mu_h - \mu), \nabla v_h\rangle + \langle (b(\phi_h) - b(\phi))\nabla\mu, \nabla v_h\rangle. \tag{30}$$

By the properties of the discrete dual norm $\|\cdot\|_{-1,h}$ and standard approximation error estimates, see Lemma 13, the residual $\hat r_{1,h}$ can further be bounded by

$$\begin{aligned}\|r_{1,h}\|_{-1,h}^2 &\le C\|\partial_t\hat\phi_h - \partial_t\phi\|_{-1,h}^2 + C(b_2)\|\nabla\hat\mu_h - \nabla\mu\|_0^2 + C(b_3)\|\nabla\mu\|_{0,3}^2(\|\hat\phi_h - \phi\|_{0,6}^2 + \|\phi_h - \hat\phi_h\|_{0,6}^2)\\ &\le Ch^4(\|\partial_t\phi\|_1^2 + \|\mu\|_3^2 + (1 + \|\mu\|_{1,3}^2)\|\phi\|_3^2) + C'\|\mu\|_{1,3}^2\,\mathcal{E}_\alpha(\phi_h|\hat\phi_h),\end{aligned} \tag{31}$$

with constants C, C' depending only on bounds on the coefficients, the domain Ω, the mesh regularity, and the constant $C_T(\|\phi_0\|_3)$ for the solution in Lemma 2. We can now use Lemma 12 to obtain the following bounds for the discrete error.

Lemma 14. *Let (A1)–(A4) hold and let (ϕ, μ) be a solution with regular initial value $\phi_0 \in H_p^3(\Omega)$. Further, let $(\hat\phi_h, \hat\mu_h)$ be the discrete approximations from above and let (ϕ_h, μ_h) be the solution of Problem 10 with initial value $\phi_{0,h} = \pi_h^1\phi_0$. Then*

$$\|\phi_h - \hat\phi_h\|_{L^\infty(H_p^1)}^2 + \|\nabla\mu_h - \nabla\hat\mu_h\|_{L^2(L^2)}^2 \le C_T'(\|\phi_0\|_3)h^4,$$

with constant $C_T'(\|\phi_0\|_3)$ independent of the mesh size h.

Proof. From the discrete stability estimate of Lemma 12 and the bounds for the residual, cf. (31), derived above, we may deduce that

$$\mathcal{E}_\alpha(\phi_h(t)|\hat\phi_h(t)) + \int_0^t \mathcal{D}_{\phi_h(s)}(\mu_h(s)|\hat\mu_h(s))\,\mathrm{d}s \le C\mathcal{E}_\alpha(\phi_h(0)|\hat\phi_h(0)) + C'\int_0^t \|\hat r_{1,h}(s)\|_{-1,h}^2\,\mathrm{d}s$$

$$\leq C''h^4 \int_0^t \|\partial_t \phi\|_1^2 + \|\mu\|_3^2 + (1+\|\mu\|_{1,3}^2)\|\phi\|_3^2 \,\mathrm{d}s + C''' \int_0^t \|\mu\|_{1,3}^2 \mathcal{E}_\alpha(\phi_h(s)|\hat{\phi}_h(s))\,\mathrm{d}s.$$

Since we assumed $\mu \in L^2(W_p^{1,3})$, the last term can be eliminated *via* the Gronwall inequality (A.1), which we here employ with the choices $u(t) = \mathcal{E}_\alpha(\phi_h(t)|\hat{\phi}_h(t))$, $\beta(t) = C'''\|\mu(t)\|_{1,3}^2$, and $\alpha(t) = C\mathcal{E}_\alpha(\phi_h(0)|\hat{\phi}_h(0)) - \int_0^t \mathcal{D}_{\phi_h(s)}(\mu_h(s)|\hat{\mu}_h(s))\,\mathrm{d}s + C''h^4 \int_0^t \|\partial_t\phi\|_1^2 + \|\mu\|_3^2 + (1+\|\mu\|_{1,3}^2)\|\phi\|_3^2\,\mathrm{d}s$. The assertion then follows by the lower bounds (13), cf. Lemma 5, and (16) for the relative energy and dissipation functionals. □

By combination of the previous estimates we now immediately obtain the following error bounds for the Galerkin semi-discretization with quadratic finite elements.

Theorem 15. *Let (A1)–(A4) hold and let (ϕ,μ) denote the unique periodic weak solution of (1) and (2) with $\phi(0) = \phi_0 \in H_p^3(\Omega)$. Moreover, let (ϕ_h,μ_h) be the corresponding semi-discrete solution of Problem 10 with initial value $\phi_{h,0} = \pi_h^1\phi_0$. Then*

$$\|\phi - \phi_h\|_{L^\infty(H_p^1)}^2 + \|\mu - \mu_h\|_{L^2(H_p^1)}^2 \leq C_T'(\|\phi_0\|_3)h^4$$

with a constant $C_T'(\|\phi_0\|_3)$ independent of the mesh size h.

Remark 16. The convergence rates in the theorem are optimal with respect to the approximation properties of quadratic finite elements. Moreover, the regularity assumption on the initial value is necessary to establish the predicted convergence rates. The convergence result is both, *order optimal* and *sharp*, *i.e.*, obtained under minimal smoothness assumptions on the problem data. The constant C_T' depends exponentially on T and γ^{-1}.

5. Fully discrete approximation

We now turn to the time discretization, for which we again employ a variational method. For a given step size $\tau = T/N$, $N \in \mathbb{N}$, we define discrete time points $t^n := n\tau$ and denote by $\mathcal{I}_\tau := \{0 = t^0, t^1, \ldots, t^N = T\}$ the corresponding partition of the time interval $[0,T]$. We write $\Pi_k(\mathcal{I}_\tau;\mathcal{V}_h)$ for the space of piecewise polynomials of degree k over the time grid $\mathcal{I}_\tau$ with values in $\mathcal{V}_h$, and denote by $\Pi_k^c(\mathcal{I}_\tau;\mathcal{V}_h) = \Pi_k(\mathcal{I}_\tau;\mathcal{V}_h) \cap C(0,T;\mathcal{V}_h)$ the corresponding sub-space of continuous functions. Furthermore, we use a bar symbol $\bar{g}$ to denote piecewise constant functions of time. We search for approximations $(\phi_{h,\tau},\bar{\mu}_{h,\tau})$ for (ϕ,μ) in

$$\mathbb{W}_{h,\tau}(0,T) := \Pi_1^c(\mathcal{I}_\tau;\mathcal{V}_h) \quad \text{and} \quad \mathbb{Q}_{h,\tau}(0,T) := \Pi_0(\mathcal{I}_\tau;\mathcal{V}_h).$$

Let us emphasize that functions in $\mathbb{W}_{h,\tau}(0,T)$ are continuous in time and piecewise linear, while functions $\bar{q}_{h,\tau} \in \mathbb{Q}_{h,\tau}$ are piecewise constant in time, which is designated by the bar symbol. The discrete approximation for (1) and (2) then is the following.

Problem 17. *Let $\phi_{0,h} \in \mathcal{V}_h$ be given. Find $\phi_{h,\tau} \in \mathbb{W}_{h,\tau}(0,T)$, $\bar{\mu}_{h,\tau} \in \mathbb{Q}_{h,\tau}(0,T)$ such that $\phi_{h,\tau}(0) = \phi_{0,h}$ and for all $\bar{v}_{h,\tau}, \bar{w}_{h,\tau} \in \mathbb{Q}_{h,\tau}$ and $n \geq 1$, there holds*

$$\int_{t^{n-1}}^{t^n} \langle \partial_t\phi_{h,\tau}, \bar{v}_{h,\tau}\rangle + \langle b(\phi_{h,\tau})\nabla\bar{\mu}_{h,\tau}, \nabla\bar{v}_{h,\tau}\rangle\,\mathrm{d}s = 0, \tag{32}$$

$$\int_{t^{n-1}}^{t^n} \langle \bar{\mu}_{h,\tau}, \bar{w}_{h,\tau}\rangle - \langle \gamma\nabla\phi_{h,\tau}, \nabla\bar{w}_{h,\tau}\rangle - \langle f'(\phi_{h,\tau}), \bar{w}_{h,\tau}\rangle\,\mathrm{d}s = 0. \tag{33}$$

Remark 18. By the discontinuity of the test functions $\bar{v}_{h,\tau}$, $\bar{w}_{h,\tau}$ in time, this method amounts to an implicit time-stepping scheme, similar to the Crank–Nicolson or average vector field methods; see [1,38] for details.

