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A Second Order Accurate in Time, Energy Stable Finite Element Scheme for the Flory-Huggins-Cahn-Hilliard Equation

Maoqin Yuan[1,5], Wenbin Chen[2,*], Cheng Wang[3], Steven M. Wise[4] and Zhengru Zhang[5]

[1] *School of Science & Arts, China University of Petroleum-Beijing at Karamay, Karamay, Xinjiang 834000, China*
[2] *Shanghai Key Laboratory of Mathematics for Nonlinear Sciences, School of Mathematical Sciences, Fudan University, Shanghai 200433, China*
[3] *Department of Mathematics, The University of Massachusetts, North Dartmouth, MA 02747, USA*
[4] *Department of Mathematics, The University of Tennessee, Knoxville, TN 37996, USA*
[5] *School of Mathematical Sciences, Beijing Normal University and Laboratory of Mathematics and Complex Systems, Ministry of Education, Beijing 100875, China*

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Abstract. In this paper, we propose and analyze a second order accurate in time, mass lumped mixed finite element scheme for the Cahn-Hilliard equation with a logarithmic Flory-Huggins energy potential. The standard backward differentiation formula (BDF) stencil is applied in the temporal discretization. In the chemical potential approximation, both the logarithmic singular terms and the surface diffusion term are treated implicitly, while the expansive term is explicitly updated via a second-order Adams-Bashforth extrapolation formula, following the idea of the convex-concave decomposition of the energy functional. In addition, an artificial Douglas-Dupont regularization term is added to ensure the energy dissipativity. In the spatial discretization, the mass lumped finite element method is adopted. We provide a theoretical justification of the unique solvability of the mass lumped finite element scheme, using a piecewise linear element. In particular, the positivity is always preserved for the logarithmic arguments in the sense that the phase variable is always located between -1 and 1. In fact, the singular nature of the implicit terms and the mass lumped approach play an essential role in the positivity preservation in the discrete setting. Subsequently, an unconditional energy stability is proven for the proposed numerical scheme. In addition, the convergence analysis and error estimate of the numerical scheme are also presented. Two numerical experiments are carried out to verify the theoretical properties.

*Corresponding author.
Emails: mqyuan@mail.bnu.edu.cn (M. Yuan), wbchen@fudan.edu.cn (W. Chen), cwang1@umassd.edu (C. Wang), swise1@utk.edu (S. Wise), zrzhang@bnu.edu.cn (Z. Zhang)

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1 Introduction

The Cahn-Hilliard equation plays an important role in materials science and biological applications. It was constructed by Cahn and Hilliard [9] as a conserved gradient flow with respect to the free energy of an isothermal, isotropic fluid. Usually, the evolution of the system is driven by the gradient of the singular Flory-Huggins free energy and describes phase separation processes with respect to the concentration ϕ. Phase separation can be observed, e.g., when a binary alloy is cooled down sufficiently. One then may observe spinodal decomposition, whereby the material quickly becomes inhomogeneous, forming a fine-grained structure in which each of the two phases appears in a more or less alternating pattern. In the second stage, which is called coarsening, and which occurs at a slower time scale, the average size of phases in the microstructure grows with time. Such phenomena play an essential role in the structural and mechanical properties of the material [4, 17, 38]. The equation is flexible, allowing several variants–based on the choices of mobility and free energy density–which are relevant in different contexts and for disparate physical and biological processes in which phase separation and coarsening/clustering processes can be observed (see [34, 37]).

There have been a lot of theoretical analyses and numerical approximations for these gradient flows in the two-phase case. The existence of solutions and attractors to the Cahn-Hilliard equation with degenerate mobility and logarithmic nonlinearities has been proved in [24,36,44,45]. For the time integration, several numerical techniques have been applied to design the energy dissipative schemes for gradient flows [2,5,6,10,15,29,54], including convex splitting [25,55,57], stabilization [29,49], auxiliary variable approaches [1] (such as invariant energy quadrature method [60, 64] and scalar auxiliary variable version [16,46–48]). In particular, the convex splitting method has been widely used to solve various phase field equations by virtue of its theoretical advantages [11, 13, 26, 30, 31, 50, 52]. Meanwhile, the IEQ and SAV approaches can be used to design linear and energy stable numerical schemes, which can improve the computational efficiency of many relatively complex problems [41, 43, 48, 51, 56, 61], and have been rapidly developed in recent years. And also, the stabilization method turns out to be a useful tool to extend the above methods to a higher-order accuracy of time [28, 29, 48, 58, 59]. These numerical techniques possess two main features: mass conservation and energy dissipativity (conditionally/unconditionally).

Meanwhile, most above-mentioned works have been focused on the physical model with a polynomial approximation in the energy potential expansion. For the Cahn-Hilliard equation with the original Flory-Huggins logarithmic energy potential, a theoretical justification of the positivity-preserving property for the logarithmic arguments has always been an essential difficulty, at both the analytic and numerical levels. There have been quite a few works on the positivity-preserving analysis of the numerical solutions for the Cahn-Hilliard equation with logarithmic free energy. In [18], a finite element scheme was proposed, based on the backward Euler temporal discretization for the Flory-Huggins-Cahn-Hilliard equation, and the positivity-preserving property of the numerical solution was proven under a constraint on the time step. In fact, such a time step constraint comes from the explicit treatment of the concave expansive term, so that the monotone property of the implicit parts is not automatically ensured. To overcome this shortcoming, Chen et al. [14] applied the convex splitting approach to the equation, combined with finite difference spatial discretization, in which the singular logarithmic terms and the surface diffusion part are computed implicitly, while an explicit update is applied to the explicit part. In turn, both the unconditionally unique solvability and positivity-preserving feature have been theoretically justified for the numerical scheme, and an optimal convergence estimate has been derived in the $\ell^\infty(0,T;H^{-1})\cap\ell^2(0,T;H^1)$ norm. Following similar theoretical framework, more positivity-preserving numerical schemes have been proposed and analyzed for a variety of the Cahn-Hilliard type equations with singular energy potential, with finite difference spatial discretization; see the related works [12, 19–21, 32, 33, 40, 42, 62, 63] and the reference therein. It is noticed that these approaches have been based on the implicit treatment of the singular logarithmic terms, due to their convexity. On the other hand, there have also been some works of positivity-preserving numerical schemes for certain gradient flows with logarithmic energy potential, such as [27] for the Poisson-Nernst-Planck system, based on the Lagrange multiplier method. The energy functional has to be modified in this work, because of the scalar auxiliary variable (SAV) method used.

In fact, most existing numerical works of positivity-preserving analysis for gradient flows with singular energy potential have been focused on the finite difference spatial discretization, because of its simplicity in the numerical representation. In comparison with the finite difference approximation, the finite element (FEM) method allows for flexible, adaptive meshes and has a systematic theoretical framework. Inspired by the scientific idea in [14], we would like to extend the theoretical framework of positivity preserving scheme to the fully discrete finite element scheme. However, a direct extension to the FEM method would face a serious difficulty in the numerical analysis. It is well-known that the standard-conforming FEM fails to satisfy the discrete maximum principle, thus it is a great challenge to derive the rigid theoretical analysis of positivity preserving in the finite element framework. The main contribution of this paper is that we propose a second order accurate in time, mass-lumped FEM numerical scheme for the Cahn-Hilliard equation with logarithmic free energy. In more details, the standard backward differentiation formula (BDF) stencil is applied in the temporal discretization. In the chemical potential approximation, both the logarithmic singular terms and the surface diffusion term are treated implicitly, while the expansive term is explicitly updated via a second-order Adams-Bashforth extrapolation formula, following the idea of the convex-concave decomposition of the energy functional. In addition, an artificial Douglas-Dupont regularization term is added to ensure the energy dissipativity. Meanwhile, as mentioned earlier, a direct application of the positivity-preserving analysis techniques for the finite difference method, as reported in [14], is not available to the standard FEM method, due to the difficulty to ensure the point-wise positivity of the numerical solution in the standard FEM because of the non-diagonal mass matrix. Instead, a lumped mass FEM is chosen to diagonalize the mass matrix, that is, the diagonal elements are the row sums of the original mass matrix [53]. With the mass lumped FEM approximation, the positivity-preserving analysis of the numerical scheme could be theoretically justified, with the help of the singular nature of the logarithmic terms as the phase variable approaches the singular limit values of 1 and -1. A modified energy stability of the proposed mass-lumped FEM will be proven, with the help of the artificial Douglas-Dupont regularization term. In addition, the convergence analysis and error estimate will be theoretically established, in the $\ell^\infty(0,T;H^{-1})\cap\ell^2(0,T;H^1)$ norm.

The rest of this article is organized as follows. In Section 2, we review the Sobolev spaces and the corresponding weak form, as well as the mass lumped FEM method. In Section 3, we propose the fully discrete numerical scheme, demonstrate the positivity-preserving property of the numerical solutions. The modified energy stability analysis and the optimal rate convergence analysis are provided in Section 4. Finally, this paper ends with some concluding remarks in the last section.

2 The weak formulation

In this section, we provide a review on the basic property of the Cahn-Hilliard equation with the logarithmic potential, as well as the corresponding weak formulation. To this end, we consider the following (total) free energy:

$$E(\phi)=\int_\Omega f(\phi)+\frac{\varepsilon^2}{2}|\nabla\phi|^2 d\mathbf{x}, \tag{2.1a}$$

$$f(\phi)=(1+\phi)\ln(1+\phi)+(1-\phi)\ln(1-\phi)-\frac{\theta_0}{2}\phi^2, \tag{2.1b}$$

where ϕ is the phase variable and $f(\phi)$ is a double-well logarithmic potential, often approximated by a smooth polynomial function, with minimums located at the two attraction points that represent pure phases $\phi=\pm 1$, and ε, θ_0 are positive constants associated with the diffuse interface width. In turn, the Cahn-Hilliard equation with respect to the energy functional (2.1) is defined as

$$\partial_t\phi=\nabla\cdot(\mathcal{M}(\phi)\nabla\mu) \tag{2.2}$$

subject to the initial condition

$$\phi(\mathbf{x},0)=\phi_0(\mathbf{x}),\quad \mathbf{x}\in\Omega. \tag{2.3}$$

For simplicity, we are using periodic boundary conditions on square area $\Omega = [0,L]^2$. The variable μ is the chemical potential

$$\mu := \delta_\phi E = \ln(1+\phi) - \ln(1-\phi) - \theta_0\phi - \varepsilon^2\Delta\phi. \tag{2.4}$$

$\mathcal{M}(\phi) > 0$ is the mobility function, which is often taken to be either constant [22,23,39] or of degenerate type [3,4,8,14,24]. Eq. (2.2) has been proposed to model phase separation in a binary mixture composed of two species which is quenched into an unstable state. It can be regarded as a type of H^{-1} (conserved) gradient flow with respect to the energy functional (2.1), satisfying the following properties:

- mass conservation

$$\int_\Omega \phi(\mathbf{x},t)d\mathbf{x} = \int_\Omega \phi(\mathbf{x},0)d\mathbf{x}, \quad \forall t > 0,$$

- energy dissipation

$$\frac{d}{dt}E(\phi(t)) = -\int_\Omega \mathcal{M}(\phi)|\nabla\mu|^2 d\mathbf{x} \le 0.$$

Now, we use standard notation for the function spaces and norms. In particular, we denote the standard norms for the Sobolev spaces $W^{m,p}(\Omega)$ by $\|\cdot\|_{m,p}$. When $p=2$, $W^{m,2}(\Omega)$ is a Hilbert space denoted by $H^m(\Omega)$ with the norm $\|\cdot\|_m$. Let $C^\infty_{per}(\Omega)$ be the set of all restrictions onto Ω of all real-valued, L-periodic, $C^\infty(\Omega)$-functions on $\mathbb{R}^2$. For each integer $q \ge 0$, let $H^q_{per}(\Omega)$ be the closure of $C^\infty_{per}(\Omega)$ in the usual Sobolev norm $\|\cdot\|_q$, and $H^{-q}_{per}(\Omega)$ be the dual space of $H^q_{per}(\Omega)$. Note that $H^0_{per}(\Omega) = L^2(\Omega)$, and denote by $(\cdot,\cdot)$ the L^2 inner-product on domain Ω, which, naturally induces the L^2 norm $\|\cdot\|$.

