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A POSITIVITY-PRESERVING, ENERGY STABLE AND CONVERGENT NUMERICAL SCHEME FOR THE CAHN-HILLIARD EQUATION WITH A FLORY-HUGGINS-DEGENNES ENERGY*

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Abstract. This article is focused on the bound estimate and convergence analysis of an unconditionally energy-stable scheme for the MMC-TDGL equation, a Cahn-Hilliard equation with a Flory-Huggins-deGennes energy. The numerical scheme, a finite difference algorithm based on a convex splitting technique of the energy functional, was proposed in [Sci. China Math., 59:1815, 2016]. We provide a theoretical justification of the unique solvability for the proposed numerical scheme, in which a well-known difficulty associated with the singular nature of the logarithmic energy potential has to be handled. Meanwhile, a careful analysis reveals that, such a singular nature prevents the numerical solution of the phase variable reaching the limit singular values, so that the positivity-preserving property could be proved at a theoretical level. In particular, the natural structure of the deGennes diffusive coefficient also ensures the desired positivity-preserving property. In turn, the unconditional energy stability becomes an outcome of the unique solvability and the convex-concave decomposition for the energy functional. Moreover, an optimal rate convergence analysis is presented in the $\ell^\infty(0,T;H_h^{-1})\cap\ell^2(0,T;H_h^1)$ norm, in which the the convexity of nonlinear energy potential has played an essential role. In addition, a rewritten form of the surface diffusion term has facilitated the convergence analysis, in which we have made use of the special structure of concentration-dependent deGennes type coefficient. Some numerical results are presented as well.

Keywords. Cahn-Hilliard equation; Flory-Huggins energy; deGennes diffusive coefficient; energy stability; positivity-preserving; convergence analysis.

AMS subject classifications. 60F10; 60J75; 62P10; 92C37.

1. Introduction

Composite hydrogel is an important material in the polymeric field, such as topological gels (TP), nanocomposite hydrogels (NC), macromolecular microspheres (MMSs), and so on [35]. Phase transition is the foundational phenomena of these materials. It is urgently expected to understand the progress of phase transition and find the important microscopic factors to determine the microstructure and property of hydrogels. Here we present a numerical approximation of the phase transition of the macromolecular microsphere composite (MMC) hydrogel, which has a well-defined reticular structure and high mechanical strength [22]. Zhai and Zhang [43] have developed a reticular free energy according to the structures of the MMC hydrogel, based on Boltzmann entropy theory. Then they presented a mathematical model to state the phase transition of the MMC hydrogels, so-called MMC-TDGL equation and also similar to the Cahn-Hilliard equation. However, it possesses the reticular Flory-Huggins-deGennes free energy and variable diffusive coefficient, called deGennes diffusion coefficient. Zhang et al. [24, 26] present some numerical approximations to perfectly simulate this MMC-TDGL equation.

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Allen-Cahn and Cahn-Hilliard equations are traditional phase field models with Ginzburg-Landau or Flory-Huggins energy density [19]. In some cases, certain stochastic force term has been added in the model, such as Cahn-Hilliard-Cook model, and these models can be used to describe the structural evolution of mixtures with polymers and block copolymers [19]. Concerning the computation and analysis of these models, Du et al. had a series of works [9, 10, 16]. Yang et al. presented invariant energy quadratization(IEQ) approximation [41, 42, 45–47]. Chen et al. used the phase field method to investigate composite materials and presented some numerical methods [15]. Shen et al. designed a few high-order energy-stable numerical schemes and provided the corresponding error estimates [29–34]. These works investigated the nucleation by using string method in virtue of stochastic Allen-Cahn and Cahn-Hilliard equations [44].

Since the pioneering work by Elliott [17] and Eyre [18], the convex splitting approximation has been a popular numerical approach to solve gradient flows with energy stability. The fundamental observation is that the energy E admits a splitting into purely convex and concave parts, that is, $E = E_c - E_e$, where E_c and E_e are both convex. Such an idea has also been applied to a wide class of gradient flows in recent years. Both first and second order accurate in time algorithms have been developed. See the related works for the PFC equation and the modified PFC (MPFC) equation [14, 37, 38, 40]; the epitaxial thin film growth models [1, 4, 7, 23, 28, 36], the Cahn-Hilliard flow and its coupling with fluid motion [2, 3, 6, 12, 13, 21, 27, 39], etc.