Lemma 19. *Let (A1)–(A4) hold. Then for any $\phi_{0,h} \in \mathcal{V}_h$ and any $\tau > 0$, Problem 17 has at least one solution. Moreover, any solution $(\phi_{h,\tau}, \bar{\mu}_{h,\tau})$ of (32) and (33) satisfies $\int_\Omega \phi_{h,\tau}(t^n)\,\mathrm{d}x = \int_\Omega \phi_{0,h}\,\mathrm{d}x$ and $\mathcal{E}(\phi_{h,\tau}(t^n)) + \int_0^{t^n} \mathcal{D}_{\phi_{h,\tau}}(\bar{\mu}_{h,\tau})\,\mathrm{d}s = \mathcal{E}(\phi_{0,h})$ for all $0 \le t^n \le T$, and as a direct consequence, we obtain uniform bounds*

$$\|\phi_{h,\tau}\|_{L^\infty(H^1)} + \|\bar{\mu}_{h,\tau}\|_{L^2(H^1)} \le C(\|\phi_{0,h}\|_1). \tag{34}$$

Proof. Conservation of mass and dissipation of energy follow again by testing (32) and (33), now with $(\bar{v}_{h,\tau}, \bar{w}_{h,\tau}) = (1, 0)$ and $(\bar{v}_{h,\tau}, \bar{w}_{h,\tau}) = (\bar{\mu}_{h,\tau}, \partial_t \phi_{h,\tau})$, which are admissible test functions in (32) and (33). To show existence, we use an induction argument. Let $\phi_{h,\tau}(t^{n-1})$ be given. Then in the nth time step, only the function values $\phi_h^n := \phi_{h,\tau}(t^n)$ and $\mu_h^{n-1/2} := \bar{\mu}_{h,\tau}(t^n - \tau/2)$ are to be determined. From the discrete energy-dissipation identity, the bounds for the coefficients, and the equivalence of norms on finite dimensional spaces, one can deduce that potential solutions are necessarily bounded. Existence of a solution for the nth time step then follows from Brouwer's fixed-point theorem. The uniform bounds for the solution, finally, follow directly from the energy-dissipation identity and using (13) and (16). □

Remark 20. Uniqueness of the discrete solution can be shown under a mild restriction $\tau \le \tau_0(h)$ on the time step size. In Section 5.4 below, we will show that uniqueness holds for $\tau \le ch^\alpha$ with some $\alpha \le 1$, if the solution (ϕ, μ) is sufficiently regular. The choice $\tau = ch$, which seems reasonable in view of the estimates of Theorem 27, therefore will lead to unique solutions for the fully discrete problem.

In the following, we first establish a discrete analogue of the stability estimate derive in Theorem 6, and then derive convergence rates for the fully-discrete scheme.

5.1. Discrete stability

For any pair $(\hat{\phi}_{h,\tau}, \hat{\bar{\mu}}_{h,\tau}) \in \mathbb{W}_{h,\tau}(0,T) \times \mathbb{Q}_{h,\tau}(0,T)$, we define discrete residuals $(\bar{r}_{1,h,\tau}, \bar{r}_{2,h,\tau}) \in \mathbb{Q}_{h,\tau}(0,T) \times \mathbb{Q}_{h,\tau}(0,T)$ *via*

$$\int_{t^{n-1}}^{t^n} \langle \partial_t \hat{\phi}_{h,\tau}, \bar{v}_{h,\tau}\rangle + \langle b(\phi_{h,\tau})\nabla \hat{\bar{\mu}}_{h,\tau}, \nabla \bar{v}_{h,\tau}\rangle\,\mathrm{d}s =: \langle \bar{r}_{1,h,\tau}, \bar{v}_{h,\tau}\rangle, \tag{35}$$

$$\int_{t^{n-1}}^{t^n} \langle \hat{\bar{\mu}}_{h,\tau}, \bar{w}_{h,\tau}\rangle - \langle \gamma \nabla \hat{\phi}_{h,\tau}, \nabla \bar{w}_{h,\tau}\rangle - \langle f'(\hat{\phi}_{h,\tau}), \bar{w}_{h,\tau}\rangle\,\mathrm{d}s =: \langle \bar{r}_{2,h,\tau}, \bar{w}_{h,\tau}\rangle, \tag{36}$$

for $\bar{v}_{h,\tau}, \bar{w}_{h,\tau} \in \Pi_0(t^{n-1}, t^n; \mathcal{V}_h)$, and all $0 < t^n \le T$. Note that the residuals $\bar{r}_{1,h,\tau}$, $\bar{r}_{2,h,\tau}$ are defined as piecewise constant functions of time, which we again designate by bar symbols. With similar arguments as used for the derivation of the stability estimates in the previous sections, we now obtain the following result.

Lemma 21. *Let (A1)–(A4) hold and $(\phi_{h,\tau}, \bar{\mu}_{h,\tau})$ be a solution of Problem 17 with step size $0 < \tau \le \tau_0$ sufficiently small. Let $(\hat{\phi}_{h,\tau}, \hat{\bar{\mu}}_{h,\tau}) \in \mathbb{W}_{h,\tau}(0,T) \times \mathbb{Q}_{h,\tau}(0,T)$ be given and $(\bar{r}_{1,h,\tau}, \bar{r}_{2,h,\tau})$ be the corresponding residuals defined by (35) and (36). Then*

$$\begin{aligned} &\mathcal{E}_\alpha(\phi_{h,\tau}(t^n)|\hat{\phi}_{h,\tau}(t^n)) + \int_0^{t^n} \mathcal{D}_{\phi_{h,\tau}(s)}(\bar{\mu}_{h,\tau}(s)|\hat{\bar{\mu}}_{h,\tau}(s))\,\mathrm{d}s \\ &\qquad \le e^{ct^n}\mathcal{E}_\alpha(\phi_{h,\tau}(0)|\hat{\phi}_{h,\tau}(0)) + Ce^{ct^n}\int_0^{t^n} \|\bar{r}_{1,h,\tau}(s)\|_{-1}^2 + \|\bar{r}_{2,h,\tau}(s)\|_1^2\,\mathrm{d}s \end{aligned}$$

for all $0 \le t^n \le T$ with constants $c = c_0 + c_1\|\partial_t \hat{\phi}_{h,\tau}\|_{L^\infty(L^2)}$, and c_0, c_1, C depending only on the bounds for the coefficients, the domain Ω, and the uniform bounds for $(\phi_{h,\tau}, \mu_{h,\tau})$ and $(\hat{\phi}_{h,\tau}, \hat{\mu}_{h,\tau})$ in $L^\infty(H^1) \times L^2(H^1)$.

Remark 22. We will see that the estimate of Lemma 21 holds uniformly for all $h > 0$ and $0 < \tau \leq \tau_0$ depending on the bounds for the coefficients, the domain Ω, the time horizon T, as well as the uniform bounds for $(\phi_{h,\tau}, \mu_{h,\tau})$ and $(\hat{\phi}_{h,\tau}, \hat{\mu}_{h,\tau})$ in $L^\infty(H^1) \times L^2(H^1)$ and on the bound for $\|\partial_t \hat{\phi}_{h,\tau}\|_{L^\infty(L^2)}$. Thus, the scheme is unconditionally stable, *i.e.*, τ can be chosen independent of h.

Proof. By the fundamental theorem of calculus, we obtain

$$\begin{aligned}
\mathcal{E}_\alpha(\phi_{h,\tau}|\hat{\phi}_{h,\tau})\big|_{t^{n-1}}^{t^n} &= \int_{t^{n-1}}^{t^n} \frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}_\alpha(\phi_{h,\tau}|\hat{\phi}_{h,\tau})\,\mathrm{d}s \\
&= \int_{t^{n-1}}^{t^n} \gamma\langle \nabla\phi_{h,\tau} - \nabla\hat{\phi}_{h,\tau}, \nabla\partial_t\phi_{h,\tau} - \nabla\partial_t\hat{\phi}_{h,\tau}\rangle + \langle f'(\phi_{h,\tau}) - f'(\hat{\phi}_{h,\tau}), \partial_t\phi_{h,\tau} - \partial_t\hat{\phi}_{h,\tau}\rangle \\
&\quad + \alpha\langle \phi_{h,\tau} - \hat{\phi}_{h,\tau}, \partial_t\phi_{h,\tau} - \partial_t\hat{\phi}_{h,\tau}\rangle \\
&\quad + \langle f'(\phi_{h,\tau}) - f'(\hat{\phi}_{h,\tau}) - f''(\hat{\phi}_{h,\tau})(\phi_{h,\tau} - \hat{\phi}_{h,\tau}), \partial_t\hat{\phi}_{h,\tau}\rangle\,\mathrm{d}s \\
&= \int_{t^{n-1}}^{t^n} \langle \bar{\mu}_{h,\tau} - \hat{\bar{\mu}}_{h,\tau} + \bar{r}_{2,h,\tau}, \partial_t\phi_{h,\tau} - \partial_t\hat{\phi}_{h,\tau}\rangle + \alpha\langle \phi_{h,\tau} - \hat{\phi}_{h,\tau}, \partial_t\phi_{h,\tau} - \partial_t\hat{\phi}_{h,\tau}\rangle \\
&\quad + \langle f'(\phi_{h,\tau}) - f'(\hat{\phi}_{h,\tau}) - f''(\hat{\phi}_{h,\tau})(\phi_{h,\tau} - \hat{\phi}_{h,\tau}), \partial_t\hat{\phi}_{h,\tau}\rangle\,\mathrm{d}s = (*).
\end{aligned}$$