The mixed weak formulation of Cahn-Hilliard equation (2.2) is defined as follows: find $(\phi,\mu) \in L^2(0,T;H^1_{per}(\Omega))$, with $\phi_t \in L^2(0,T;H^{-1}_{per}(\Omega))$, satisfying

$$\begin{cases} (\phi_t,v) + (\mathcal{M}(\phi)\nabla\mu,\nabla v) = 0, & \forall v \in H^1_{per}(\Omega), \\ (\mu,w) = (g(\phi) - \theta_0\phi,w) + \varepsilon^2(\nabla\phi,\nabla w), & \forall w \in H^1_{per}(\Omega), \end{cases} \tag{2.5}$$

for almost every $t \in [0,T]$, where

$$g(u) = \ln(1+u) - \ln(1-u).$$

Let $\mathcal{T}_h = K$ be a quasi-uniform, shape-regular triangulation of Ω, with mesh size h. By h_e we denote the diameter of each triangle $e \in \mathcal{T}_h$. The symbol Δ_e denotes the area of e. Then, as usual,

$$h = \max_{e \in \mathcal{T}_h} h_e.$$

Since the mesh is shape regular, we can assume that $\frac{h_e^2}{\Delta_e}$ is uniformly bounded by one constant

$$C_{\mathcal{T}}: \frac{h_e^2}{\Delta_e} \leq C_{\mathcal{T}}.$$

Based on the quasi-uniform triangulated mesh $\mathcal{T}_h$, the finite element space is defined as

$$S_h := \left\{ v \in H^1_{per}(\Omega) | v \text{ is piecewise linear on each } e \in \mathcal{T}_h \right\} = \text{span}\left\{ \chi_j | j = 1, \cdots, N_p \right\},$$

where $\chi_j \in S_h$ is the j^{th} Lagrange nodal basis function, which has the property $\chi_j(P_i) = \delta_{i,j}$. Define

$$\mathring{S}_h := S_h \cap L^2_0(\Omega) \quad \text{with } L^2_0(\Omega) = \left\{ v \in L^2(\Omega) | (v,1) = 0 \right\}$$

the function space with zero mean in $L^2(\Omega)$.

The standard mixed finite element scheme of (2.5) will lead to a theoretical difficulty with regard to justifying the positivity-preserving property. To overcome this difficulty, we apply a mass lumped FEM instead, which is a modification of standard FEM for solving parabolic equations. It simplifies the computation for the inverse of mass matrix and overcomes the shortcoming of the standard FEM that it cannot preserve the maximum principle for homogeneous parabolic equations. In more details, let $P_{e,k}$, $k=1,2,3$, be the three vertices of triangle e. The construction of the lumped mass inner product can be carried out as follows: we first introduce the quadrature formula on e,

$$Q_h(f) := \sum_{e \in \mathcal{T}_h} Q_e(f), \quad \forall f \in C(\Omega; \mathbb{R}), \tag{2.6}$$

where

$$Q_e(f) := \frac{\Delta_e}{3} \sum_{k=i}^{3} f(P_{e,k}) \approx \int_e f d\mathbf{x}.$$

It is straightforward to confirm that $Q_h(\chi_j \chi_k) = 0$ for $k \neq j$, so that Q_h has the following diagonalization property:

$$Q_h(\chi_j \chi_k) = \delta_{j,k} Q_h(\chi_j^2), \quad j,k = 1, \cdots, N_p. \tag{2.7}$$

Furthermore,

$$Q_h(\chi_j^2) = \sum_{e \in \mathcal{T}_h} Q_e\left(\chi_j^2\right) = \frac{1}{3} \text{area}\left(D_j\right), \quad D_j := \text{supp}(\chi_j). \tag{2.8}$$

We may now define an approximation of the canonical inner product on S_h by

$$(\psi, \eta)_Q := Q_h(\psi \eta), \quad \forall \psi, \eta \in S_h. \tag{2.9}$$

Likewise, we define $\|\eta\|_Q := \sqrt{(\eta,\eta)_Q}$ for any $\eta \in S_h$. This norm is observed to be equivalent to the standard $\|\cdot\|_{L^2}$ norm on S_h by considering each triangle separately.

To facilitate the analysis below, we have to modify the definition of the discrete Laplacian operator and the discrete H^{-1} norm. In fact, the primary difference is in the integral definition.

Definition 2.1. *The discrete Laplacian operator* $\Delta_h : S_h \to \mathring{S}_h$ *is defined as follows: for any* $v_h \in S_h$, $\Delta_h v_h \in \mathring{S}_h$ *denotes the unique solution to the problem*

$$(\Delta_h v_h, \chi)_Q = -(\nabla v_h, \nabla \chi), \quad \forall \chi \in S_h.$$

It is straightforward to show that, by restricting the domain, $\Delta_h : \mathring{S}_h \to \mathring{S}_h$ is invertible, and for any $v_h \in \mathring{S}_h$, we have

$$\left(\nabla(-\Delta_h)^{-1} v_h, \nabla \chi\right) = (v_h, \chi)_Q, \quad \forall \chi \in S_h.$$

Definition 2.2. *The discrete* H^{-1} *norm* $\|\cdot\|_{-1,Q}$, *is defined as follows:*

$$\|v_h\|_{-1,Q} := \sqrt{(v_h, (-\Delta_h)^{-1} v_h)_Q}, \quad \forall v_h \in \mathring{S}_h. \tag{2.10}$$

3 The fully discrete numerical scheme

In this section, we propose the fully discrete scheme based on the lumped mass FEM, and establish the positivity-preserving property, energy stability and convergence analysis at the theoretical level. For simplicity, we consider the mobility $\mathcal{M}(\phi) = 1$, and propose the following second order accurate in time, fully discrete finite element numerical scheme for the Cahn-Hilliard equation (2.5): given $\phi_h^n, \phi_h^{n-1} \in S_h$, find $\phi_h^{n+1}, \mu_h^{n+1} \in S_h$, such that

$$\begin{cases} \left(\dfrac{\frac{3}{2}\phi_h^{n+1} - 2\phi_h^n + \frac{1}{2}\phi_h^{n-1}}{\tau}, v_h\right)_Q + (\nabla \mu_h^{n+1}, \nabla v_h) = 0, & \forall v_h \in S_h, \\ (\mu_h^{n+1}, w_h)_Q = \left(g(\phi_h^{n+1}) - \theta_0 \check{\phi}_h^{n+1}, w_h\right)_Q + \varepsilon^2 (\nabla \phi_h^{n+1}, \nabla w_h) & \\ \qquad\qquad + A\tau(\nabla(\phi_h^{n+1} - \phi_h^n), \nabla w_h), & \forall w_h \in S_h, \end{cases} \tag{3.1}$$

where $\check{\phi}_h^{n+1} = 2\phi_h^n - \phi_h^{n-1}$. Obviously, the scheme requires an initialization step for $n=0$. To this end, we introduce the Ritz projection operator $R_h : H^1_{per}(\Omega) \to S_h$, satisfying

$$(\nabla(R_h u - u), \nabla \chi) = 0, \quad \forall \chi \in S_h, \quad (R_h u - u, 1) = 0. \tag{3.2}$$

The initial data are chosen so that $\phi_h^0 = R_h \phi^0$.

If a solution to the proposed numerical scheme (3.1) exists, it is clear that, for any $n \in \mathbb{N}$,

$$\bar{\phi}_h^0 := |\Omega|^{-1}(\phi_h^0, 1)_Q = |\Omega|^{-1}(\phi_h^1, 1)_Q = \cdots = |\Omega|^{-1}(\phi_h^n, 1)_Q = \bar{\phi}_h^n,$$

with $|\bar{\phi}_h^n| < 1$. Thus we expect

$$(\phi_h^n - \bar{\phi}_h^0, 1)_Q = 0.$$

In addition, the following technical lemmas are needed in the positivity-preserving analysis.

The following lemma is one finite element version of Lemma 2.8 in [14] where the Fourier analysis was used, here we use the discrete Gagliard-Nirenberg inequality.

Lemma 3.1. *Suppose that $\xi_1,\xi_2\in S_h$ with $(\xi_1-\xi_2,1)=0$, that is, $\xi_1-\xi_2\in\mathring{S}_h$, and assume that $\|\xi_1\|_\infty<1$, $\|\xi_2\|_\infty\le M$. Then, we have the following estimate:*

$$\left\|-\Delta_h^{-1}(\xi_1-\xi_2)\right\|_\infty\le C_1, \tag{3.3}$$

where $C_1>0$ depends only upon M and Ω. In particular, C_1 is independent of the mesh spacing h.

Proof. By the discrete Gagliard-Nirenberg inequality (for example, see Theorem 2.8 in [35]): if Ω is convex and polyhedral, then for any $\Psi_h\in S_h$,

$$\|\Psi_h\|_{L^\infty}\le C\|\Delta_h\Psi_h\|^{\frac{d}{2(6-d)}}\|\Psi_h\|_{L^6}^{\frac{3(4-d)}{2(6-d)}}+C\|\Psi_h\|_{L^6},\quad (d=2,3).$$

Now combining with the following L^p interpolation inequality

$$\|\Psi_h\|_{L^6}\le\|\Psi_h\|^{\frac{1}{3}}\|\Psi_h\|_{L^\infty}^{\frac{2}{3}},$$

and by simple calculations, we have another discrete Gagliard-Nirenberg inequality:

$$\|\Psi_h\|_{L^\infty}\le C\|\Delta_h\Psi_h\|^{\frac{d}{4}}\|\Psi_h\|^{1-\frac{d}{4}}+C\|\Psi_h\|,\quad (d=2,3). \tag{3.4}$$

It is obvious that $\xi_1-\xi_2\in\mathring{S}_h$, let $\Psi_h:=-\Delta_h^{-1}(\xi_1-\xi_2)$, we directly obtain

$$\|-\Delta_h^{-1}(\xi_1-\xi_2)\|_{L^\infty}\le C\|\xi_1-\xi_2\|_{L^2}\le C(\|\xi_1\|_{L^\infty}+\|\xi_2\|_{L^\infty})\le C(M+1):=C_1,$$

where the estimate $\|-\Delta_h^{-1}(\xi_1-\xi_2)\|\le C\|\xi_1-\xi_2\|$ is used. $\square$

Lemma 3.2. *For any $\phi\in S_h$ and any piecewise linear Lagrange nodal basis element χ_j, we have*

$$(\nabla\phi,\nabla\chi_j)\le\sum_{e\in D_j}\frac{h_e^2}{2\Delta_e}\sum_{i=1}^{3}\phi(P_{e,i}) \tag{3.5}$$

on $\mathcal{T}_h$ with mesh size h_e.

Proof. Let $P_i=(x_i,y_i)$, $(i=1,2,3)$ be the three vertex points of e, then

$$\begin{aligned}\frac{\partial\phi}{\partial x}&=\frac{1}{2\Delta_e}(\phi(P_1)(y_2-y_3)+\phi(P_2)(y_3-y_1)+\phi(P_3)(y_1-y_2)),\\ \frac{\partial\phi}{\partial y}&=\frac{1}{2\Delta_e}(\phi(P_1)(x_3-x_2)+\phi(P_2)(x_1-x_3)+\phi(P_3)(x_2-x_1)),\end{aligned}$$

which implies

$$(\nabla\phi,\nabla\chi_j)=\sum_{e\in\mathcal{T}_h}\int_e\nabla\phi\cdot\nabla\chi_jd\mathbf{x}=\sum_{e\in D_j}\int_e\frac{\partial\phi}{\partial x}\frac{\partial\chi_j}{\partial x}+\frac{\partial\phi}{\partial y}\frac{\partial\chi_j}{\partial y}d\mathbf{x}\le\sum_{e\in D_j}\frac{h_e^2}{2\Delta_e}\sum_{i=1}^{3}\phi(P_{e,i}). \tag{3.6}$$

The proof is finished. $\square$

The positivity-preserving property of the proposed numerical scheme (3.1) is stated in the following theorem.

Theorem 3.1. *Given $\phi_h^k \in S_h$ with $\|\phi_h^k\|_\infty \le M$, $k=n,n-1$, for some $M>0$ and $|\bar{\phi}_h^n| = |\bar{\phi}_h^{n-1}| < 1$, there exists a unique solution $\phi_h^{n+1} \in S_h$ to (3.1), with $\phi_h^{n+1} - \bar{\phi}_h^n \in \mathring{S}_h$ and $\|\phi_h^{n+1}\|_\infty < 1$.*

Proof. In fact, the numerical solution of (3.1) is a minimizer of the following discrete energy functional

$$
\begin{aligned}
\mathcal{J}^n(\phi) :=& \frac{1}{3\tau} \left\| \frac{3}{2}\phi - 2\phi_h^n + \frac{1}{2}\phi_h^{n-1} \right\|_{-1,Q}^2 + (1+\phi, \ln(1+\phi))_Q + (1-\phi, \ln(1-\phi))_Q \\
&+ \frac{\varepsilon^2 + A\tau}{2} \|\nabla \phi\|_2^2 + (\phi, A\tau \Delta \phi_h^n) - \left(\theta_0 \check{\phi}_h^{n+1}, \phi \right)_Q
\end{aligned}
\tag{3.7}
$$

over the admissible set

$$
A_h := \left\{ \phi \in S_h \,|\, \|\phi\|_\infty \le 1,\ (\phi - \bar{\phi}_h^0, 1)_Q = 0 \right\} \subset \mathbb{R}^{N_p^2}.
$$

Observe that $\mathcal{J}^n$ is a strictly convex function over this domain.