For the MMC-TDGL equation, a convex splitting of the discrete energy in temporal approximation, combined with the centered difference discretization in space, was proposed and studied in [25]. This scheme was proved to be unconditionally energy-stable, provided that the positivity-preserving property is valid for the numerical solution of the phase variable. On the other hand, although this property was extensively demonstrated in the numerical experiments [25], a theoretical justification has not been available. One well-known challenge for the numerical scheme with the Flory-Huggins energy density has always been associated with the singularity of the numerical solution as the phase variable approaches limit values. In an earlier work [8], the authors analyzed a fully discrete finite element scheme based on the backward Euler approximation for the Cahn-Hilliard equation with a logarithmic free energy; some theoretical results about the positivity property of the numerical solution were obtained. On the other hand, as stated in a remark in [8]: *our analysis requires the condition* $k < 4\gamma/\theta_c^2$. *This is a consequence of the non-convexity of the free energy. Even though it is independent of the spatial mesh, this condition is restrictive because* $\gamma \ll 1$. In addition, an energy stability analysis has not been justified for the fully discrete scheme in [8], either, due to the implicit treatment of the concave expansive term. In a more recent work [5], the authors presented a finite difference scheme based on the convex-concave decomposition of the free energy with logarithmic potential and established a theoretical justification of the positivity property, regardless of time step size. This improvement has been based on the following fact: *the singular nature of the logarithmic term around the boundary values prevents the numerical solution from reaching these singular values, so that the numerical scheme is always well-defined as long as the numerical solution stays similarly bounded at the previous time step.*

In this article, we perform a theoretical investigation of the numerical scheme proposed and studied in [25]. In fact, this scheme is equivalent to a minimization of a strictly convex discrete energy functional at each time step. Then we can transform the positivity-preserving analysis of the numerical solution into the minimization problem of this functional, via a rigorous proof by contradiction. Because of the implicit treatment for the logarithmic terms, which comes from the convex splitting approach, we can make use of the following subtle fact: the singular feature of the logarithmic function guarantees that such a minimizer could not occur on a limit value at all. In fact, such an estimate could not pass through if the logarithmic term is explicitly updated. Moreover, the term associated with the deGennes diffusive coefficient $\kappa(\phi)=1/[36\phi(1-\phi)]$ is very challenging, due to its singularity. With the help of the following inequality: $\frac{1}{2}\kappa'(\phi_1)(\phi_2-\phi_1)\le\kappa(\phi_2), \forall\phi_1,\phi_2\in(0,1)$, for the deGennes coefficient, which plays an essential role in the analysis, we can establish the positivity-preserving property for the numerical solution.

In addition to the existence, uniqueness, positivity-preserving property and unconditional energy stability of the numerical scheme, we also provide an optimal rate convergence analysis, which has not been reported for the MMC-TDGL equation in the existing literature. The key difficulty in the convergence analysis has always been associated with the logarithmic potential term. In general, if the nonlinear term is a polynomial approximation, an estimate of the ℓ^∞ bound for the numerical solution enables one to justify the convergence analysis. However, such an ℓ^∞ bound turns out to be not sufficient to derive the convergence analysis with the logarithmic potential, due to the singular nature as the numerical solution approaches the limit values. Here we treat the three nonlinear logarithmic terms as a whole, and make full use of the convexity of the associated nonlinear terms, which indicates that the corresponding nonlinear error of the inner product is always non-negative. Moreover, a control of the linear expansive term is not available using a standard convexity analysis. To overcome this subtle difficulty, we divide the surface diffusion term into two convex parts: one term can be analyzed in a manner similar to the logarithmic term, with the help of its convexity property, and the other term can be used to control the explicit error estimate associated with the Huggins interaction. In turn, the convergence analysis could go through at a theoretical level.

The rest of the paper is organized as follows. In Section 2, we present the mathematical model of the phase transition of the MMC hydrogel. In Section 3, we review the unconditional energy-stable numerical scheme proposed in [25], and state the main theoretical results. The detailed proof for the positivity-preserving property of the numerical solution is provided in Section 4, and the detailed convergence analysis is given by Section 5. The numerical simulation results are presented in Section 6. Finally, some concluding remarks are given in Section 7.

2. The model equation: MMC-TDGL equation

We consider a bounded domain $\Omega\subset\mathbb{R}^2$. For any $\phi\in H^1(\Omega)$, with a point-wise bound, $\phi\in(0,1/\rho)\subset(0,1)$, the energy functional is given by

$$E(\phi)=\int_\Omega\left(S(\phi)+H(\phi)+\kappa(\phi)|\nabla\phi|^2\right)d\mathbf{x}, \tag{2.1}$$

where $S(\phi)+H(\phi)$ is the reticular free energy density for the MMC hydrogels

$$S(\phi)=\frac{\phi}{\tau}\ln\frac{\alpha\phi}{\tau}+\frac{\phi}{N_1}\ln\frac{\beta\phi}{\tau}+(1-\rho\phi)\ln(1-\rho\phi),\quad H(\phi)=\chi\phi(1-\rho\phi), \tag{2.2}$$