In the last step, we use the identities (33) and (36) with $\bar{w}_{h,\tau} = \partial_t\phi_{h,\tau} \in \mathbb{Q}_{h,\tau}$. Since the function $\partial_t\phi_{h,\tau} - \partial_t\hat{\phi}_{h,\tau}$ is piecewise constant in time, we can replace

$$\int_{t^{n-1}}^{t^n} \alpha\langle \phi_{h,\tau} - \hat{\phi}_{h,\tau}, \partial_t\phi_{h,\tau} - \partial_t\hat{\phi}_{h,\tau}\rangle\,\mathrm{d}t = \int_{t^{n-1}}^{t^n} \alpha\langle \bar{\pi}_\tau^0\phi_{h,\tau} - \bar{\pi}_\tau^0\hat{\phi}_{h,\tau}, \partial_t\phi_{h,\tau} - \partial_t\hat{\phi}_{h,\tau}\rangle\,\mathrm{d}t$$

where $\bar{\pi}_\tau^0 : \mathbb{W}_{h,\tau} \to \mathbb{Q}_{h,\tau}$ denotes the L^2-orthogonal projection in time onto piecewise constants. Employing $\bar{v}_{h,\tau} = \bar{\mu}_{h,\tau} - \hat{\bar{\mu}}_{h,\tau} + \bar{r}_{2,h,\tau} + \alpha\bar{\pi}_\tau^0(\phi_{h,\tau} - \hat{\phi}_{h,\tau}) \in \mathbb{Q}_{h,\tau}$ as a test function in the identities (32) and (35), we obtain

$$\begin{aligned}
(*) = \int_{t^{n-1}}^{t^n} &-\langle b(\phi_{h,\tau})\nabla(\bar{\mu}_{h,\tau} - \hat{\bar{\mu}}_{h,\tau}), \nabla(\bar{\mu}_{h,\tau} - \hat{\bar{\mu}}_{h,\tau} + \bar{r}_{2,h,\tau})\rangle - \langle \bar{r}_{1,h,\tau}, \bar{\mu}_{h,\tau} - \hat{\bar{\mu}}_{h,\tau} + \bar{r}_{2,h,\tau}\rangle \\
&- \alpha\langle b(\phi_{h,\tau})\nabla(\bar{\mu}_{h,\tau} - \hat{\bar{\mu}}_{h,\tau}), \nabla(\phi_{h,\tau} - \hat{\phi}_{h,\tau})\rangle - \alpha\langle \bar{r}_{1,h,\tau}, \phi_{h,\tau} - \hat{\phi}_{h,\tau}\rangle \\
&+ \langle f'(\phi_{h,\tau}) - f'(\hat{\phi}_{h,\tau}) - f''(\hat{\phi}_{h,\tau})(\phi_{h,\tau} - \hat{\phi}_{h,\tau}), \partial_t\hat{\phi}_{h,\tau}\rangle\,\mathrm{d}s.
\end{aligned}$$

At this point, we can start to estimate the individual terms in the same manner, as in the proof of Theorem 6. In this way, we arrive at

$$\begin{aligned}
\mathcal{E}_\alpha(\phi_{h,\tau}|\hat{\phi}_{h,\tau})\big|_{t^{n-1}}^{t^n} &+ \int_{t^{n-1}}^{t^n} \mathcal{D}_{\phi_{h,\tau}(s)}(\bar{\mu}_{h,\tau}(s)|\hat{\bar{\mu}}_{h,\tau}(s))\,\mathrm{d}s \\
&\leq \int_{t^{n-1}}^{t^n} c\mathcal{E}_\alpha(\phi_{h,\tau}(s)|\hat{\phi}_{h,\tau}(s))\,\mathrm{d}s + \int_{t^{n-1}}^{t^n} C_1\|\bar{r}_{1,h,\tau}(s)\|_{-1}^2 + C_2\|\bar{r}_{2,h,\tau}(s)\|_1^2\,\mathrm{d}s,
\end{aligned}$$

where we may choose $c = c_1 + c_2\|\partial_t\hat{\phi}_{h,\tau}(s)\|_{L^\infty(L^2)}$ here with c_1, c_2 and also C_1, C_2 depending only on the uniform $L^\infty(H^1) \times L^2(H^1)$ bounds for $(\phi_{h,\tau}, \bar{\mu}_{h,\tau})$ and $(\hat{\phi}_{h,\tau}, \hat{\bar{\mu}}_{h,\tau})$, as well as on the bounds for the coefficients, and the domain Ω, and the time horizon. Using the uniform $L^\infty(H^1)$ bounds for $\phi_{h,\tau}$ and $\hat{\phi}_{h,\tau}$ and (13), we can further estimate the first term on the right-hand side of the previous inequality by

$$\int_{t^{n-1}}^{t^n} \mathcal{E}_\alpha(\phi_{h,\tau}|\hat{\phi}_{h,\tau})\,\mathrm{d}s \leq c(\gamma)\tau(\mathcal{E}_\alpha(\phi_{h,\tau}|\hat{\phi}_{h,\tau})(t^n) + \mathcal{E}_\alpha(\phi_{h,\tau}|\hat{\phi}_{h,\tau})(t^{n-1})).$$

Under the assumption that $\tau \le 1/(2c(\gamma)c) =: \tau_0$, we can rewrite the estimate into

$$u^n + b^n \le e^{\lambda} u^{n-1} + d^n,$$

with $u^n = \mathcal{E}_\alpha(\phi_{h,\tau}(t^n)|\hat{\phi}_{h,\tau}(t^n))$, $b^n = e^{\gamma\tau}\int_{t^{n-1}}^{t^n} \mathcal{D}_{\phi_{h,\tau}}(s)\,\mathrm{d}s$, and $d^n = e^{\gamma\tau}\int_{t^{n-1}}^{t^n} C_1\|\bar{r}_{1,h,\tau}(s)\|_{-1}^2 + C_2\|\bar{r}_{2,h,\tau}(s)\|_1^2\,\mathrm{d}s$, and $e^{\gamma\tau} = \frac{1+c(\gamma)c\tau}{1-c(\gamma)c\tau}$, which corresponds to $\gamma \approx 2c(\gamma)c$. The assertion then follows by the discrete Gronwall inequality (A.2) and the bounds (13) and (16) for the relative energy and dissipation functionals. □

5.2. Auxiliary results

Similar to the semi-discrete case, we use certain projections to define suitable approximations $\hat{\phi}_{h,\tau}$ and $\hat{\bar{\mu}}_{h,\tau}$ for solutions (ϕ,μ) to (1) and (2) that allow us to take advantage of the discrete stability estimate. So, let

$$I_\tau^1 : H^1(0,T) \to \Pi_1^c(\mathcal{I}_\tau), \qquad I_\tau^1 u(t^n) = u(t^n)$$

denote the piecewise linear interpolation with respect to time. Furthermore, let

$$\bar{\pi}_\tau^0 : L^2(0,T) \to \Pi_0(I_\tau), \qquad \bar{\pi}_\tau^0 u(t) = \frac{1}{\tau}\int_{t^{n-1}}^{t^n} u(t)\,\mathrm{d}t, \qquad t \in (t^{n-1}, t^n),$$

be the L^2-orthogonal projection to piecewise constant functions in time. For later reference, we summarize some important properties of these operators.

Lemma 23. *For $u \in W^{1,q}(0,T)$, $1 \le p, q \le \infty$, there holds*

$$\|u - \bar{\pi}_\tau^0 u\|_{L^p(0,T)} \le C\tau^{1+1/p-1/q}\|\partial_t u\|_{L^q(0,T)}, \tag{37}$$

and for $u \in W^{r,q}(0,T)$ with $1 \le r \le 2$ and $1 \le p \le q \le \infty$, one has

$$\|u - I_\tau^1 u\|_{L^p(0,T)} \le C\tau^{1/p-1/q+r}\|u\|_{W^{r,q}(0,T)}. \tag{38}$$

Moreover, interpolation and projection commutes with differentiation, i.e.,

$$\partial_t(I_\tau^1 u) = \bar{\pi}_\tau^0(\partial_t u). \tag{39}$$

The proof for these standard results can be found, *e.g.*, in [10]. The interpolation operator naturally extends to vector valued functions, and we use the same symbol in that case. For the piecewise constant L^2-projection we can show the following estimate for the product error; see Appendix B for a proof.

Lemma 24. *Let $u, v \in W^{2,p}(0,T)$ and $\bar{a} = \bar{\pi}_\tau^0 a$ denote the L^2-orthogonal projection onto piecewise constants. Then*

$$\|\bar{u}\bar{v} - \overline{uv}\|_{L^p(0,T)} \le C\tau^2\|u\|_{W^{2,p}(0,T)}\|v\|_{W^{2,p}(0,T)} \tag{40}$$

with a constant C independent of τ and p as well as the functions u and v.

As fully discrete approximations $(\hat{\phi}_{h,\tau}, \hat{\bar{\mu}}_{h,\tau}) \in \mathbb{W}_{h,\tau} \times \mathbb{Q}_{h,\tau}$ for solutions (ϕ,μ) of (1) and (2), to be used in the subsequent error analysis, we now define

$$\hat{\phi}_{h,\tau} = I_\tau^1 \pi_h^1 \phi \quad \text{and} \quad \hat{\bar{\mu}}_{h,\tau} = \bar{\pi}_\tau^0 \pi_h^0 \mu. \tag{41}$$

For this particular choice, we can make the following observation.