To facilitate the analysis below, we transform the minimization problem into an equivalent one. Consider the functional

$$
\begin{aligned}
\mathcal{F}^n(\varphi) :=& \mathcal{J}^n\left(\varphi + \bar{\phi}_h^0\right) \\
=& \frac{1}{3\tau} \left\| \frac{3}{2}\left(\varphi + \bar{\phi}_h^0\right) - 2\phi_h^n + \frac{1}{2}\phi_h^{n-1} \right\|_{-1,Q}^2 \\
&+ \left(1 + \varphi + \bar{\phi}_h^0, \ln\left(1 + \varphi + \bar{\phi}_h^0\right)\right)_Q + \left(1 - \varphi - \bar{\phi}_h^0, \ln\left(1 - \varphi - \bar{\phi}_h^0\right)\right)_Q \\
&+ \frac{\varepsilon^2 + A\tau}{2} \|\nabla \varphi\|_2^2 + \left(\varphi + \bar{\phi}_h^0, A\tau \Delta \phi_h^n\right) - \left(\theta_0 \check{\phi}^{n+1}, \varphi + \bar{\phi}_h^0 \right)_Q
\end{aligned}
\tag{3.8}
$$

defined on the set

$$
\mathring{A}_h := \left\{ \varphi \in \mathring{S}_h \,|\, -1 - \bar{\phi}_h^0 \le \varphi \le 1 - \bar{\phi}_h^0 \right\} \subset \mathbb{R}^{N_p^2}.
$$

If φ minimizes $\mathcal{F}^n$, then $\phi := \varphi + \bar{\phi}_h^0 \in A_h$ minimizes $\mathcal{J}^n$, and vice versa. Next, we prove that there exists a minimizer of $\mathcal{F}^n$ over the domain $\mathring{A}_h$. The following closed domain is taken into consideration, for $\delta \in (0,1/2)$:

$$
\mathring{A}_{h,\delta} := \left\{ \varphi \in \mathring{S}_h \,|\, \delta - 1 - \bar{\phi}_h^0 \le \varphi \le 1 - \bar{\phi}_h^0 - \delta \right\} \subset \mathbb{R}^{N_p^2}.
\tag{3.9}
$$

Since $\mathring{A}_{h,\delta}$ is a bounded, compact, and convex set in the subspace $\mathring{S}_h$, there exists a (not necessarily unique) minimizer of $\mathcal{F}^n$ over $\mathring{A}_{h,\delta}$. The key point of the positivity analysis is that such a minimizer could not occur on the boundary of $\mathring{A}_{h,\delta}$, if δ is sufficiently small.

To be more explicit, by the boundary of $A_{h,\delta}$, we mean the locus of points $\psi\in\mathring{A}_{h,\delta}$ such that $\|\psi+\bar{\phi}_h^0\|_\infty=1-\delta$, precisely.

To get a contradiction, suppose that the minimizer of $\mathcal{F}^n$, call it $\varphi^\star$ occurs at a boundary point of $\mathring{A}_{h,\delta}$. There is at least one grid point $P_{\alpha_0}=(i_0,j_0)$ such that

$$|\varphi^\star|_{\alpha_0}+\bar{\phi}_h^0|=1-\delta.$$

First, let us assume that $\varphi^\star|_{\alpha_0}+\bar{\phi}_h^0=\delta-1$, so that the grid function $\varphi^\star$ has a global minimum at α_0. Suppose that $P_{\alpha_1}=(i_1,j_1)$ is a grid point at which φ achieves its maximum. By the fact that $\bar{\varphi}^\star$, it is obvious that

$$1-\delta\geq\varphi^\star|_{\alpha_1}+\bar{\phi}_h^0\geq\bar{\phi}_h^0.$$

Since $\mathcal{F}^n$ is smooth over $\mathring{A}_{h,\delta}$, for all $\psi\in\mathring{S}_h$, the directional derivative becomes

$$\begin{aligned}
&d_S\mathcal{F}^n(\varphi^\star+s\psi)|_{s=0}\\
=&\big(\ln\big(1+\varphi^\star+\bar{\phi}_h^0\big)-\ln\big(1-\varphi^\star-\bar{\phi}_h^0\big),\psi\big)_Q\\
&+(A\tau\Delta\phi_h^n,\psi)-\theta_0\left(\check{\phi}^{n+1},\psi\right)_Q+\big(\varepsilon^2+A\tau\big)(\nabla\varphi^\star,\nabla\psi)\\
&+\frac{1}{\tau}\left((-\Delta)^{-1}\left(\frac{3}{2}\big(\varphi^\star+\bar{\phi}_h^0\big)-2\phi_h^n+\frac{1}{2}\phi_h^{n-1}\right),\psi\right).
\end{aligned}\tag{3.10}$$

This time, due to $\varphi_1^\star+s\psi\in\mathring{A}_{h,\delta}$, let us pick the direction

$$\psi=\delta_{\alpha_0}-C_2\delta_{\alpha_1},\quad C_2=\frac{\text{area}(D_{\alpha_0})}{\text{area}(D_{\alpha_1})},\tag{3.11}$$

where δ_{α_0} and δ_{α_1} are the basis functions on α_0 and α_1, D_{α_0} and D_{α_1} are the support of δ_{α_0} and δ_{α_1}, respectively.

For simplicity, now let us write $\phi^\star:=\varphi^\star+\bar{\phi}_h^0$. Since $\phi^\star|_{\alpha_0}=-1+\delta$ and $\phi^\star|_{\alpha_1}\geq\bar{\phi}_h^0$, we have

$$\begin{aligned}
&(\ln(1+\phi^\star)-\ln(1-\phi^\star),\psi)_Q\\
=&\sum_{e\in\mathcal{T}_h}\frac{1}{3}\Delta_e\sum_{j=1}^{3}(\ln(1+\phi^\star)-\ln(1-\phi^\star))\psi(P_{e,j})\\
=&\frac{1}{3}\text{area}(D_{\alpha_0})((\ln(1+\phi^\star)-\ln(1-\phi^\star))|_{\alpha_0}-(\ln(1+\phi^\star)-\ln(1-\phi^\star))|_{\alpha_1})\\
\leq&\frac{1}{3}\text{area}(D_{\alpha_0})\Big(\ln\frac{\delta}{2-\delta}-\ln\frac{1+\bar{\phi}_h^0}{1-\bar{\phi}_h^0}\Big).
\end{aligned}\tag{3.12}$$

Furthermore, an application of Lemma 3.2 gives the following estimate

$$\begin{aligned}(\Delta\phi_h^n,\psi)=&-(\nabla\phi_h^n,\nabla\psi)=-(\nabla\phi_h^n,\nabla\delta_{\alpha_0})+C_2(\nabla\phi_h^n,\nabla\delta_{\alpha_1})\\ \le&-\sum_{e\in D_{\alpha_0}}\frac{h_e^2}{2\Delta_e}\sum_{i=1}^3\phi_h^n(P_{e,i})+C_2\sum_{e\in D_{\alpha_1}}\frac{h_e^2}{2\Delta_e}\sum_{i=1}^3\phi_h^n(P_{e,i})\\ \le&-\sum_{e\in D_{\alpha_0}}\frac{3Mh_e^2}{2\Delta_e}+C_2\sum_{e\in D_{\alpha_1}}\frac{3Mh_e^2}{2\Delta_e}\le\frac{3M\tilde{C}_{\mathcal{T}}}{2},\end{aligned}\tag{3.13}$$

where

$$\tilde{C}_{\mathcal{T}}:=C_{\mathcal{T}}\Big(\sum_{e\in D_{\alpha_0}}1|_e+C_2\sum_{e\in D_{\alpha_1}}1|_e\Big).$$

For the numerical solution ϕ_h^k, $k=n,n-1$, at the previous time steps, the a priori assumption $\|\phi_h^k\|_\infty\le M$ yields

$$-2M\le\phi_h^k|_{\alpha_0}-\phi_h^k|_{\alpha_1}\le 2M,\tag{3.14}$$

so that

$$\begin{aligned}\Big(\theta_0\phi_h^k,\psi\Big)_Q=&\theta_0\sum_{e\in\mathcal{T}_h}\frac{1}{3}\Delta_e\sum_{j=1}^3\phi_h^k\psi(P_{e,j})\\ =&\frac{\theta_0}{3}\mathrm{area}(D_{\alpha_0})\Big(\phi_h^k|_{\alpha_0}-\phi_h^k|_{\alpha_1}\Big)\\ \le&\frac{2M\theta_0}{3}\mathrm{area}(D_{\alpha_0}).\end{aligned}\tag{3.15}$$

This in turn leads to the estimate for the third term in (3.10):

$$-6M\mathrm{area}(D_{\alpha_0})\le(\check{\phi}_h^{n+1},\psi)_Q\le 6M\mathrm{area}(D_{\alpha_0}).\tag{3.16}$$

For the fourth term, we easily obtain

$$(\nabla\varphi^\star,\nabla\psi)=(\nabla\varphi^\star,\nabla\delta_{\alpha_0})-C_2(\nabla\varphi^\star,\nabla\delta_{\alpha_1})\le 0.\tag{3.17}$$

For the last term, an application of Lemma 3.1 reveals that

$$\begin{aligned}&\left((-\Delta)^{-1}\left(\frac{3}{2}(\phi^\star)-2\phi_h^n+\frac{1}{2}\phi_h^{n-1}\right),\psi\right)_Q\\ =&\sum_{e\in\mathcal{T}_h}\frac{1}{3}\Delta_e\sum_{j=1}^3\left((-\Delta)^{-1}\left(\frac{3}{2}(\phi^\star)-2\phi_h^n+\frac{1}{2}\phi_h^{n-1}\right)\psi(P_{e,j})\right)\\ =&\frac{1}{3}\mathrm{area}(D_{\alpha_0})\left((-\Delta)^{-1}\left(\frac{3}{2}(\phi^\star)-2\phi_h^n+\frac{1}{2}\phi_h^{n-1}\right)\Big|_{\vec{\alpha}_0}\right.\\ &\left.\qquad-(-\Delta)^{-1}\left(\frac{3}{2}(\phi^\star)-2\phi_h^n+\frac{1}{2}\phi_h^{n-1}\right)|_{\vec{\alpha}_1}\right)\\ \le&\frac{5C_3\mathrm{area}(D_{\alpha_0})}{3}.\end{aligned}\tag{3.18}$$

Subsequently, a substitution of (3.13)-(3.18), (3.12) and (3.17) into (3.10) yields the following bound on the directional derivative:

$$\begin{aligned} & d_S\mathcal{F}^n(\varphi^\star+s\psi)|_{s=0} \\ \leq & \operatorname{area}(D_{\alpha_0})\left(\frac{1}{3}\ln\frac{\delta}{2-\delta}-\frac{1}{3}\ln\frac{1+\bar{\phi}_0}{1-\bar{\phi}_0}+6M\theta_0+\frac{5C_3}{3\tau}\right)+\frac{3A\tau M\tilde{C}_{\mathcal{T}}}{2}. \end{aligned} \tag{3.19}$$

We denote

$$r_1=-\ln\frac{1+\bar{\phi}_h^0}{1-\bar{\phi}_h^0}+18M\theta_0+5C_3\tau^{-1}+\frac{9A\tau M\tilde{C}_{\mathcal{T}}}{2}(\operatorname{area}(D_{\alpha_0}))^{-1}.$$

Note that r_1 is a constant for a fixed τ, though it becomes singular as $\tau\to 0$. However, for any fixed τ, we may choose $\delta\in(0,1/2)$ sufficiently small so that

$$\ln\frac{\delta}{2-\delta}+r_1<0. \tag{3.20}$$

This in turn shows that, provided δ satisfies (3.20) such that

$$d_s\mathcal{F}^n(\varphi^\star+s\psi)|_{s=0}<0. \tag{3.21}$$

As before, this contradicts the assumption that $\mathcal{F}^n$ has a minimum at $\varphi^\star$, since the directional derivative is negative in a direction pointing into the interior of $\mathring{A}_{h,\delta}$.