Lemma 25. *Let (ϕ,μ) be a sufficiently regular periodic solution of (7) and (8), and let $(\hat\phi_{h,\tau},\hat{\bar\mu}_{h,\tau})$ be defined as above. Then (35) and (36) holds with residuals*

$$\int_{t^{n-1}}^{t^n}\langle\bar r_{1,h,\tau},\bar v_{h,\tau}\rangle\,\mathrm{d}s=\int_{t^{n-1}}^{t^n}\langle\partial_t(\pi_h^1\phi-\phi),\bar v_{h,\tau}\rangle+\langle b(\phi_{h,\tau})\nabla\hat{\bar\mu}_{h,\tau}-b(\phi)\nabla\mu,\nabla\bar v_{h,\tau}\rangle\,\mathrm{d}s$$
$$\int_{t^{n-1}}^{t^n}\langle\bar r_{2,h,\tau},\bar w_{h,\tau}\rangle\,\mathrm{d}s=\int_{t^{n-1}}^{t^n}\langle\hat{\bar\mu}_{h,\tau}-I_\tau^1\mu,\bar w_{h,\tau}\rangle+\gamma\langle\nabla(\hat\phi_{h,\tau}-I_\tau^1\phi),\nabla\bar w_{h,\tau}\rangle+\langle f'(\hat\phi_{h,\tau})-I_\tau^1f'(\phi),\bar w_{h,\tau}\rangle\,\mathrm{d}s.$$

Proof. Testing (7) with $v=\bar v_{h,\tau}$ and integration over time yields

$$\int_{t^{n-1}}^{t^n}\langle\partial_t\phi,\bar v_{h,\tau}\rangle+\langle b(\phi)\nabla\mu,\nabla\bar v_{h,\tau}\rangle=0.$$

The first identity then follows by subtracting (35), and noting that

$$\int_0^{t^n}\langle\partial_t\hat\phi_{h,\tau},\bar v_{h,\tau}\rangle\,\mathrm{d}s=\int_0^{t^n}\langle\partial_tI_\tau^1\pi_h^1\phi,\bar v_{h,\tau}\rangle\,\mathrm{d}s=\int_0^{t^n}\langle\partial_t\pi_h^1\phi,\bar v_{h,\tau}\rangle\,\mathrm{d}s,$$

which follows from (39) and $\bar v_{h,\tau}$ being piecewise constant in time. Testing (8) at t^{n-1}, t^n with $\bar w_{h,\tau}$, and noting that $\int_{t^{n-1}}^{t^n}a(t)\bar b(t)\,\mathrm{d}t=\frac{\tau}{2}(a(t^n)+a(t^{n-1}))b(t^n-\tau/2)$ for all $a\in\Pi_1(t^{n-1},t^n)$ and $\bar b\in\Pi_0(t^{n-1},t^n)$, one finds

$$\int_{t^{n-1}}^{t^n}\langle I_\tau^1\mu,\bar w_{h,\tau}\rangle+\gamma\langle\nabla I_\tau^1\phi,\nabla\bar w_{h,\tau}\rangle+\langle I_\tau^1f'(\phi),\bar w_{h,\tau}\rangle\,\mathrm{d}s=0.$$

Combination with (36) then yields the second identity. □

As a next step, we derive bounds for the discrete residuals in terms of interpolation and projection errors. For ease of notation, we will write $W^{k,p}(X)=W^{k,p}(a,b;X)$ for different choices of the time interval (a,b), which will be clear from the context.

Lemma 26. *Let (ϕ,μ) be a sufficiently regular periodic solution of (7) and (8). Then*

$$\int_{t^{n-1}}^{t^n}\|\bar r_{1,h,\tau}\|_{-1,h}^2\,\mathrm{d}s\le C_0(\phi,\mu)\tau^4+C_1(\phi,\mu)h^4+C(b,\mu)\int_{t^{n-1}}^{t^n}\mathcal{E}_\alpha(\phi_{h,\tau}(s)|\hat\phi_{h,\tau}(s))\,\mathrm{d}s,$$
$$\int_{t^{n-1}}^{t^n}\|\bar r_{2,h,\tau}\|_1^2\,\mathrm{d}s\le C_2(\phi,\mu)\tau^4+C_3(\phi)h^4$$

for all $0<t^n\le T$ with constants $C(\cdot)$ independent of h, τ, and t^n.

Proof. Since $\bar v_{h,\tau}$ is piecewise constant in time, we can use (39), the definition of $\hat\phi_{h,\tau}$, and the bounds for the H^1-projection error, to estimate the residual by

$$\begin{aligned}\int_{t^{n-1}}^{t^n}\|\bar r_{1,h,\tau}\|_{-1,h}^2\,\mathrm{d}s&\le C\int_{t^{n-1}}^{t^n}\|\partial_t(\pi_h^1\phi-\phi)\|_{-1}^2+\|\overline{b(\phi_{h,\tau})}\nabla\hat{\bar\mu}_{h,\tau}-\overline{b(\phi)\nabla\mu}\|_0^2\,\mathrm{d}s\\&\le Ch^4\|\partial_t\phi\|_{L^2(H_p^1)}^2+C(*)^2.\end{aligned}$$

Here and in the following, we use $\overline{a}=\bar\pi_\tau^0a$ to abbreviate the projection onto piecewise constant functions in time and all Bochner-norms refer to the time interval (t^{n-1},t^n) under consideration. The remaining term can be further estimated by

$$\begin{aligned}(*)^2&\le\|\overline{b(\phi_{h,\tau})}\nabla(\hat{\bar\mu}_{h,\tau}-\overline{\mu})\|_{L^2(L^2)}^2+\|(\overline{b(\phi_{h,\tau})}-\overline{b(\phi)})\nabla\overline{\mu}\|_{L^2(L^2)}^2+\|\overline{b(\phi)\nabla\mu}-\overline{b(\phi)}\;\overline{\nabla\mu}\|_{L^2(L^2)}^2\\&=\text{(i)}+\text{(ii)}+\text{(iii)}.\end{aligned}$$

Using the boundedness of b, the definition of $\hat{\bar\mu}_{h,\tau}$, and the stability and error estimates for the L^2-projection (24), we immediately obtain

$$\text{(i)} \le C(b_2)\|\nabla(\pi_h^0\mu - \mu)\|^2_{L^2(L^2)} \le C'(b_2)h^4\|\mu\|^2_{L^2(H_p^3)}.$$

For the second term, we use a triangle inequality, the error bounds (26) for the H^1-projection, the interpolation error estimate (38), and the lower bound (13) for the relative energy. In summary, this leads to

$$\text{(ii)} \le C(b_3)\|\phi_{h,\tau} - \phi\|^2_{L^2(L^6)}\|\mu\|^2_{L^\infty(W_p^{1,3})} \le C(b_3)\|\mu\|_{L^\infty(W_p^{1,3})}(h^4\|\phi\|^2_{L^2(H_p^3)} + \tau^4\|\phi\|^2_{H^2(H_p^1)} + \gamma\mathcal{E}_\alpha(\phi_{h,\tau}|\hat\phi_{h,\tau})),$$

For the third term, we observe that this is a second order approximation on the midpoint of the time interval and using the estimate (40) we obtain

$$\text{(iii)} \le C\tau^4\|b(\phi)\nabla\mu\|^2_{H^2(L^2)} \le C(b_2, b_3, \|\mu\|_{L^\infty(W_p^{1,3})})\tau^4(\|\mu\|^2_{H^2(H_p^1)} + \|\phi\|^2_{H^2(H_p^1)}).$$

To estimate $H^2(L^2)$ norm of $b(\phi)\nabla\mu$, we differentiate $b(\phi)\nabla\mu$ in time and use triangle inequalities, the uniform bounds for $b(\cdot)$, and the Hlder inequalities in space and time. The critical terms are the higher order terms $b(\phi)\partial_{tt}\nabla\mu, b'(\phi)\nabla\mu\partial_{tt}\phi$, which are estimated in $L^2(L^2)$. Indeed, they can be bounded by $C\|\mu\|_{H^2(H^1)}$ and $C\|\mu\|_{L^\infty(W_p^{1,3})}\|\phi\|_{H^2(L^6)}$. By combination of the previous estimates, we thus obtain

$$\int_{t^{n-1}}^{t^n}\|\bar r_{1,h,\tau}\|^2_{-1,h}\,\mathrm{d}s \le C_0(\phi,\mu)\tau^4 + C_1(\phi,\mu)h^4 + C(b,\mu)\int_{t^{n-1}}^{t^n}\mathcal{E}_\alpha(\phi_{h,\tau}(s)|\hat\phi_{h,\tau}(s))\,\mathrm{d}s,$$

with $C_0 = C(\|\phi\|_{H^2(H_p^1)}, \|\mu\|_{H^2(H_p^1)})$, $C_1(\phi,\mu) = C(\|\partial_t\phi\|_{L^2(H_p^1)}, \|\mu\|_{L^2(H_p^3)}, \|\phi\|^2_{L^2(H_p^3)})$ and constant $C(b,\mu) = C(b_3, \|\mu\|_{L^\infty(W_p^{1,3})})$ independent of h and τ.

Before turning to the bound for the second residual, let us observe that

$$\int_{t^{n-1}}^{t^n}\langle\nabla(\hat\phi_{h,\tau} - I_\tau^1\phi), \nabla\bar w_{h,\tau}\rangle\,\mathrm{d}s = \int_{t^{n-1}}^{t^n}\langle I_\tau^1\phi - \hat\phi_{h,\tau}, \bar w_{h,\tau}\rangle\,\mathrm{d}s, \tag{42}$$

which follows from the definition of $\hat\phi_{h,\tau}$ and the variational characterization (25) of π_h^1. The second residual can then be expressed equivalently in strong form as

$$\bar r_{2,h,\tau} = (\overline{\pi_h^0\mu} - \overline{I_\tau^1\pi_h^0\mu}) + (\overline{I_\tau^1\phi} - \overline{\hat\phi_{h,\tau}}) + (\overline{f'(\hat\phi_{h,\tau})} - \overline{I_\tau^1 f'(\phi)}),$$

where $\overline{g} = \bar\pi_\tau^0 g$ denotes the piecewise constant projection of g with respect to time. This point wise representation allows us to estimate the second residual by

$$\begin{aligned}\int_{t^{n-1}}^{t^n}\|\bar r_{2,h,\tau}\|_1^2\,\mathrm{d}s \le \|\pi_h^0\mu - I_\tau^1\pi_h^0\mu\|^2_{L^2(H_p^1)} + \|I_\tau^1\phi - \hat\phi_{h,\tau}\|^2_{L^2(H_p^1)} \\ + \|f'(\hat\phi_{h,\tau}) - I_\tau^1 f'(\phi)\|^2_{L^2(H_p^1)} = \text{(i)} + \text{(ii)} + \text{(iii)}.\end{aligned}$$

We again estimate the individual terms separately. For the first, we use the contraction property of the L^2-projection π_h^0 and the interpolation error estimate (38) to obtain

$$\text{(i)} \le \|\mu - I_\tau^1\mu\|^2_{L^2(H_p^1)} \le C\tau^4\|\mu\|^2_{H^2(H_p^1)}.$$

By the estimate (26) for the H^1-projection π_h^1 to obtain for the second term

$$\text{(ii)} \le \|\phi - \pi_h^1\phi\|^2_{L^\infty(H_p^1)} \le Ch^4\|\phi\|^2_{L^\infty(H_p^3)}.$$

For the third term, we use that ϕ and its discrete counterpart $\hat{\phi}_{h,\tau} = I_\tau^1 \phi_h^1 \phi$ can be uniformly bounded in $L^\infty(0,T;W_p^{1,\infty}(\Omega))$. Therefore, all terms $f^{(k)}(\cdot)$ appearing in the following can be bounded uniformly by a constant $C(f)$. This leads to

$$\begin{aligned}
\text{(iii)} &\leq \|f'(\hat{\phi}_{h,\tau}) - f'(\phi)\|_{L^2(H_p^1)}^2 + \|f'(\phi) - I_\tau^1 f'(\phi)\|_{L^2(H_p^1)}^2 \\
&\leq C_1(f)\|\hat{\phi}_{h,\tau} - \phi\|_{L^2(H_p^1)}^2 + \tau^4 \|f'(\phi)\|_{H^2(H_p^1)}^2 \\
&\leq C(f)(h^4\|\phi\|_{L^2(H_p^3)} + \tau^4\|\phi\|_{H^2(H_p^1)}) + \tau^4\|f'(\phi)\|_{H^2(H_p^1)}^2.
\end{aligned}$$

A quick inspection of the last term shows that its evaluation involves up to cubic products of ϕ and its derivatives, with the highest order terms given by $\phi^2\partial_{tt}\nabla\phi$, $(\partial_t\phi)^2\nabla\phi$, and $\phi\partial_t\phi\nabla\partial_t\phi$, respectively. This allows to establish the following bounds

$$\|f'(\phi)\|_{H^2(H_p^1)} \leq C(f)(1 + \|\phi\|_{H^2(H^1)} + \|\phi\|_{H^1(H^3)})^3.$$

In summary, the second residual can thus be bounded by

$$\int_{t^{n-1}}^{t^n} \|\bar{r}_{2,h,\tau}\|_1^2 \,\mathrm{d}s \leq C_2(\phi,\mu)\tau^4 + C_3(\phi)h^4,$$

with the two solution dependent constants given by $C_2(\phi,\mu) = C(\|\mu\|_{H^2(H_p^1)}, \|\phi\|_{H^2(H_p^1)}, \|\phi\|_{H^1(H_p^3)})$ and $C_3(\phi) = C(\|\phi\|_{L^\infty(H_p^3)}, \|\phi\|_{L^2(H_p^3)})$ independent of h and τ. □

5.3. Error estimates

Together with the discrete stability estimate of Lemma 21 and a Gronwall-type argument, similar as already used in the proof of that result, we can now obtain the following convergence rate estimates.

Theorem 27. *Let (ϕ,μ) be a regular periodic weak solution of (1) and (2) with initial value $\phi_0 \in H_p^3(\Omega)$ satisfying*

$$\begin{aligned}
\phi &\in H^2(0,T;H_p^1(\Omega)) \cap H^1(0,T;H_p^3(\Omega)), \\
\mu &\in H^2(0,T;H_p^1(\Omega)) \cap L^\infty(0,T;W_p^{1,3}(\Omega)),
\end{aligned}$$

and let $(\phi_{h,\tau}, \bar{\mu}_{h,\tau})$ be a solution of (32) and (33) with $\phi_{h,\tau}(0) = \pi_h^1\phi_0$. Then

$$\max_{t^n\in\mathcal{I}_\tau} \|\phi_{h,\tau}(t^n) - \phi(t^n)\|_1^2 + \|\bar{\mu}_{h,\tau} - \bar{\mu}\|_{L^2(0,T;H_p^1)}^2 \leq C_T'(h^4 + \tau^4),$$

with C_T' depending on the norms of the solution (ϕ,μ), but independent of h and τ.

As in the semi-discrete case the constant C_T' depends exponentially on T and γ^{-1}.

Proof. We may proceed almost verbatim to the proof of Lemma 21 and insert the above estimates for the residual terms, to see that

$$\begin{aligned}
\mathcal{E}_\alpha(\phi_{h,\tau}|\hat{\phi}_{h,\tau})\Big|_{t^{n-1}}^{t^n} &+ \int_{t^{n-1}}^{t^n} \mathcal{D}_{\phi_{h,\tau}(s)}(\bar{\mu}_{h,\tau}(s)|\hat{\bar{\mu}}_{h,\tau}(s))\,\mathrm{d}s \\
&\leq C_1'\tau^4 + C_2'h^4 + \int_{t^{n-1}}^{t^n} C(b,\mu)\mathcal{E}_\alpha(\phi_{h,\tau}(s)|\hat{\phi}_{h,\tau}(s))\,\mathrm{d}s,
\end{aligned}$$

with $C(b,\mu) = c_0 + c_1\|\partial_t\hat{\phi}_{h,\tau}\|_{L^\infty(L^2)} + c_2\|\mu\|_{L^\infty(W_p^{1,3})}$ bounded uniformly in time. The proof of the assertion then follows in the same manner as that of Lemma 21. Note that it suffices to consider the case that $\tau \leq \tau_0$ is sufficiently small, since for large τ the result already follows from the *a priori* estimates. □

5.4. Uniqueness of the fully discrete solution

As a final step of our analysis, we now establish uniqueness of the discrete solution under a mild restriction on the time step size; see Remark 20. Let us start with the observation that under the conditions of the previous theorem, $\bar{\mu}_{h,\tau}$ is uniformly bounded in the norm of $L^\infty(W_p^{1,3})$. To see this, note that

$$\|\bar{\mu}_{h,\tau}\|_{L^\infty(W_p^{1,3})} \le \|\bar{\mu}_{h,\tau} - \pi_h^0\bar{\mu}\|_{L^\infty(W_p^{1,3})} + \|\pi_h^0\bar{\mu} - \bar{\mu}\|_{L^\infty(W_p^{1,3})} + \|\bar{\mu}\|_{L^\infty(W_p^{1,3})}.$$

The last two terms are uniformly bounded by assumption and standard projection error estimates. For the first term on the right-hand side, we use the second inverse inequality in (27) with $p = 3, q = 2, d \le 3$ in space and with $p = \infty, q = 2, d = 1$ in time, as well as the convergence estimates of the previous theorem, to see that

$$\|\bar{\mu}_{h,\tau} - \pi_h^0\bar{\mu}\|_{L^\infty(W_p^{1,3})} \le C\tau^{-1/2}h^{-1/2}\|\bar{\mu}_{h,\tau} - \pi_h^0\bar{\mu}\|_{L^2(H_p^1)} \le C_1'h^{-1/2}\tau^{3/2} + C_2'h^{3/2}\tau^{-1/2}.$$

For any choice $ch^3 \le \tau \le Ch^{1/3}$, one can thus conclude that $\|\bar{\mu}_{h,\tau}\|_{L^\infty(W_p^{1,3})} \le C'$.