Using very similar arguments, we can also prove that the global minimum of $\mathcal{F}^n$ over $\mathring{A}_{h,\delta}$ could not occur at a boundary point $\varphi^\star$ such that $\varphi^\star|_{\alpha_0}+\bar{\phi}_h^0=1-\delta$, for some α_0, so that the grid function $\varphi^\star$ has a global maximum at α_0. The details are left to interested readers. A combination of these two facts shows that, the global minimum of $\mathcal{F}^n$ over $\mathring{A}_{h,\delta}$ could only possibly occur at interior point

$$\varphi\in\operatorname{interior}(\mathring{A}_{h,\delta})\subset\operatorname{interior}(\mathring{A}_h).$$

We conclude that there must be a solution $\phi=\varphi+\bar{\phi}^0\in A_h$ that minimizes $\mathcal{J}^n$ over A_h, which is equivalent to the numerical solution of (3.1). The existence of the numerical solution is established. In addition, since $\mathcal{J}^n$ is a strictly convex function over A_h, the uniqueness analysis for this numerical solution is straightforward. $\square$

4 The energy stability and convergence analysis

In this section, we derive the discrete energy stability of the proposed numerical scheme (3.1), as well as the convergence analysis. The discrete energy is defined as

$$E_h(\phi)=(1+\phi,\ln(1+\phi))_Q+(1-\phi,\ln(1-\phi))_Q+\frac{\varepsilon^2}{2}\|\nabla\phi\|^2-\frac{\theta_0}{2}\|\phi\|_Q^2. \tag{4.1}$$

Now, we will establish a modified energy stability for the numerical algorithm (3.1), provided that $A\geq\frac{\theta_0^2}{16}$. This result is stated in the following theorem.

Theorem 4.1. *We have the stability analysis of the following modified energy functional for the proposed numerical scheme* (3.1)*:*

$$\tilde{E}_h\left(\phi_h^{n+1},\phi_h^n\right) \leq \tilde{E}_h\left(\phi_h^n,\phi_h^{n-1}\right), \quad \textit{if}\ \ A \geq \frac{\theta_0^2}{16}, \tag{4.2}$$

with

$$\tilde{E}_h\left(\phi_h^{n+1},\phi_h^n\right) = E_h\left(\phi_h^{n+1}\right) + \frac{1}{4\tau}\left\|\phi_h^{n+1}-\phi_h^n\right\|_{-1,Q}^2 + \frac{\theta_0}{2}\left\|\phi_h^{n+1}-\phi_h^n\right\|_Q^2. \tag{4.3}$$

Proof. In (3.1), by choosing

$$v = (-\Delta_h)^{-1}(\phi_h^{n+1}-\phi_h^n) \quad \text{and} \quad w = \phi_h^{n+1}-\phi_h^n,$$

we could derive the following inequalities:

$$\begin{aligned}
&\left(\frac{\frac{3}{2}\phi_h^{n+1}-2\phi_h^n+\frac{1}{2}\phi_h^{n-1}}{\tau},(-\Delta_h)^{-1}\left(\phi_h^{n+1}-\phi_h^n\right)\right)_Q \\
&= \frac{3}{2\tau}\left\|\phi_h^{n+1}-\phi_h^n\right\|_{-1,Q}^2 - \frac{1}{2\tau}\left(\phi_h^n-\phi_h^{n-1},(-\Delta_h)^{-1}(\phi_h^{n+1}-\phi_h^n)\right)_Q \\
&\geq \frac{1}{\tau}\left(\frac{5}{4}\left\|\phi_h^{n+1}-\phi_h^n\right\|_{-1,Q}^2 - \frac{1}{4}\left\|\phi_h^n-\phi_h^{n-1}\right\|_{-1,Q}^2\right), &(4.4a)\\
&\left(\phi_h^{n+1}-\phi_h^n,g(\phi_h^{n+1})\right)_Q = \left(\phi_h^{n+1}-\phi_h^n,\ln\left(1+\phi_h^{n+1}\right)-\ln\left(1-\phi_h^{n+1}\right)\right)_Q \\
&\geq \left(1+\phi_h^{n+1},\ln\left(1+\phi_h^{n+1}\right)\right)_Q - \left(1-\phi_h^{n+1},\ln\left(1-\phi_h^{n+1}\right)\right)_Q \\
&\qquad -(1+\phi_h^n,\ln(1+\phi_h^n))_Q-(1-\phi_h^n,\ln(1-\phi_h^n))_Q, &(4.4b)\\
&-\left(\check{\phi}_h^{n+1},\left(\phi_h^{n+1}-\phi_h^n\right)\right)_Q = -\left(2\phi_h^n-\phi_h^{n-1},\left(\phi_h^{n+1}-\phi_h^n\right)\right)_Q \\
&\geq -\frac{1}{2}\left(\left\|\phi_h^{n+1}\right\|_Q^2-\|\phi_h^n\|_Q^2\right)-\frac{1}{2}\left\|\phi_h^n-\phi_h^{n-1}\right\|_Q^2, &(4.4c)\\
&(\nabla\phi_h^{n+1},\nabla\left(\phi_h^{n+1}-\phi_h^n\right)) = \frac{1}{2}\left(\left\|\nabla\phi_h^{n+1}\right\|^2-\|\nabla\phi_h^n\|^2+\left\|\nabla\left(\phi_h^{n+1}-\phi_h^n\right)\right\|^2\right), &(4.4d)\\
&(\nabla(\phi_h^{n+1}-\phi_h^n),\nabla\left(\phi_h^{n+1}-\phi_h^n\right)) = \|\nabla(\phi_h^{n+1}-\phi_h^n)\|^2. &(4.4e)
\end{aligned}$$

Meanwhile, an application of Cauchy inequality indicates the following estimate:

$$\frac{1}{\tau}\left\|\phi_h^{n+1}-\phi_h^n\right\|_{-1,Q}^2 + A\tau\left\|\nabla\left(\phi_h^{n+1}-\phi_h^n\right)\right\|^2 \geq 2A^{1/2}\left\|\phi_h^{n+1}-\phi_h^n\right\|_Q^2. \tag{4.5}$$

Therefore, a combination of (4.4a)-(4.5) yields

$$\begin{aligned}
&E_h\left(\phi_h^{n+1}\right)-E_h(\phi_h^n)+\frac{1}{4\tau}\left(\left\|\phi_h^{n+1}-\phi_h^n\right\|_{-1,Q}^2-\left\|\phi_h^n-\phi_h^{n-1}\right\|_{-1,Q}^2\right)\\
&\quad+\frac{\theta_0}{2}\left(\left\|\phi_h^{n+1}-\phi_h^n\right\|_Q^2-\left\|\phi_h^n-\phi_h^{n-1}\right\|_Q^2\right)\\
\le&\left(-2A^{1/2}+\frac{\theta_0}{2}\right)\left\|\phi_h^{n+1}-\phi_h^n\right\|_Q^2\le 0, \qquad (4.6)
\end{aligned}$$

provided that $A\ge\frac{\theta_0^2}{16}$. Therefore, by denoting a modified energy as given by (4.3), we get the energy estimate (4.2). □

Next, we will provide a convergence analysis for the proposed numerical scheme (3.1), in the $\ell^\infty\left(0,T;H^{-1}\right)\cap\ell^2\left(0,T;H^1\right)$ norm. We denote the exact solution as $\phi^n=\phi(x,t_n)$ at $t=t_n$. As usual, a regularity assumption has to be made in the error analysis, and we denote all the upper bounds for the exact solution as C_0. The following estimates hold for Ritz projection [7]:

$$\|R_h\varphi\|_{1,p}\le C\|\varphi\|_{1,p,}, \qquad \forall 1<p\le\infty, \qquad (4.7a)$$

$$\|\varphi-R_h\varphi\|_p+h\|\varphi-R_h\varphi\|_{1,p}\le Ch^{q+1}\|\varphi\|_{q+1,p,}, \qquad \forall 1<p\le\infty. \qquad (4.7b)$$

Suppose that $\phi\in L^\infty(0,T;W^{1,p}(\Omega))$. By combining (4.7a) and the Sobolev imbedding theorem: $W^{1,p}(\Omega)\hookrightarrow L^\infty(\Omega)$, for $d<p\le\infty$, there are constants $C_3,C_4>0$, such that

$$\|\phi^n\|_\infty\le C\|\phi^n\|_{1,p}\le C_3, \quad \|R_h\phi^n\|_\infty\le C\|R_h\phi^n\|_{1,p}\le C\|\phi^n\|_{1,p}\le C_4. \qquad (4.8)$$

Lemma 4.1. *If $\phi\in H^2(\Omega)$, where $\Omega\in R^d$, and $\|\phi\|_{L^\infty}\le 1-\delta$ where $\delta>0$, then there exists $0<h_0<1$ such that for any $h\le h_0$,*

$$\|R_h\phi\|_{L^\infty}\le 1-\frac{1}{2}\delta. \qquad (4.9)$$

Proof. For any $v_h\in S_h$,

$$\|R_h\phi\|_{L^\infty}\le\|R_h\phi-v_h\|_{L^\infty}+\|v_h\|_{L^\infty}\le Ch^{-\frac{d}{2}}\|R_h\phi-v_h\|+\|v_h\|_{L^\infty}.$$

We can choose v_h as the standard Lagrange linear interpolation, and

$$\|v_h\|_{L^\infty}\le\|\phi\|_{L^\infty} \quad \text{and} \quad \|v_h-\phi\|\le Ch^2\|\phi\|_{H^2}.$$

By the approximation of R_h (see (4.7b)),

$$\|R_h\phi\|_{L^\infty}\le\|\phi\|_{L^\infty}+Ch^{2-\frac{d}{2}}\|\phi\|_{H^2}.$$

For $d=2,3$, we can choose h_0 such that

$$Ch_0^{\frac{1}{2}}\|\phi\|_{H^2}\leq\frac{\delta}{2},$$

then

$$\|R_h\phi\|_{L^\infty}\leq 1-\frac{\delta}{2}.$$

Thus, we complete the proof. □

By (ϕ,μ) we denote the exact solution to the weak formulation (2.5). We say that the solution pair belongs to regularity of class $\mathcal{C}^2$ if and only if

$$\begin{aligned}
&\phi\in W^{3,\infty}\left(0,T;L^2_{per}(\Omega)\right)\bigcap W^{1,\infty}\left(0,T;H^2_{per}(\Omega)\right),\\
&\mu\in L^\infty\left(0,T;H^2_{per}(\Omega)\right).
\end{aligned}$$

On the other hand, the solution of (3.1) is also mass conservative at the discrete level:

$$\bar{\phi}^{n+1}=\bar{\phi}^n=\bar{\phi}^{n-1},\quad \forall n\in\mathbb{N}. \tag{4.10}$$

Lemma 4.2 ([53]). *Let $\kappa_h(\cdot,\cdot)=(\cdot,\cdot)-(\cdot,\cdot)_Q$ denote the quadrature error in* (2.6). *We then have*

$$|\kappa_h(\psi,\chi)|\leq Ch^2\|\nabla\psi\|\|\nabla\chi\|,\quad \forall\psi,\chi\in S_h. \tag{4.11}$$

Lemma 4.3. *Suppose $g(\cdot)\in W^{2,\infty}(\mathbb{R})$ and $\kappa_h(g(\cdot),\cdot)=(g(\cdot),\cdot)-(g(\cdot),\cdot)_Q$, then we have*

$$|\kappa_h(g(\psi),\chi)|\leq C_5h^2(\|\nabla\psi\|^2_{L^4}\|\chi\|+\|\nabla\psi\|\|\nabla\chi\|),\quad \forall\psi,\chi\in S_h, \tag{4.12}$$

where $C_5=C\max\{\|g''\|_{L^\infty},\|g'\|_{L^\infty}\}$ is independent of h.