Uniqueness can now be deduced as follows: Let the assumptions of Theorem 27 be valid. Furthermore, let $(\phi_{h,\tau}, \bar{\mu}_{h,\tau}) \in \mathbb{W}_{h,\tau}(0,T) \times \mathbb{Q}_{h,\tau}(0,T)$ and $(\hat{\phi}_{h,\tau}, \hat{\bar{\mu}}_{h,\tau}) \in \mathbb{W}_{h,\tau}(0,T) \times \mathbb{Q}_{h,\tau}(0,T)$ denote two solutions of Problem 17 with the same initial data $\phi_{h,\tau}(0) = \hat{\phi}_{h,\tau}(0)$ and with time step size $ch^3 \le \tau \le Ch^{1/3}$ and $\tau \le \tau_0$ sufficiently small. Then the residuals defined by (35) and (36) are $\bar{r}_{2,h,\tau} = 0$ and

$$\int_{t^{n-1}}^{t^n} \langle \bar{r}_{1,h,\tau}, \bar{v}_{h,\tau}\rangle \,\mathrm{d}s = \int_{t^{n-1}}^{t^n} \langle (b(\phi_{h,\tau}) - b(\hat{\phi}_{h,\tau}))\nabla\hat{\bar{\mu}}_{h,\tau}, \bar{v}_{h,\tau}\rangle \,\mathrm{d}s,$$

for all $\bar{v}_{h,\tau} \in \Pi_0(t^{n-1}, t^n; \mathcal{V}_h)$. Using the bounds for the coefficients and (13), the residual term $\bar{r}_{1,h,\tau}$ can be further estimated by

$$\int_{t^{n-1}}^{t^n} \|\bar{r}_{1,h,\tau}\|_{-1,h}^2 \,\mathrm{d}s \le C(b_3)\|\hat{\bar{\mu}}_{h,\tau}\|_{L^\infty(W_p^{1,3})}^2 \int_{t^{n-1}}^{t^n} \mathcal{E}(\phi_{h,\tau}(s)|\hat{\phi}_{h,\tau}(s)) \,\mathrm{d}s.$$

The last term can be treated by a Gronwall estimate, similar as in the proof of Lemma 21 and Theorem 27. Together with $\phi_{h,\tau}(0) = \hat{\phi}_{h,\tau}(0)$, we thus obtain

$$\mathcal{E}_\alpha(\phi_{h,\tau}(t^n)|\hat{\phi}_{h,\tau}(t^n)) + \int_0^{t^n} \mathcal{D}_{\phi_{h,\tau}}(\bar{\mu}_{h,\tau}|\hat{\bar{\mu}}_{h,\tau}) \,\mathrm{d}s \le 0.$$

By the lower bounds (13) and (16) for the relative energy and dissipation terms, this implies that $\nabla\bar{\mu}_{h,\tau} \equiv \nabla\hat{\bar{\mu}}_{h,\tau}$ and $\phi_{h,\tau}(t^n) = \hat{\phi}_{h,\tau}(t^n)$ for all n, from which one can deduce that $\phi_{h,\tau} \equiv \hat{\phi}_{h,\tau}$ and $\bar{\mu}_{h,\tau} \equiv \hat{\bar{\mu}}_{h,\tau}$.

Remark 28. A brief inspection of the arguments reveal, that the regularity assumptions on the true solution could be somewhat relaxed, which will however lead to tighter bounds $ch^\alpha \le \tau \le Ch^{1/\alpha}$ with $1 \le \alpha \le 3$ for the admissible time step sizes. The choice $\tau = ch$, seems reasonable and leads to a uniqueness result under minimal regularity assumptions. If the mobility function $b(\phi) \equiv b$ is independent of the concentration, then the above considerations become obsolete, since the relevant terms in the stability estimate vanish.

6. Numerical validation

The aim of this section is to illustrate our theoretical results, in particular, the convergence rate estimates obtained in Theorems 15 and 27. We solve a typical test problem, which is specified as follows: The interface parameter γ is set to $\gamma = 0.003$, the potential and mobility functions are defined as

$$f(\phi) = 0.3(\phi - 0.99)^2(\phi + 0.99)^2 \quad \text{and} \quad b(\phi) = (1-\phi)^2(1+\phi)^2 + 10^{-3}.$$

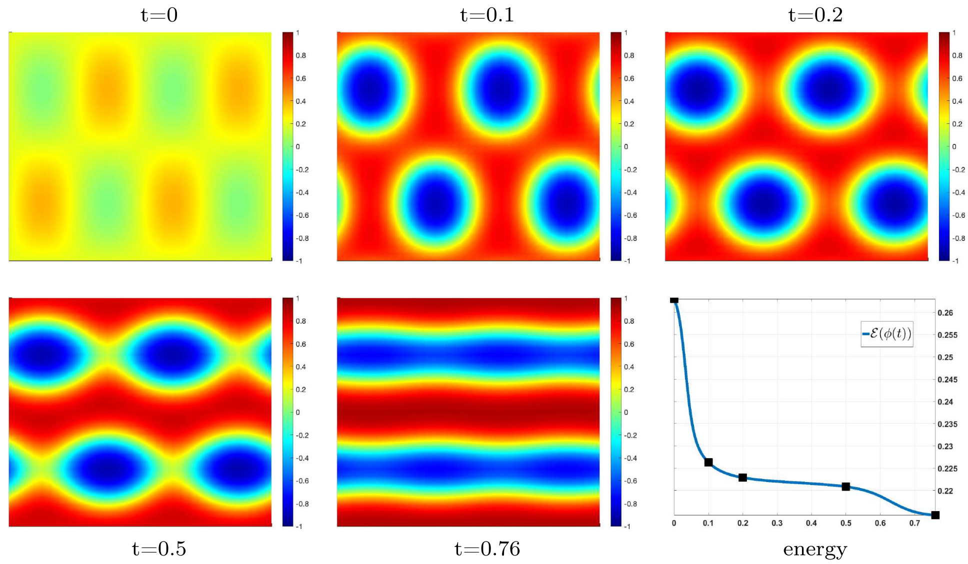

FIGURE 1. Snapshots of the phase fraction $\phi_{h,\tau}$ and time evolution of the energy.

The computational domain Ω is a unit square, $\Omega = (0,1)^2$. The system (1) and (2) is complemented by periodic boundary conditions and following initial data for the phase fraction ϕ

$$\phi_0(x,y) = 0.1\sin(4\pi x)\sin(2\pi y) + 0.6.$$

For all our computations, we use the fully discrete approximation of Problem 17 on a sequence of uniformly refined triangulations $\mathcal{T}_h$ in space and equidistant grids $\mathcal{I}_\tau$ in time. The arising nonlinear systems at each discrete time step are solved by the Newton method with absolute residual tolerance 10^{-12}. Since in our test problem the nonlinearities are polynomial, all integrals appearing in the discrete scheme can be evaluated exactly. For more general nonlinearities numerical integration can be used. Integration errors and iteration errors of the Newton method can be analyzed with slight modifications of the above-mentioned proofs.

Time snapshot of the phase fraction $\phi_{h,\tau}$ computed by our Petrov–Galerkin method are depicted in Figure 1. One can clearly observe the expected evolution from a rather uniform distribution to an almost completely separated configuration. As predicted by our theoretical results, the solution remains smooth over the whole time interval.

We now turn to the validation of the convergence rates. The parameter functions and initial conditions are chose as described above and the final time is set to $T = 0.76$. Since no analytical solution is available, the discretization error is estimated by comparing the computed solutions $(\phi_{h,\tau}, \bar{\mu}_{h,\tau})$ with those computed on uniformly refined grids in space and time. In accordance with our convergence analysis, the error quantities for the fully-discrete scheme are thus defined by

$$e_{h,\tau} = \max_{t^n \in \mathcal{I}_\tau} \|\phi_{h,\tau}(t^n) - \phi_{h/2,\tau/2}(t^n)\|_{H^1_p} + \|\bar{\mu}_{h,\tau} - \bar{\mu}_{h/2,\tau/2}\|_{L^2(0,T;H^1_p)}.$$

In order to evaluate the convergence rates of the semi-discrete scheme, we choose a very small step size τ^*, and define the corresponding error quantities as

$$e_h = \max_{t^n \in \mathcal{I}_{\tau^*}} \|\phi_{h,\tau^*}(t^n) - \phi_{h/2,\tau^*}(t^n)\|_{H^1_p} + \|\bar{\mu}_{h,\tau^*} - \bar{\mu}_{h/2,\tau^*}\|_{L^2(0,T;H^1_p)}.$$

TABLE 1. Errors and convergence rates for the semi-discrete and fully-discrete approximations.

k	e_h	eoc	$e_{h,\tau}$	eoc
0	1.4794×10^{-0}	–	1.5183×10^{-0}	–
1	3.7373×10^{-1}	1.98	3.7896×10^{-1}	2.00
2	9.2554×10^{-2}	2.01	9.2797×10^{-2}	2.02
3	2.3622×10^{-2}	1.97	2.3795×10^{-2}	1.96
4	5.9391×10^{-3}	1.99	6.0902×10^{-3}	1.96

In Table 1, we summarize the results of our computations obtained on a sequence of uniformly refined meshes with mesh size $h_k = 2^{-(3+k)}$, $k = 0, \ldots, 5$ and time steps $\tau_k = 0.16 \cdot h_k$. For the results concerning the semi-discretization, the time step is chosen $\tau^* = 0.16 \cdot 2^{-9}$. Since nested grids are used in all our computations, the error quantities defined above can be computed exactly.

The experimental order of convergence (eoc) is computed by comparing the errors of two consecutive refinements. In perfect agreement with the theoretical predictions of Theorems 15 and 27, we observe second order convergence for the total errors in space and time. The same convergence rates are obtained for each error term separately that arises in the definition of the discrete error measures e_h respectively $e_{h,\tau}$.

7. Discussion

In this paper, we studied the stability, regularity, and uniqueness of solutions to the Cahn–Hilliard equation with concentration-dependent mobility. The variational characterization of weak solutions and relative energy estimates were used as the main ingredients of our analysis, and the latter greatly simplified the handling of nonlinear terms in the problem. The basic tools of our analysis are applicable almost verbatim to discretization schemes based on variational principles, *i.e.*, Galerkin finite-element approximations in space and Petrov–Galerkin approximation in time. The variational time discretization, which is tightly related to the average vector field methods, leads to fully-implicit schemes which, however, can be solved efficiently by Newton-iterations, and which allows for a structured and transparent error analysis. The convergence results obtained in the paper are of optimal order and the result for the semi-discretization is sharp concerning regularity requirements of the solution. Some additional regularity is required for the fully-discrete scheme, which can be explained by the lack of strong stability of the Petrov–Galerkin time discretization; see [2] for details. In principle, the proposed schemes can be extended immediately to higher order in space and time. Further investigations in this direction and the extension to more complex multiphase problems, *e.g.*, the Cahn–Hilliard Navier–Stokes equations, will be topics of future research.

Appendix A. Gronwall lemmas

Let us start with recalling the following classical version of Gronwall's lemma.

Lemma 29. *Let $T > 0$, $v, g \in C[0, T]$ and $\lambda \in L^1(0, T)$ be given. Further, assume that*

$$v(t) \leq g(t) + \int_0^t \lambda(s)v(s)\,\mathrm{d}s, \qquad 0 \leq t \leq T,$$

and that $\lambda(t) \geq 0$ for a.a. $0 \leq t \leq T$. Then

$$v(t) \leq g(t) + \int_0^t g(s)\lambda(s)e^{\int_s^t \lambda(r)\,\mathrm{d}r}\,\mathrm{d}s, \qquad 0 \leq t \leq T. \tag{A.1}$$

A proof can be found in Chapter 29 of [39]. A similar result also holds on the discrete level.

Lemma 30. *Let $(u_n)_n$, $(b_n)_n$, $(c_n)_n$, and $(\lambda_n)_n$ be given positive sequences, satisfying*

$$u_n + b_n \le e^{\lambda_n} u_{n-1} + c_n, \qquad n \ge 0.$$

Then

$$u_n + \sum_{k=1}^{n} e^{\sum_{j=k+1}^{n} \lambda_j} b_k \le e^{\sum_{j=1}^{n} \lambda_j} u_0 + \sum_{k=0}^{n} e^{\sum_{j=k+1}^{n} \lambda_j} c_k, \quad n > 0. \tag{A.2}$$

Proof. The result follows immediately by induction. □

Appendix B. Proof of Lemma 24

We start with considering a single element $J = (t^{n-1}, t^n)$ and show that

$$\|\bar{u}\bar{v} - \overline{uv}\|_{0,p} \le C\tau^2(\|u\|_{2,p}\|v\|_{1,\infty} + \|u\|_{1,\infty}\|v\|_{2,p}), \tag{B.1}$$

where $\|\cdot\|_{k,p} = \|\cdot\|_{W^{k,p}(J)}$ and $\bar{a} = \bar{\pi}_\tau^0 a$ denotes the average of a over J. In addition, we denote by $\tilde{a} = a(t^{n-1/2})$ the constant interpolant at $t^{n-1/2} = (t^n + t^{n-1})/2$. Then we have

$$\begin{aligned}\|\bar{u}\bar{v} - \overline{uv}\|_{0,p} &\le \|\bar{u}\bar{v} - \tilde{u}\bar{v}\|_{0,p} + \|\tilde{u}\bar{v} - \tilde{u}\tilde{v}\|_{0,p} + \|\tilde{u}\tilde{v} - \widetilde{uv}\|_{0,p} + \|\widetilde{uv} - \overline{uv}\|_{0,p} \\ &= \text{(i)} + \text{(ii)} + \text{(iii)} + \text{(iv)}.\end{aligned}$$

In order to bound the individual terms, we utilize the super-closeness estimate

$$\|\bar{a} - \tilde{a}\|_{0,p} \le C\tau^2\|a\|_{2,p}, \tag{B.2}$$

which follows by observing that $\bar{a} - \tilde{a} = 0$ for $a \in P_1(J)$ and using the Bramble–Hilbert lemma and a scaling argument; see [10] for details. We can then estimate the first term in the above error expansion by

$$\text{(i)} \le \|\bar{u} - \tilde{u}\|_{0,p}\|\bar{v}\|_{0,\infty} \le C\tau^2\|u\|_{2,p}\|v\|_{0,\infty},$$

and similarly, we see that (ii) $\le Ch^2\|u\|_{0,\infty}\|v\|_{2,p}$. The third term vanishes identically, *i.e.*, (iii) $= 0$, and using (B.2) again, the last term can be bounded by

$$\text{(iv)} \le C\tau^2\|uv\|_{2,p} \le C'\tau^2(\|u\|_{2,p}\|v\|_{1,\infty} + \|u\|_{1,\infty}\|v\|_{2,p}).$$

This proves the estimate (B.1) for one single element $J = (t^{n-1}, t^n)$. The global projection estimate (40) then follows by summation over the elements and using the bounds for the continuous embedding $\|a\|_{L^\infty(0,T)} \le \|a\|_{W^{1,\infty}(0,T)} \le C\|a\|_{W^{2,p}(0,T)}$. □

Appendix C. Regularity

We now discuss improved regularity results for the weak solution (ϕ, μ) of (1), (2) and the initial data are given by $\phi_0 \in H_p^k(\Omega)$, $k \in \{2, 3\}$. The basic argument relies on Galerkin approximation and uniform *a priori* estimates, which are obtained by testing the discretized variational problems with approximations for higher order derivatives and using energy-type estimates and Gronwall-type inequalities.

Using simplifications of the results and proofs presented in [8], one can see that for initial value $\phi_0 \in H_p^2(\Omega)$ the Galerkin approximations (ϕ_N, μ_N) satisfy

$$\phi_N \in L^\infty(0, T; H_p^2(\Omega)) \cap L^2(0, T; H_p^4(\Omega)), \tag{C.1}$$

$$\partial_t\phi_N \in L^2(0, T; L^2(\Omega)), \tag{C.2}$$

$$\mu_N \in L^\infty(0,T;L^2(\Omega)) \cap L^2(0,T;H^2_p(\Omega)), \tag{C.3}$$

with uniform bounds for the respective norms, *i.e.*, independent of the level N of the approximation. This immediately leads to the bounds of Lemma 2 for $k=2$. Let us note that in three space dimensions, the maximal time T of validity has to be chosen sufficiently small, depending on the norm of the initial data, while in two space dimensions T can be chosen arbitrary; we refer to [8] for details.

Now assume that $\phi_0 \in H^3_p(\Omega)$. We may then test the Galerkin approximation of the weak formulation (7) with $v_N = -\Delta^3\phi_N$, and obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\|\nabla\Delta\phi_N\|_0^2 - \langle \nabla\operatorname{div}(m(\phi_N)\nabla\mu_N), \nabla\Delta^2\phi_N\rangle = 0.$$

By elementary computations, one can verify that

$$\begin{aligned}\nabla\operatorname{div}(m(\phi_N)\nabla\mu_N) &= b(\phi_N)\nabla\Delta\mu_N + 2b'(\phi_N)\nabla\phi_N\Delta\mu_N + b'(\phi_N)\Delta\phi_N\nabla\mu_N + b''(\phi_N)|\nabla\phi_N|^2\nabla\mu_N\\ &= \text{(i)} + \text{(ii)} + \text{(iii)} + \text{(iv)}.\end{aligned}$$

From the regularity result for $k=2$ and standard embedding results, we already know that ϕ_N is bounded in $L^\infty(0,T;L^\infty(\Omega))$. We can then decompose the first term by

$$\text{(i)} = -b(\phi_N)\nabla\Delta^2\phi_N + \nabla\Delta(f'(\phi_N)),$$

and further estimate the Laplacian of f' by

$$\begin{aligned}\|\nabla\Delta(f'(\phi_N))\|_0^2 &\le C(f^{(4)})\|\nabla\phi_N\|_{0,6}^6 + C(f^{(3)})\|\nabla\phi_N\Delta\phi_N\|_0^2 + C(f^{(2)})\|\nabla\Delta\phi_N\|_0^2\\ &\le C(f^{(4)})\|\nabla\phi_N\|_{0,6}^6 + C(f^{(3)})\|\nabla\Delta\phi_N\|_{0,2}^2\|\nabla\phi_N\|_{0,4}^2 + C(f^{(2)})\|\nabla\Delta\phi_N\|_0^2.\end{aligned}$$

Using the improved bounds for ϕ_N for $k=2$, we can also estimate the other terms by

$$\begin{aligned}\langle\text{(ii)},\nabla\Delta^2\phi_N\rangle &\le \delta\|\nabla\Delta^2\phi_N\|_0^2 + C(b_3,\delta)\|\Delta\mu_N\nabla\phi_N\|_0^2 \le \delta\|\nabla\Delta^2\phi_N\|_0^2 + C(b_3,\delta)\|\Delta\mu_N\|_{0,4}\|\nabla\phi_N\|_{0,4}^2\\ &\le 2\delta\|\nabla\Delta^2\phi_N\|_0^2 + C(b_3,\delta)\|\Delta\mu_N\|_{0,2}^2\|\nabla\phi_N\|_{0,4}^2 + C(b_3,\delta)\|\nabla\Delta(f'(\phi_N))\|_0\|\nabla\phi_N\|_{0,4}^2,\\ \langle\text{(iii)},\nabla\Delta^2\phi_N\rangle &\le \delta\|\nabla\Delta^2\phi_N\|_0^2 + C(b_3,\delta)\|\Delta\phi_N\nabla\mu_N\|_0^2 \le \delta\|\nabla\Delta^2\phi_N\|_0^2 + C(b_3,\delta)\|\nabla\Delta\phi_N\|_0^2\|\nabla\mu_N\|_{0,4}^2,\\ \langle\text{(iv)},\nabla\Delta^2\phi_N\rangle &\le \delta\|\nabla\Delta^2\phi_N\|_0^2 + C(b_4,\delta)\||\nabla\phi_N|^2\nabla\mu_N\|_0^2 \le \delta\|\nabla\Delta^2\phi_N\|_0^2 + C(b_4,\delta)\|\nabla\phi_N\|_{0,8}^4\|\nabla\mu_N\|_{0,4}^2.\end{aligned}$$