Proof. Since the quadrature formula (2.6) is exact for f linear we have, by transformation to a fixed reference triangle e_0 and using the Bramble-Hilbert lemma and the Sobolev inequality

$$\|f\|_{L^\infty(e_0)}\leq C\|f\|_{W^2_1(e_0)},$$

that

$$\left|Q_e(f)-\int_e f d\mathbf{x}\right|\leq Ch^2\sum_{|\alpha|=2}\|D^\alpha f\|_{L^1(e)}.$$

After application to $f=g(\psi)\chi$ this implies, that

$$\left|Q_e(g(\psi)\chi)-\int_e g(\psi)\chi d\mathbf{x}\right|\leq Ch^2\sum_{|\alpha|=2}\|D^\alpha(g(\psi)\chi)\|_{L^1(e)}.$$

Next, we will continuous to expand every term in the right hand of the above: if $\alpha=(1,0)$, then

$$D^\alpha(g(\psi)\chi)=g'\psi_x\chi+g\chi_x,$$

since both ψ and χ are linear in e, $\alpha=(2,0)$ implies that

$$D^\alpha(g(\psi)\chi)=g''\psi_x^2\chi+2g'\psi_x\chi_x.$$

Then

$$\begin{aligned}\|D^\alpha(g(\psi)\chi)\|_{L^1(e)}\le&\int_e|g''\psi_x^2\chi|d\mathbf{x}+2\int_e|g'\psi_x\chi_x|d\mathbf{x}\\ \le&\|g''\|_{L^\infty(e)}\|\psi_x\|^2_{L^4(e)}\|\chi\|_{L^2(e)}+2\|g'\|_{L^\infty(e)}\|\psi_x\|_{L^2(e)}\|\chi_x\|_{L^2(e)}.\end{aligned}$$

Similarly, for $\alpha=(1,1)$, then

$$\begin{aligned}\|D^\alpha(g(\psi)\chi)\|_{L^1(e)}\le&\|g''\|_{L^\infty(e)}\|\psi_x\psi_y\|_{L^2(e)}\|\chi\|_{L^2(e)}\\ &+\|g'\|_{L^\infty(e)}(\|\psi_x\|_{L^2(e)}\|\chi_y\|_{L^2(e)}+\|\psi_y\|_{L^2(e)}\|\chi_x\|_{L^2(e)}),\end{aligned}$$

and $\alpha=(0,2)$

$$\|D^\alpha(g(\psi)\chi)\|_{L^1(e)}\le\|g''\|_{L^\infty(e)}\|\psi_y\|^2_{L^4(e)}\|\chi\|_{L^2(e)}+2\|g'\|_{L^\infty(e)}\|\psi_y\|_{L^2(e)}\|\chi_y\|_{L^2(e)}.$$

Here we have at once

$$\begin{aligned}&\left|Q_e(g(\psi)\chi)-\int_e g(\psi)\chi d\mathbf{x}\right|\\ \le&Ch^2(\|g''\|_{L^\infty(e)}\|\nabla\psi\|^2_{L^4(e)}\|\chi\|_{L^2(e)}+\|g'\|_{L^\infty(e)}\|\nabla\psi\|_{L^2(e)}\|\nabla\chi\|_{L^2(e)}).\end{aligned}$$

Then, we conclude that

$$\begin{aligned}|\kappa_h(g(\psi),\chi)|\le&Ch^2\sum_{e\in\mathcal{T}_h}(\|g''\|_{L^\infty(e)}\|\nabla\psi\|^2_{L^4(e)}\|\chi\|_{L^2(e)}+\|g'\|_{L^\infty(e)}\|\nabla\psi\|_{L^2(e)}\|\nabla\chi\|_{L^2(e)})\\ \le&Ch^2(\|g''\|_{L^\infty}\|\nabla\psi\|^2_{L^4}\|\chi\|+\|g'\|_{L^\infty}\|\nabla\psi\|\|\nabla\chi\|)\\ \le&C_5h^2(\|\nabla\psi\|^2_{L^4}\|\chi\|+\|\nabla\psi\|\|\nabla\chi\|),\end{aligned}$$

where $C_5=C\max\{\|g''\|_{L^\infty},\|g'\|_{L^\infty}\}$ is independent of h. □

Before proceeding into the convergence analysis, we introduce a new norm from [59]. Let $\mathbf{p}=[u,v]^T\in\left[L^2(\Omega)\right]^2$, where Ω represents an arbitrary bounded domain. Define the G-norm to be a weighted inner product

$$\|\mathbf{p}\|^2_{\mathrm{G}}=(\mathbf{p},\mathrm{G}(-\Delta_h)^{-1}\mathbf{p})_Q,\quad \mathrm{G}=\begin{bmatrix}\frac{1}{2}&-1\\-1&\frac{5}{2}\end{bmatrix}.$$

Since G is symmetric positive definite, the norm is well-defined. Moreover,

$$\mathrm{G}=\begin{bmatrix} \frac{1}{2} & -1 \\ -1 & \frac{5}{2} \end{bmatrix}=\begin{bmatrix} \frac{1}{2} & -1 \\ -1 & 2 \end{bmatrix}+\begin{bmatrix} 0 & 0 \\ 0 & \frac{1}{2} \end{bmatrix}=:\mathrm{G}_1+\mathrm{G}_2.$$

By the positive semi-definiteness of G_1, we immediately have

$$\|\mathbf{p}\|_{\mathrm{G}}^2=\Big(\mathbf{p},(\mathrm{G}_1+\mathrm{G}_2)(-\Delta_h)^{-1}\mathbf{p}\Big)_Q\geq\Big(\mathbf{p},\mathrm{G}_2(-\Delta_h)^{-1}\mathbf{p}\Big)_Q=\frac{1}{2}\|v\|_{-1,Q}^2. \tag{4.13}$$

For any $v_i\in H_{per}^1(\Omega)$, $i=0,1,2$, the following equality is valid:

$$\left(\frac{3}{2}v_2-2v_1+\frac{1}{2}v_0,(-\Delta_h)^{-1}v_2\right)_Q=\frac{1}{2}\left(\|\mathbf{p}^2\|_{\mathrm{G}}^2-\left\|\mathbf{p}^1\right\|_{\mathrm{G}}^2\right)+\frac{\|v_2-2v_1+v_0\|_{-1,Q}^2}{4}, \tag{4.14}$$

where $\mathbf{p}^2=[v_1,v_2]^T$, $\mathbf{p}^1=[v_0,v_1]^T$, especially, when $v_0=0$,

$$\|\mathbf{p}^1\|_{\mathrm{G}}^2=\frac{5}{2}\|v_1\|_{-1,Q}^2.$$

Subsequently, the convergence result is stated in the following theorem.

Theorem 4.2. *Suppose that the exact solution pair (ϕ,μ) is in the regularity class $\mathcal{C}_2$, for the fixed final time $T>0$. Let $\phi^n=\phi(t_n)$ and ϕ_h^n be the solution at time $t=t_n$ to the fully discrete numerical scheme* (3.1)*, for $1\leq n\leq N$, with $N\cdot\tau=T$, provided that τ and h are sufficiently small, then we have the error estimate*

$$\|\phi^{n+1}-\phi_h^{n+1}\|_{-1,Q}+\left(\tau\varepsilon^2\sum_0^n\|\nabla(\phi^{n+1}-\phi_h^{n+1})\|^2\right)^{\frac{1}{2}}\leq C(T,\varepsilon)(\tau^2+h^2)$$

for some constant $C(T,\varepsilon)>0$ that is independent of τ and h.

Proof. We define $\xi^{n+1}=\phi^{n+1}-\phi_h^{n+1}$ and $\eta^{n+1}=\mu^{n+1}-\mu_h^{n+1}$. The following error evolutionary equation could be derived:

$$\left\{\begin{aligned} &(\delta_\tau\xi^{n+1},v_h)_Q+(\nabla\eta^{n+1},\nabla v_h)=-(R_1^{n+1},v_h)-\kappa_h(\delta_\tau\phi^{n+1},v_h),\\ &(\eta^{n+1},w_h)_Q+\kappa_h(\mu^{n+1},w_h)=(g(\phi^{n+1})-g(\phi_h^{n+1}),w_h)_Q+\kappa_h(g(\phi^{n+1}),w_h)\\ &\qquad\qquad-\theta_0(R_2^{n+1},w_h)_Q-\theta_0(T_1^{n+1},w_h)_Q-\theta_0\kappa_h(\phi^{n+1},w_h)\\ &\qquad\qquad+\varepsilon^2(\nabla\xi^{n+1},\nabla w_h)+\tau(\nabla T_2^{n+1},\nabla w_h)+(R_3^{n+1},w_h), \end{aligned}\right. \tag{4.15}$$

where

$$\delta_\tau v^{n+1} := \begin{cases} \dfrac{3v^{n+1}-4v^n+v^{n-1}}{2\tau}, & n\geq 1, \\ \dfrac{v^1-v^0}{\tau}, & n=0, \end{cases} \qquad R_1^{n+1} := \partial_t \phi^{n+1} - \delta_\tau \phi^{n+1},$$

$$R_2^{n+1} := \phi^{n+1} - \begin{cases} 2\phi^n - \phi^{n-1}, & n\geq 1, \\ \phi^0, & n=0, \end{cases} \qquad R_3^{n+1} := \begin{cases} A\tau\Delta\left(\phi^{n+1}-\phi^n\right), & n\geq 1, \\ 0, & n=0, \end{cases}$$

$$T_1^{n+1} := \begin{cases} 2\xi^n - \xi^{n-1}, & n\geq 1, \\ \xi^0, & n=0, \end{cases} \qquad T_2^{n+1} := \begin{cases} A\left(\xi^{n+1}-\xi^n\right), & n\geq 1, \\ 0, & n=0. \end{cases}$$

By the Cauchy-Schwarz inequality, we have the following estimate (see [59]):

$$\left\|R_1^{n+1}\right\|^2 \leq 32\tau^3 \int_{t_{n-1}}^{t_{n+1}} \|\partial_{ttt}\phi\|^2 dt \leq 32\tau^3 \int_{t_{n-1}}^{t_{n+1}} \|\partial_{ttt}\phi\|^2 dt, \qquad \text{if } n\geq 1, \tag{4.16a}$$

$$\left\|R_1^{n+1}\right\|^2 \leq \frac{\tau}{3}\int_0^{t_1} \|\partial_{tt}\phi\|^2 dt \leq \frac{\tau^2}{3}\|\phi\|_{W^{2,\infty}(0,T;L^2)} \leq C_9\tau^2, \qquad \text{if } n=0. \tag{4.16b}$$

An analogous estimate is available for the second remainder term:

$$\left\|\nabla R_2^{n+1}\right\|^2 \leq \begin{cases} 32\tau^3 \displaystyle\int_{t_{n-1}}^{t_{n+1}} \|\partial_{tt}\nabla\phi\|^2 dt, & n\geq 1, \\ C_{10}\tau^2, & n=0. \end{cases} \tag{4.17}$$

In fact, the estimate for $n=0$ is based on the fact that

$$\|\nabla R_2^1\|^2 = \|\nabla(\phi^1-\phi^0)\|^2 \leq \tau \int_{t_0}^{t_1} \|\partial_t \nabla\phi\|^2 dt \leq \tau^2 \|\phi\|_{W^{1,\infty}(0,T;H^1_{per}(\Omega))} \leq C_{10}\tau^2.$$

For the third remainder term, we obtain the estimate

$$\left\|R_3^{n+1}\right\|^2 \leq \begin{cases} A^2\tau^3 \displaystyle\int_{t_n}^{t_{n+1}} \|\partial_t\Delta\phi\|^2 dt, & n\geq 1, \\ 0, & n=0. \end{cases} \tag{4.18}$$

Using the definitions of Ritz projection and combining the lumped version definition of the discrete Laplacian operator, it holds that

$$(\Delta_h v_h, \chi)_Q = -(\nabla v_h, \nabla \chi)$$

for $\forall v_h,\chi\in S_h$,

$$\begin{aligned}\left(\nabla\eta^{n+1},\nabla v_h\right)&=\left(\nabla\mu^{n+1}-\nabla R_h\mu^{n+1},\nabla v_h\right)+\left(\nabla R_h\mu^{n+1}-\nabla\mu_h^{n+1},\nabla v_h\right)\\&=\left(\nabla\left(R_h\mu^{n+1}-\mu_h^{n+1}\right),\nabla v_h\right)\\&=\left(R_h\mu^{n+1}-\mu_h^{n+1},-\Delta_h v_h\right)_Q\\&=\left(\mu^{n+1}-\mu_h^{n+1}+R_h\mu^{n+1}-\mu^{n+1},-\Delta_h v_h\right)_Q\\&=\left(\eta^{n+1},-\Delta_h v_h\right)_Q-\left(\mu^{n+1}-R_h\mu^{n+1},-\Delta_h v_h\right)_Q.\end{aligned}\tag{4.19}$$

Denote $\rho_\phi^{n+1}:=\phi^{n+1}-R_h\phi^{n+1}$, $\sigma_\phi^{n+1}:=R_h\phi^{n+1}-\phi_h^{n+1}$, taking $w_h=\Delta_h v_h$ in (4.15) and using (4.19), we have

$$\begin{aligned}&(\delta_\tau\sigma_\phi^{n+1},v_h)_Q-\varepsilon^2(\nabla\sigma_\phi^{n+1},\nabla(\Delta_h v_h))\\=&-(R_1^{n+1},v_h)+(g(\phi^{n+1})-g(\phi_h^{n+1}),\Delta_h v_h)_Q-\theta_0(R_2^{n+1},\Delta_h v_h)_Q-\theta_0(T_1^{n+1},\Delta_h v_h)_Q\\&+(R_3^{n+1},\Delta_h v_h)+(\mu-R_h\mu^{n+1},-\Delta_h v_h)_Q-\kappa_h(\delta_\tau\phi^{n+1},v_h)\\&-\kappa_h(\mu^{n+1},\Delta_h v_h)+\kappa_h(g(\phi^{n+1}),\Delta_h v_h)-\theta_0\kappa_h(\phi^{n+1},\Delta_h v_h)\\&+\tau(\nabla T_2^{n+1},\nabla(\Delta_h v_h))-(\delta_\tau\rho_\phi^{n+1},v_h)_Q.\end{aligned}\tag{4.20}$$

In turn, taking $v_h=(-\Delta_h)^{-1}\sigma_\phi^{n+1}$, Eq. (4.20) can be written as follows

$$\begin{aligned}&(\delta_\tau\sigma_\phi^{n+1},-\Delta_h^{-1}\sigma_\phi^{n+1})_Q+\varepsilon^2(\nabla\sigma_\phi^{n+1},\nabla\sigma_\phi^{n+1})+\tau(\nabla T_2^{n+1},\nabla\sigma_\phi^{n+1})\\=&-(R_1^{n+1},-\Delta_h^{-1}\sigma_\phi^{n+1})-(g(\phi^{n+1})-g(\phi_h^{n+1}),\sigma_\phi^{n+1})_Q+\theta_0(R_2^{n+1},\sigma_\phi^{n+1})_Q\\&+\theta_0(T_1^{n+1},\sigma_\phi^{n+1})_Q+(\mu^{n+1}-R_h\mu^{n+1},\sigma_\phi^{n+1})_Q-\kappa_h(\delta_\tau\phi^{n+1},-\Delta_h^{-1}\sigma_\phi^{n+1})+\kappa_h(\mu^{n+1},\sigma_\phi^{n+1})\\&-\kappa_h(g(\phi^{n+1}),\sigma_\phi^{n+1})+\theta_0\kappa_h(\phi^{n+1},\sigma_\phi^{n+1})-(\delta_\tau\rho_\phi^{n+1},-\Delta_h^{-1}\sigma_\phi^{n+1})_Q-(R_3^{n+1},\sigma_\phi^{n+1})\\=&J_1+J_2+J_3+J_4+J_5+J_6+J_7+J_8+J_9+J_{10}+J_{11}:=J.\end{aligned}\tag{4.21}$$

Now look at the left-hand side of (4.21). From (4.14), we have

$$\begin{aligned}&\left(\delta_\tau\sigma_\phi^{n+1},-\Delta_h^{-1}\sigma_\phi^{n+1}\right)_Q\\=&\begin{cases}\dfrac{1}{2\tau}\left(\|\mathbf{p}^{n+1}\|_G^2-\|\mathbf{p}^n\|_G^2\right)+\dfrac{1}{4\tau}\left\|\sigma_\phi^{n+1}-2\sigma_\phi^n+\sigma_\phi^{n-1}\right\|_{-1,Q}^2, & n\geq 1,\\ \dfrac{1}{2\tau}\left(\left\|\sigma_\phi^1\right\|_{-1,Q}^2-\left\|\sigma_\phi^0\right\|_{-1,Q}^2\right)+\dfrac{1}{2\tau}\left\|\sigma_\phi^1-\sigma_\phi^0\right\|_{-1,Q}^2, & n=0,\end{cases}\end{aligned}\tag{4.22}$$

where

$$\mathbf{p}^{k+1}=[\sigma_\phi^k,\sigma_\phi^{k+1}]^T.$$

Using the equality (3.2) indicates that

$$\begin{aligned}\tau(\nabla T_2^{n+1},\nabla\sigma_\phi^{n+1}) &= A\tau(\nabla(\zeta^{n+1}-\zeta^n),\nabla\sigma_\phi^{n+1})\\ &= A\tau(\nabla(\rho_\phi^{n+1}-\rho_\phi^n),\nabla\sigma_\phi^{n+1})+A\tau(\nabla(\sigma_\phi^{n+1}-\sigma_\phi^n),\nabla\sigma_\phi^{n+1})\\ &\geq \frac{1}{2}A\tau(\|\nabla\sigma_\phi^{n+1}\|^2-\|\nabla\sigma_\phi^n\|^2). \end{aligned} \tag{4.23}$$

Meanwhile, the estimate for the term associated with the surface diffusion is straightforward:

$$\varepsilon^2(\nabla\sigma_\phi^{n+1},\nabla\sigma_\phi^{n+1})=\varepsilon^2\|\nabla\sigma_\phi^{n+1}\|^2. \tag{4.24}$$

A combination with of (4.22), (4.23) and (4.24) reveals that, the left-hand side of (4.21) is bounded from below:

$$\begin{aligned}&\frac{1}{2\tau}\left(\left\|\mathbf{p}^{n+1}\right\|_{\mathrm{G}}^2-\|\mathbf{p}^n\|_{\mathrm{G}}^2\right)+\frac{1}{2}A\tau\left(\left\|\nabla\sigma_\phi^{n+1}\right\|^2-\left\|\nabla\sigma_\phi^n\right\|^2\right)\\ &\quad+\epsilon^2\left\|\nabla\sigma_\phi^{n+1}\right\|^2\leq J \quad \text{for} \ \ n\geq 1. \end{aligned} \tag{4.25}$$

Observe that $\sigma_\phi^0\equiv 0$ for $n=0$, and we know that $A=0$. As a result, we get

$$\frac{1}{2\tau}(\|\sigma_\phi^1\|_{-1,Q}^2-\|\sigma_\phi^0\|_{-1,Q}^2+\|\sigma_\phi^1-\sigma_\phi^0\|_{-1,Q}^2)+\varepsilon^2\|\nabla\sigma_\phi^1\|^2\leq J, \tag{4.26a}$$

$$\frac{1}{2\tau}\|\sigma_\phi^1\|_{-1,Q}^2+\varepsilon^2\|\nabla\sigma_\phi^1\|^2\leq J. \tag{4.26b}$$

Next, we study the eleven terms on the right-hand side of (4.21). Employing the (4.16a) and Young inequality reveals that

$$J_1\leq\|R_1^{n+1}\|_{-1,Q}\|\sigma_\phi^{n+1}\|_{-1,Q}\leq\begin{cases}64\tau^3\displaystyle\int_{t_{n-1}}^{t_{n+1}}\|\partial_{ttt}\phi\|^2dt+\frac{1}{8}\left\|\sigma_\phi^{n+1}\right\|_{-1,Q}^2, & n\geq 1,\\ 2C_9\tau^3+\dfrac{1}{8\tau}\left\|\sigma_\phi^1\right\|_{-1,Q}^2, & n=0.\end{cases} \tag{4.27}$$

For the nonlinear term J_2, we begin with an application of the mean value theorem:

$$g(\phi^{n+1})-g(R_h\phi^{n+1})=\frac{2(\phi^{n+1}-R_h\phi^{n+1})}{1-(\lambda^{n+1})^2},$$

where $\lambda^{n+1}\in S_h$ is between ϕ^{n+1} and $R_h\phi^{n+1}$. Moreover, from the positivity analysis, suppose there exists a constant $\delta>0$, $\|\phi^{n+1}\|_{L^\infty}\leq 1-\delta$. In turn, we get

$$\|R_h\phi^{n+1}\|_{L^\infty}\leq 1-\frac{1}{2}\delta,$$

if h is small enough, by Lemma 4.1. Therefore,

$$\|\frac{2}{1-(\lambda^{n+1})^2}\|\leq\frac{2}{1-(1-\frac{1}{2}\delta)^2}:=\tilde{C}_8. \tag{4.28}$$

Moreover, the convex nature of logarithmic term implies the following results:

$$\big(g(R_h\phi^{n+1})-g(\phi_h^{n+1}),\sigma_\phi^{n+1}\big)\geq 0. \tag{4.29}$$

Immediately, using the above inequality and Poincare's inequality yields the following result

$$\begin{aligned}
J_2=&-(g(\phi^{n+1})-g(\phi_h^{n+1}),\sigma_\phi^{n+1})_Q\\
=&-(g(\phi^{n+1})-g(R_h\phi^{n+1}),\sigma_\phi^{n+1})_Q-(g(R_h\phi^{n+1})-g(\phi_h^{n+1}),\sigma_\phi^{n+1})_Q\\
\leq&\tilde{C}_8\|\rho_\phi^{n+1}\|\|\sigma_\phi^{n+1}\|\leq C\tilde{C}_8\|\rho_\phi^{n+1}\|\|\nabla\sigma_\phi^{n+1}\|\\
\leq&\frac{C_8Ch^4}{2\varepsilon^2}\|\phi^{n+1}\|_{H^2}^2+\frac{\varepsilon^2}{8}\|\nabla\sigma_\phi^{n+1}\|^2,
\end{aligned} \tag{4.30}$$

where $C_8=(C\tilde{C}_8)^2$.

The standard finite element approximation estimate could be applied to handle the term J_5:

$$\begin{aligned}
J_5=&(\mu^{n+1}-R_h\mu^{n+1},\sigma_\phi^{n+1})_Q\\
\leq&\|(I-R_h)\mu^{n+1}\|_{-1,Q}\|\nabla\sigma_\phi^{n+1}\|\\
\leq&\frac{4Ch^4}{\varepsilon^2}\|\mu^{n+1}\|_{H^2}^2+\frac{\varepsilon^2}{16}\|\nabla\sigma_\phi^{n+1}\|^2.
\end{aligned} \tag{4.31}$$

By Lemma 4.2, we have

$$\begin{aligned}
J_6=&-\kappa_h(\delta_\tau\phi^{n+1},-\Delta_h^{-1}\sigma_\phi^{n+1})\\
\leq&Ch^2\|\nabla\delta_\tau\phi^{n+1}\|\|\nabla(\Delta_h^{-1}\sigma_\phi^{n+1})\|\\
\leq&Ch^2\|\nabla\delta_\tau\phi^{n+1}\|\|\sigma_\phi^{n+1}\|_{-1,Q}\\
\leq&\frac{2Ch^4}{\tau}\int_{t_n}^{t_{n+1}}\|\partial_t\nabla\phi\|^2dt+\frac{1}{8}\|\sigma_\phi^{n+1}\|_{-1,Q}^2.
\end{aligned} \tag{4.32}$$

Similarly, the following bounds could be derived:

$$J_7=\kappa_h(\mu^{n+1},\sigma_\phi^{n+1})\leq\frac{4Ch^4}{\varepsilon^2}\|\nabla\mu^{n+1}\|^2+\frac{\varepsilon^2}{16}\|\nabla\sigma_\phi^{n+1}\|^2, \tag{4.33a}$$

$$J_9=\theta_0\kappa_h(\phi^{n+1},\sigma_\phi^{n+1})\leq\frac{4Ch^4\theta_0^2}{\varepsilon^2}\|\nabla\phi^{n+1}\|^2+\frac{\varepsilon^2}{16}\|\nabla\sigma_\phi^{n+1}\|^2. \tag{4.33b}$$

Moreover, an application of Lemma 4.3 yields

$$\begin{aligned}J_8 \le& \kappa_h(g(\phi^{n+1}),\sigma_\phi^{n+1})\\ \le& C_5h^2(\|\nabla\phi^{n+1}\|_{L^4}^2\|\sigma_\phi^{n+1}\|+\|\nabla\phi^{n+1}\|\|\nabla\sigma_\phi^{n+1}\|)\\ \le& \frac{8(CC_5)^2h^4}{\varepsilon^2}(\|\nabla\phi^{n+1}\|_{L^4}^4+\|\nabla\phi^{n+1}\|^2)+\frac{\varepsilon^2}{16}\|\nabla\sigma_\phi^{n+1}\|^2. \end{aligned} \tag{4.34}$$