Setting $y(t) = \|\nabla\Delta\phi_N(t)\|_0^2$, a combination of the above estimates directly leads to

$$y(t) + (c_0b_1 - 4\delta)\int_0^t \|\nabla\Delta^2\phi_N\|_0^2 \le y(0) + C\int_0^t g(s)y(s)\,\mathrm{d}s + C\int_0^t h(s)\,\mathrm{d}s,$$

with $g(s) \le C + \|\nabla\mu_N\|_{0,4}^2 + \|\nabla\phi_N\|_{0,4}^2$ and $h(s) \le C + \|\nabla\mu_N\|_{0,4}^2\|\Delta\phi_N\|_2^4 + \|\nabla\phi_N\|_{0,4}^4$. From the improved regularity (C.1) for $k=2$, one can deduce that g,h are uniformly bounded in $L^1(0,T)$. Choosing δ sufficiently small and applying the Lemma 29 together with the previous estimates, now leads to

$$\phi_N \in L^\infty(0,T;H^3_p(\Omega)) \cap L^2(0,T;H^5_p(\Omega)), \tag{C.4}$$

$$\mu_N \in L^\infty(0,T;H^1_p(\Omega)) \cap L^2(0,T;H^3_p(\Omega)), \tag{C.5}$$

with uniform bounds (independent of N) for the corresponding norms. A straight forward computation shows

$$\partial_t\phi_N \in L^2(0,T;H^1_p(\Omega)), \tag{C.6}$$

together with corresponding uniform bounds. Taking the limit with $N\to\infty$, maybe after choosing a weakly convergent sub-sequence, shows that corresponding bounds also hold for the weak solution $u = \lim_N u_N$. Hence, at least one regular weak solution (ϕ,μ) exists satisfying the bounds of Lemma 2. Let us emphasize that the bounds hold for all $T>0$ in two space dimensions, while $T>0$ has to be chosen sufficiently small, depending on the problem data, in three dimensions.

Appendix D. Limiting process for the stability estimate

For ease of notation, we denote the space-time cylinder by $\Omega_T := \Omega \times (0,T)$ in the following. Let $(\phi,\mu) \in \mathbb{W}(0,T) \times \mathbb{Q}(0,T)$ be given a periodic weak solution of the Cahn–Hilliard system (1) and (2). Then by the mollification procedure proposed by Meyers and Serrin [36], one can construct a sequence $(\phi_n,\mu_n) \in \mathbb{W}(0,T) \cap C^\infty(\Omega_T) \times \mathbb{Q}(0,T) \cap C^\infty(\Omega_T)$ of smooth approximations, such that

$$\phi_n \to \phi \text{ in } \mathbb{W}(0,T) \quad \text{and} \quad \mu_n \to \mu \text{ in } \mathbb{Q}(0,T) \quad \text{with } n \to \infty.$$

Similar as in the proof of Theorem 6, we can define residuals $r_{1,n}$, $r_{2,n}$ such that

$$\begin{aligned} \langle \partial_t \phi_n(t), v\rangle + \langle b(\phi_n(t))\nabla\mu_n(t), \nabla v\rangle &=: \langle r_{1,n}(t), v\rangle \\ \langle \mu_n(t), w\rangle - \gamma\langle \nabla\phi_n(t), \nabla w\rangle - \langle f'(\phi_n(t)), w\rangle &=: \langle r_{2,n}(t), w\rangle \end{aligned}$$

for all test functions $v, w \in H^1_p(\Omega)$ and all $0 \le t \le T$. Since (ϕ,μ) is a periodic weak solution of (1) and (2), one can immediately see that

$$\begin{aligned} \langle r_{1,n}, v\rangle &= \langle \partial_t\phi_n - \partial_t\phi, v\rangle + \langle b(\phi_n)\nabla\mu_n - b(\phi)\nabla\mu, \nabla v\rangle \\ \langle r_{2,n}, w\rangle &= \langle \mu_n - \mu, w\rangle - \langle \nabla(\phi_n - \phi), \nabla w\rangle - \langle f'(\phi_n) - f'(\phi), w\rangle \end{aligned}$$

for all $v, w \in H^1_p(\Omega)$ and a.a. $0 \le t \le T$. From the convergence of (ϕ_n,μ_n) to (ϕ,μ) in the norms stated above, and the assumptions on the coefficients, one can deduce that

$$\lim_{n\to\infty} \|r_{1,n}\|_{-1}^2 = 0, \quad \lim_{n\to\infty} \|r_{2,n}\|_1^2 = 0.$$

Similarly, we choose for given $(\hat\phi,\hat\mu) \in \mathbb{W}(0,T) \cap W^{1,1}(0,T;L^2(\Omega) \times \mathbb{Q}(0,T)$ a sequence of smooth approximations $(\hat\phi_m,\hat\mu_m)$ such that

$$\hat\phi_m \to \hat\phi \text{ in } \mathbb{W}(0,T) \cap W^{1,1}(0,T;L^2(\Omega)) \text{ and } \hat\mu_m \to \hat\mu \text{ in } \mathbb{Q}(0,T)$$

with $m \to \infty$, and define corresponding residuals

$$\begin{aligned} \langle \partial_t\hat\phi_m, v\rangle + \langle b(\phi_n)\nabla\hat\mu_m, \nabla v\rangle &=: \langle \tilde r_{1,m}, v\rangle \\ \langle \hat\mu_m, w\rangle - \gamma\langle \nabla\hat\phi_m, \nabla w\rangle - \langle f'(\hat\phi_m), w\rangle &=: \langle \tilde r_{2,m}, w\rangle \end{aligned}$$

for all $v, w \in H^1_p(\Omega)$ and all $0 \le t \le T$. Using (10) and (11), we immediately deduce that

$$\begin{aligned} \langle \tilde r_{1,m}, v\rangle &= \langle \hat r_1, v\rangle + \langle \partial_t\hat\phi_m - \partial_t\hat\phi, v\rangle + \langle b(\phi_n)\nabla(\hat\mu_m - \hat\mu), \nabla v\rangle \\ \langle \tilde r_{2,m}, w\rangle &= \langle \hat r_2, w\rangle + \langle \hat\mu_m - \hat\mu, w\rangle - \langle \nabla(\hat\phi_m - \hat\phi), \nabla w\rangle - \langle f'(\hat\phi_m) - f'(\hat\phi), w\rangle \end{aligned}$$

for all $v, w \in H^1_p(\Omega)$ and a.a. $0 \le t \le T$. Using the convergence of $(\hat\phi_m,\hat\mu_m)$ towards $(\hat\phi,\hat\mu)$ in the corresponding norms and the assumptions on the parameters, one can see that

$$\lim_{m\to\infty} \|\tilde r_{1,m} - r_{1,m}\|_{-1}^2 = 0, \quad \lim_{m\to\infty} \|\tilde r_{2,m} - r_{2,m}\|_1^2 = 0.$$

With a slight adoption of the proof in Theorem 6, we now obtain the stability estimate

$$\begin{aligned} &\mathcal{E}_\alpha(\phi_n(t)|\hat\phi_m(t)) + \int_0^t \mathcal{D}_{\phi_n}(\mu_n(s)|\mu_m(s))\,\mathrm{d}s \\ &\qquad \le Ce^{ct}\mathcal{E}_\alpha(\phi_n(0)|\hat\phi_m(0)) + Ce^{ct}\int_0^t \|\tilde r_{1,m} - r_{1,n}\|_{-1}^2 + \|\tilde r_{2,m} - r_{2,n}\|_1^2\,\mathrm{d}s, \end{aligned}$$

with constants c, C for all n, m, only depending on the uniform bounds

$$\|\phi_n\|_{L^\infty(H^1_p)}, \|\hat{\phi}_m\|_{L^\infty(H^1_p)}, \|\partial_t\hat{\phi}_m\|_{L^1(L^2)}.$$

Hence, the constants c, C in the above estimate can be chosen independent of m, n. Using the strong convergence of the residuals in the corresponding norms, we may pass to the limit in the integral on the right-hand side. Furthermore, application of Egorov's Theorem yields almost everywhere convergence of $b(\phi_n)$. With this and standard weak convergence results using Fatou's Lemma yields

$$\int_0^t \mathcal{D}_\phi(\mu(s)|\hat{\mu}(s))\,\mathrm{d}s \leq \liminf_{m\to\infty}\liminf_{n\to\infty}\int_0^t \mathcal{D}_{\phi_n}(\mu_n(s)|\hat{\mu}_m(s))\,\mathrm{d}s,$$

which allows us to pass to the limit in the relative dissipation term. A similar process is used to derive the energy inequality for the standard weak solution of (1) and (2). By the continuous embedding of $W(0,T)$ into $C([0,T]; H^1_p(\Omega))$, we obtain convergence of the energy $\mathcal{E}_\alpha(\phi_n(t)|\hat{\phi}_m(t)) \to \mathcal{E}(\phi|\hat{\phi})$ with $m, n \to \infty$, and in summary, we thus obtain (14).

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