The term J_{10} could be analyzed in a similar manner:

$$\begin{aligned}J_{10}=&-(\delta_\tau\rho_\phi^{n+1},-\Delta_h^{-1}\sigma_\phi^{n+1})_Q\le\|\delta_\tau\rho_\phi^{n+1}\|_{-1,Q}\|\sigma_\phi^{n+1}\|_{-1,Q}\\ \le& 2\|\delta_\tau\rho_\phi^{n+1}\|_{-1,Q}^2+\frac{1}{8}\|\sigma_\phi^{n+1}\|_{-1,Q}^2\le\frac{2Ch^4}{\tau}\int_{t_n}^{t_{n+1}}\|\partial_t\phi\|^2dt+\frac{1}{8}\|\sigma_\phi^{n+1}\|_{-1,Q}^2. \end{aligned}\tag{4.35}$$

For the J_3 term, we see that

$$\begin{aligned}J_3\le&\theta_0\|\nabla R_2^{n+1}\|\|\sigma_\phi^{n+1}\|_{-1,Q}\\ \le&\begin{cases}64\theta_0^2\tau^3\displaystyle\int_{t_{n-1}}^{t_{n+1}}\|\partial_{tt}\nabla\phi\|^2dt+\frac{1}{8}\left\|\sigma_\phi^{n+1}\right\|_{-1,Q}^2, & n\ge1,\\ 2\theta_0^2C_{10}\tau^3+\dfrac{1}{8\tau}\left\|\sigma_\phi^1\right\|_{-1,Q}^2, & n=0.\end{cases}\end{aligned}\tag{4.36}$$

For the J_4 term, we define $T_{1,a}^{n+1}:=2\rho_\phi^n-\rho_\phi^{n-1}$ and $T_{1,h}^{n+1}:=2\sigma_\phi^n-\sigma_\phi^{n-1}$. It is obvious that $T_1^{n+1}=T_{1,a}^{n+1}+T_{1,h}^{n+1}$, so that the following bound is valid:

$$\begin{aligned}J_4=&\theta_0(T_1^{n+1},\sigma_\phi^{n+1})_Q=\theta_0(T_{1,a}^{n+1},\sigma_\phi^{n+1})_Q+\theta_0(T_{1,h}^{n+1},\sigma_\phi^{n+1})_Q\\ \le&\theta_0\|T_{1,a}^{n+1}\|_{-1,Q}\|\nabla\sigma_\phi^{n+1}\|+\theta_0\|T_{1,h}^{n+1}\|_{-1,Q}\|\nabla\sigma_\phi^{n+1}\|\\ \le&\begin{cases}\dfrac{\varepsilon^2}{4}\|\nabla\sigma_\phi^{n+1}\|^2+\dfrac{4\theta_0^2Ch^4}{\varepsilon^2}(4\|\phi^n\|_{H^2}^2+\|\phi^{n-1}\|_{H^2})+\dfrac{4\theta_0^2}{\varepsilon^2}(4\|\sigma_\phi^n\|_{-1,Q}^2+\|\sigma_\phi^{n-1}\|_{-1,Q}^2), & n\ge1,\\ \dfrac{3\varepsilon^2}{8}\|\nabla\sigma_\phi^1\|^2+\dfrac{2\theta_0^2Ch^4}{\varepsilon^2}\|\phi^0\|_{H^2}^2, & n=0.\end{cases}\end{aligned}$$

Lastly, repeating a similar process as in (4.18) gives an estimate for J_{11} as follows

$$\begin{aligned}J_{11}=&\tau(R_3^{n+1},\sigma_\phi^{n+1})=A\tau(\nabla(\phi^{n+1}-\phi^n),\nabla\sigma_\phi^{n+1})\le A\tau\|\nabla(\phi^{n+1}-\phi^n)\|\|\nabla\sigma_\phi^{n+1}\|\\ \le&\frac{2A^2\tau^3}{\varepsilon^2}\int_{t_n}^{t_{n+1}}\|\partial_t\nabla\phi\|^2dt+\frac{\varepsilon^2}{8}\|\nabla\sigma_\phi^{n+1}\|^2.\end{aligned}$$

Substituting these estimates into (4.21), and multiplying by 2τ on both sides, we have, for $n\geq 1$,

$$\begin{aligned}
&\left(\left\|\mathbf{p}^{n+1}\right\|_{\mathrm{G}}^{2}-\|\mathbf{p}^{n}\|_{\mathrm{G}}^{2}\right)+A\tau^{2}\left(\left\|\nabla\sigma_{\phi}^{n+1}\right\|^{2}-\left\|\nabla\sigma_{\phi}^{n}\right\|^{2}\right)+\frac{\varepsilon^{2}\tau}{2}\left\|\nabla\sigma_{\phi}^{n+1}\right\|^{2}\\
\leq&\tau\|\sigma_{\phi}^{n+1}\|_{-1,Q}^{2}+128\tau^{4}\int_{t_{n-1}}^{t_{n+1}}\|\partial_{ttt}\phi\|^{2}dt+\frac{C_{8}Ch^{4}\tau}{\varepsilon^{2}}\|\phi^{n+1}\|_{H^{2}}^{2}+128\theta_{0}^{2}\tau^{4}\int_{t_{n-1}}^{t_{n+1}}\|\partial_{tt}\nabla\phi\|^{2}dt\\
&+\frac{8\theta_{0}^{2}Ch^{4}\tau}{\varepsilon^{2}}(4\|\phi^{n}\|_{H^{2}}^{2}+\|\phi^{n-1}\|_{H^{2}})+\frac{8\theta_{0}^{2}\tau}{\varepsilon^{2}}(4\|\sigma_{\phi}^{n}\|_{-1,Q}^{2}+\|\sigma_{\phi}^{n-1}\|_{-1,Q}^{2})\\
&+\frac{8Ch^{4}\tau}{\varepsilon^{2}}\|\mu^{n+1}\|_{H^{2}}^{2}+4Ch^{4}\int_{t_{n}}^{t_{n+1}}\|\partial_{t}\nabla\phi\|^{2}dt+\frac{8Ch^{4}\tau}{\varepsilon^{2}}\|\nabla\mu^{n+1}\|^{2}+\frac{16C_{5}^{2}Ch^{4}\tau}{\varepsilon^{2}}\|\nabla\phi^{n+1}\|_{L^{4}}^{4}\\
&+\frac{8Ch^{4}\tau}{\varepsilon^{2}}(\theta_{0}^{2}+2C_{5}^{2})\|\nabla\phi^{n+1}\|^{2}+4Ch^{4}\int_{t_{n}}^{t_{n+1}}\|\partial_{t}\phi\|^{2}dt+\frac{4A^{2}\tau^{4}}{\varepsilon^{2}}\int_{t_{n}}^{t_{n+1}}\|\partial_{t}\nabla\phi\|^{2}dt. \qquad (4.37)
\end{aligned}$$

For $n=0$, a similar inequality could be derived:

$$\begin{aligned}
&\frac{1}{2}\|\sigma_{\phi}^{1}\|_{-1,Q}^{2}+\frac{\tau\varepsilon^{2}}{2}\|\nabla\sigma_{\phi}^{1}\|^{2}\\
\leq&\frac{\tau}{2}\left\|\sigma_{\phi}^{1}\right\|_{-1,Q}^{2}+\frac{C_{8}Ch^{4}\tau}{\varepsilon^{2}}\|\phi^{1}\|_{H^{2}}^{2}+\frac{4\theta_{0}^{2}Ch^{4}\tau}{\varepsilon^{2}}\|\phi^{0}\|_{H^{2}}^{2}+\frac{8Ch^{4}\tau}{\varepsilon^{2}}\|\mu^{1}\|_{H^{2}}^{2}\\
&+4Ch^{4}\int_{t_{0}}^{t_{1}}\|\partial_{t}\nabla\phi\|^{2}dt+\frac{8Ch^{4}\tau}{\varepsilon^{2}}\|\nabla\mu^{1}\|^{2}+\frac{16C_{5}^{2}Ch^{4}\tau}{\varepsilon^{2}}\|\nabla\phi^{1}\|_{L^{4}}^{4}\\
&+\frac{8Ch^{4}\tau}{\varepsilon^{2}}(\theta_{0}^{2}+2C_{5}^{2})\|\nabla\phi^{1}\|^{2}+4Ch^{4}\int_{t_{0}}^{t_{1}}\|\partial_{t}\phi\|^{2}dt+4C_{9}\tau^{4}+4\theta_{0}^{2}C_{10}\tau^{4}, \qquad (4.38)
\end{aligned}$$

or equivalently,

$$\begin{aligned}
&\frac{5}{2}\|\sigma_{\phi}^{1}\|_{-1,Q}^{2}+\frac{\tau\varepsilon^{2}}{2}\|\nabla\sigma_{\phi}^{1}\|^{2}\\
\leq&\frac{5\tau}{2}\left\|\sigma_{\phi}^{1}\right\|_{-1,Q}^{2}+\frac{5C_{8}Ch^{4}\tau}{\varepsilon^{2}}\|\phi^{1}\|_{H^{2}}^{2}+\frac{20\theta_{0}^{2}Ch^{4}\tau}{\varepsilon^{2}}\|\phi^{0}\|_{H^{2}}^{2}\\
&+\frac{40Ch^{4}\tau}{\varepsilon^{2}}\|\mu^{1}\|^{2}+20Ch^{4}\int_{t_{0}}^{t_{1}}\|\partial_{t}\nabla\phi\|^{2}dt+\frac{40Ch^{4}\tau}{\varepsilon^{2}}\|\nabla\mu^{1}\|^{2}\\
&+\frac{80C_{5}^{2}Ch^{4}\tau}{\varepsilon^{2}}\|\nabla\phi^{1}\|_{L^{4}}^{4}+\frac{40Ch^{4}\tau}{\varepsilon^{2}}(\theta_{0}^{2}+2C_{5}^{2})\|\nabla\phi^{1}\|^{2}\\
&+20Ch^{4}\int_{t_{0}}^{t_{1}}\|\partial_{t}\phi\|^{2}dt+20C_{9}\tau^{4}+20\theta_{0}^{2}C_{10}\tau^{4}, \qquad (4.39)
\end{aligned}$$

in which

$$\|\mathbf{p}^{1}\|_{\mathrm{G}}^{2}=\frac{5}{2}\|\sigma_{\phi}^{1}\|_{-1,Q}^{2}\quad\text{and}\quad\|\mathbf{p}^{n+1}\|_{\mathrm{G}}^{2}\geq\frac{1}{2}\|\sigma_{\phi}^{n+1}\|_{-1,Q}^{2}.$$

Summing (4.37) from $k=1$ to $k=n+1$, adding (4.39), keeping in mind of (4.13) (the relationship between G-norm and H^{-1}-norm), we arrive at the following estimate for $n\geq 1$:

$$\begin{aligned}&\frac{1}{2}\|\sigma_\phi^{n+1}\|_{-1,Q}^2+\frac{\varepsilon^2\tau}{2}\sum_{k=0}^{n}\|\nabla\sigma_\phi^{k+1}\|^2\\ \leq&\left\|\mathbf{p}^{n+1}\right\|_{\mathrm{G}}^2+A\tau^2\left\|\nabla\sigma_\phi^{n+1}\right\|^2+\frac{\varepsilon^2\tau}{2}\sum_{k=0}^{n}\left\|\nabla\sigma_\phi^{k+1}\right\|^2\\ \leq&\tau\|\sigma_\phi^{n+1}\|_{-1,Q}^2+\Big(\frac{5}{2}+\frac{40\theta_0^2}{\varepsilon^2}\Big)\tau\sum_{k=0}^{n-1}\left\|\sigma_\phi^{k+1}\right\|_{-1,Q}^2+\mathcal{R},\end{aligned}$$

where

$$\begin{aligned}\mathcal{R}=&\frac{40Ch^4\tau}{\varepsilon^2}\sum_{k=0}^{n}\|\mu^{k+1}\|_{H^2}^2+\frac{40Ch^4\tau}{\varepsilon^2}\sum_{k=0}^{n}\|\nabla\mu^{k+1}\|^2+128\tau^4\Big(\int_0^T\|\partial_{ttt}\phi\|^2dt+\theta_0^2\int_0^T\|\partial_{tt}\nabla\phi\|^2dt\Big)\\ &+20Ch^4\Big(\int_0^T\|\partial_t\nabla\phi\|^2dt+\int_0^T\|\partial_t\phi\|^2dt\Big)+\frac{5Ch^4\tau}{\varepsilon^2}(C_8+8\theta_0^2)\sum_{k=0}^{n}\|\phi^{k+1}\|_{H^2}^2\\ &+\frac{80Ch^4\tau}{\varepsilon^2}\sum_{k=0}^{n}\|\nabla\phi^{k+1}\|_{L^4}^4+\frac{40Ch^4\tau}{\varepsilon^2}(\theta_0^2+2C_5^2)\sum_{k=0}^{n}\|\nabla\phi^{k+1}\|^2+\frac{4A^2\tau^4}{\varepsilon^2}\int_0^T\|\partial_t\nabla\phi\|^2dt\\ &+20(C_9+\theta_0^2C_{10})\tau^4\\ \leq&C(T,\varepsilon)(\tau^4+h^4),\end{aligned}$$

where $C(T,\varepsilon)$ is independent of τ and h, under a technical assumption

$$0<\tau\leq\frac{1}{4}:=\tau_1. \tag{4.40}$$

Finally, an application of the discrete Gronwall inequality leads to the desired convergence result

$$\|\sigma_\phi^{n+1}\|_{-1,Q}^2+\varepsilon^2\tau\sum_{k=0}^{n}\|\nabla\sigma_\phi^{k+1}\|^2\leq C(T,\varepsilon)(\tau^4+h^4),$$

which completes the proof. □

Remark 4.1. Here the restriction condition (4.40) is simple and does not depend on ϵ, which may be different if the L^2 norm estimates are considered. This comes from the convexity property of the nonlinear term which has been used in H^{-1} norm analysis.

5 Numerical results

In this section, we present some numerical simulation results using the proposed scheme (3.1) to verify the theoretical results. We demonstrate, in particular, the positivity of the numerical solutions.

In the numerical test, we use a slightly different formulation of the Cahn-Hilliard equation, which allows for a comparison with the so-called obstacle potential. Specifically, we will use the standard Ginzburg-Landau free energy

$$E[\phi]=\int_\Omega\left\{f(\phi)+\frac{\varepsilon^2}{2}|\nabla\phi|^2\right\}d\mathbf{x},$$

where $f(\phi)=f_c(\phi)-f_e(\phi)$ and

$$f_c(\phi)=\frac{1}{2\theta_0}[(1-\phi)\ln(1-\phi)+(1+\phi)\ln(1+\phi)],\quad f_e(\phi)=\frac{1}{2}(\phi-1)(\phi+1). \tag{5.1}$$

Importantly, as $\theta_0\to\infty$, f tends to the obstacle potential

$$f_{\text{obs}}(\theta)=\begin{cases}\dfrac{1}{2}(\phi-1)(\phi+1), & \text{if } -1<\phi<1,\\ \infty, & \text{if } |\phi|\geq 1,\end{cases}$$

which has been investigated elsewhere [5, 6]. While we are only interested in the case of finite values of θ_0, it is interesting to explore the effects of increasing θ_0. For finite θ_0, clearly $f_e'(\phi)=\phi$ and

$$f_c'(\phi)=\frac{1}{2\theta_0}(\ln(1+\phi)-\ln(1-\phi)).$$

In turn, the chemical potential for the Cahn-Hilliard model could be expressed as

$$\mu=f_c'(\phi)-f_e'(\phi)-\varepsilon^2\Delta\phi.$$

Next, two examples will be simulated to verify the theoretical result. The first example is aimed to test the numerical convergence associated with the numerical scheme and the second one is to present some results associated with the phase evolution.

Example 5.1. Here we give a convergence test for the proposed numerical scheme. The initial condition is given by

$$\phi(x,y,0)=1.8\left(\frac{1-\cos\left(\frac{4x\pi}{3.2}\right)}{2}\right)\left(\frac{1-\cos\left(\frac{2y\pi}{3.2}\right)}{2}\right)-0.9. \tag{5.2}$$

To get the convergence rate, "the Cauchy difference", δ_ϕ, is computed between approximate solutions obtained with successively finer time sizes. Since the exact solution is unknown, we compute the errors by adjacent time step in the numerical accuracy test, where the coarse spacial step h_c is twice as much as the fine step h_f. The parameters are given by: (domain size) $L=3.2$; (interfacial parameter) $\varepsilon=0.2$; (mobility) $M\equiv 1$; (quench parameter) $\theta_0=3.0$; (final time) $T=0.4$; (Newton iteration stopping tolerance)

Table 1: Numerical errors and convergence rates for the proposed numerical scheme at $T=0.4$.

h_c	h_f	$\|e_\phi\|_\infty$	Rate	$\|e_\phi\|_2$	Rate
$\frac{3.2}{16}$	$\frac{3.2}{32}$	1.3811e-01	–	1.0976e-01	–
$\frac{3.2}{32}$	$\frac{3.2}{64}$	3.7976e-02	1.8626	3.0280e-02	1.8579
$\frac{3.2}{64}$	$\frac{3.2}{128}$	9.7227e-03	1.9657	7.7705e-03	1.9623
$\frac{3.2}{128}$	$\frac{3.2}{256}$	2.4478e-03	1.9898	1.9580e-03	1.9886
$\frac{3.2}{256}$	$\frac{3.2}{512}$	6.1343e-04	1.9965	4.9085e-04	1.9961

$\sigma=10^{-6}$; (stabilization parameter) $A=1$. The refinement path for the proposed second-order scheme is linear, $\tau=0.1h$. We only consider the periodic boundary condition, while the case of homogeneous Neumann boundary condition could be similarly handled. The test results are displayed in Table 1. We observe that the optimal convergence rate is achieved, with perfect second order accuracy in both time and space.

Example 5.2. Consider the spinodal decomposition over the domain $\Omega=(0,1)^2$, with the physical parameters $\varepsilon=5.0\times10^{-3}$, $\theta_0=3.0$, as well as the numerical resolution $h=1/256$, $\tau=5\times10^{-6}$. The initial data is given by

$$\phi(x,y,0)=0.2+r_{i,j}, \tag{5.3}$$

where $r_{i,j}$ is uniformly distributed random numbers in $[-0.02,0.02]$.

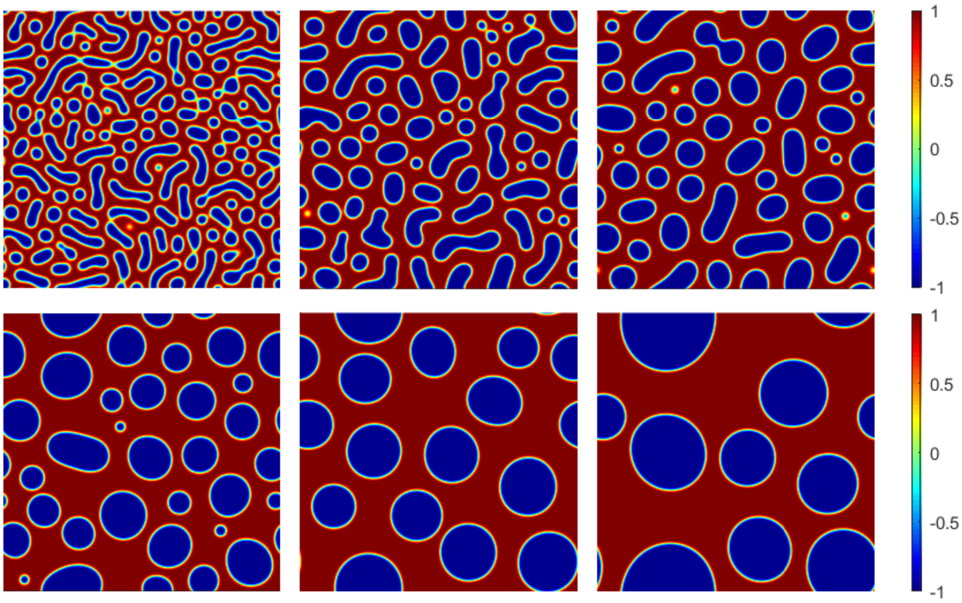
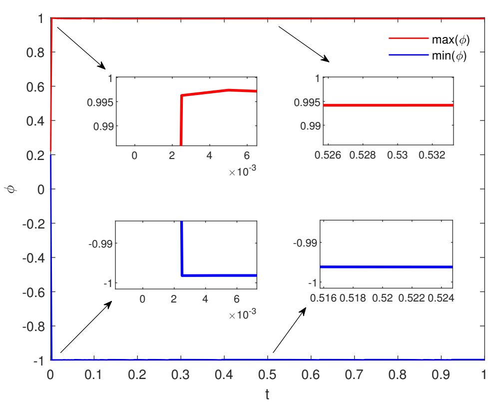
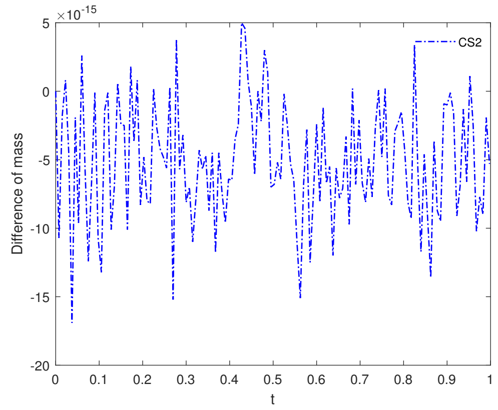


Figure 1: Evolution of phase variables at $t=0.004$, 0.01, 0.02, 0.1, 0.4 and 1, respectively.



(a)



(b)

Figure 2: (a): The time evolution of the minimum and the maximum value of ϕ; (b): The error development of the total mass for ϕ.

The second order scheme is implemented with stabilization parameter $A=1$ to show the details of spinodal decomposition with random initial data. Fig. 1 displays the snapshot plot of ϕ at t = 0.004, 0.01, 0.02, 0.1, 0.4 and 1, respectively. Moreover, the maximum values and minimum values of the phase variable are presented in Fig. 2(a). In particular, a larger version of Fig. 2(a) implies that the numerical solution is always located in the interval $(-1,1)$, which is in agreement with the theory analysis. In addition, we present the error evolution of the total mass of ϕ (away from the mass of ϕ_0) in Fig. 2(b), which demonstrates the mass conservation property. The energy evolution of the numerical solution is illustrated in Fig. 3, and a clear energy decay is observed.

6 Concluding remarks

In this paper, we propose and analyze a second-order accurate in time, mass lumped finite element numerical scheme for the Cahn-Hilliard equation with logarithmic Flory-Huggins energy potential. which contains an implicit treatment of the logarithmic term and the linear surface diffusion terms, as well as an explicit update of the concave expansive linear terms. The backward differentiation formula (BDF) stencil is applied in the temporal discretization. In the chemical potential approximation, both the logarithmic singular terms and the surface diffusion term are treated implicitly, while the expansive term is explicitly updated via a second-order Adams-Bashforth extrapolation formula. An artificial Douglas-Dupont regularization term is added to ensure the energy dissipation. Mass lumped finite element approximation and the singular nature of the logarithmic term ensure that the proposed numerical algorithm has a unique solution with preserved positivity for the logarithmic arguments, so that the finite element numeri-

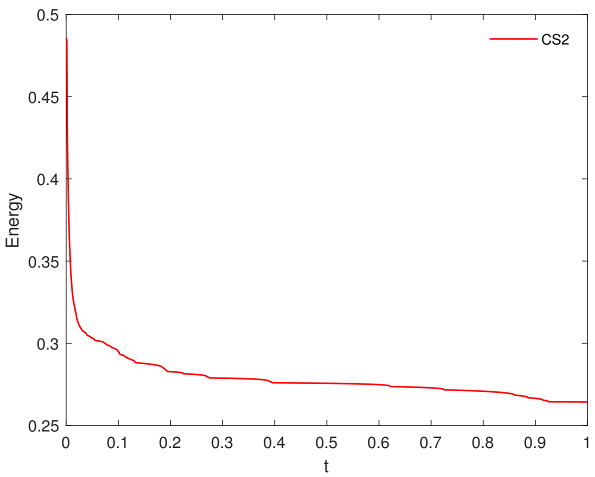


Figure 3: Evolution of the energy over time, with $\tau = 5\times 10^{-6}$.

cal solution is always located in the interval $(-1,1)$ for all time in the piecewise sense. Moreover, a modified energy stability is theoretically justified, and the convergence analysis and error estimate have been established in the $\ell^\infty(0,T;H^{-1})\cap\ell^2(0,T;H^1)$ norm. Finally, two numerical examples are carried out to show the robustness and accuracy of the proposed numerical scheme, especially the performance of the spinodal decomposition phenomenon.

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