and $\kappa(\phi)$ is the deGennes coefficient

$$\kappa(\phi)=\frac{1}{36\phi(1-\phi)}. \tag{2.3}$$

In this model, we denote by χ the Huggins interaction parameter, by N_1 the degree of polymerization of the polymer chains, and by N_2, which does not appear explicitly in (2.1), the relative volume of one macromolecular microsphere. The other numbers α,β,τ and ρ depend on N_2 and N_1, as given by

$$\alpha=\pi\left(\sqrt{\frac{N_2}{\pi}}+\frac{N_1}{2}\right)^2,\quad \beta=\frac{\alpha}{\sqrt{\pi N_2}},\quad \tau=\sqrt{\pi N_2}N_1,\quad \rho=1+\frac{N_2}{\tau}.$$

Note that all these parameters are positive. Besides, ρ is a little greater than one. The modeling detail can be referred to [43].

In turn, the MMC-TDGL equation for the MMC hydrogels becomes the following H^{-1} gradient flow associated with the given energy functional:

$$\begin{aligned}\partial_t\phi=\Delta\mu,\quad \mu:=\delta_\phi E&=S'(\phi)+H'(\phi)+\kappa'(\phi)|\nabla\phi|^2-2\nabla\cdot(\kappa(\phi)\nabla\phi)\\&=(\frac{1}{\tau}+\frac{1}{N_1})\ln\phi-\rho\ln(1-\rho\phi)-2\chi\rho\phi\\&\quad+\frac{2\phi-1}{36\phi^2(1-\phi)^2}|\nabla\phi|^2-\nabla\cdot\left(\frac{\nabla\phi}{18\phi(1-\phi)}\right).\end{aligned}\tag{2.4}$$

Also notice that we have discarded the constant terms in the representation for the chemical potential μ, since these terms will not play any role in the H^{-1} gradient flow.

3. The numerical scheme

In the spatial discretization, the centered finite difference approximation is applied. We recall some basic notations of this methodology.

3.1. Discretization of space and a few preliminary estimates. We use the notation and results for some discrete functions and operators from [20, 39, 40]. Let $\Omega=(0,L_x)\times(0,L_y)$, where for simplicity, we assume $L_x=L_y=:L>0$. Let $N\in\mathbb{N}$ be given, and define the grid spacing $h:=L/N$. We also assume-but only for simplicity of notation, ultimately-that the mesh spacing in the x and y-directions are the same. The following two uniform, infinite grids with grid spacing $h>0$, are introduced

$$E:=\{p_{i+1/2}\mid i\in\mathbb{Z}\},\quad C:=\{p_i\mid i\in\mathbb{Z}\},$$

where $p_i=p(i):=(i-1/2)\cdot h$. Consider the following 2-D discrete N^2-periodic function spaces:

$$\begin{aligned}\mathcal{C}_{\rm per}&:=\{\nu:C\times C\to\mathbb{R}\mid \nu_{i,j}=\nu_{i+\alpha N,j+\beta N},\ \forall i,j,\alpha,\beta\in\mathbb{Z}\},\\ \mathcal{E}^{\rm x}_{\rm per}&:=\left\{\nu:E\times C\to\mathbb{R}\ \middle|\ \nu_{i+\frac12,j}=\nu_{i+\frac12+\alpha N,j+\beta N},\ \forall i,j,\alpha,\beta\in\mathbb{Z}\right\}.\end{aligned}$$

Here we are using the identification $\nu_{i,j}=\nu(p_i,p_j)$, *et cetera*. The space $\mathcal{E}^{\rm y}_{\rm per}$ is analogously defined. The functions of $\mathcal{C}_{\rm per}$ are called *cell centered functions*. The functions of $\mathcal{E}^{\rm x}_{\rm per}$ and $\mathcal{E}^{\rm y}_{\rm per}$, are called *edge-centered functions*. We also define the mean-zero space

$$\mathring{\mathcal{C}}_{\rm per}:=\left\{\nu\in\mathcal{C}_{\rm per}\ \middle|\ 0=\overline{\nu}:=\frac{h^2}{|\Omega|}\sum_{i,j=1}^{N}\nu_{i,j}\right\}.$$

In addition, $\vec{\mathcal{E}}_{\rm per}$ is defined as $\vec{\mathcal{E}}_{\rm per}:=\mathcal{E}^{\rm x}_{\rm per}\times\mathcal{E}^{\rm y}_{\rm per}$.

We now introduce the difference and average operators on the spaces:

$$A_x\nu_{i+1/2,j} := \frac{1}{2}\left(\nu_{i+1,j}+\nu_{i,j}\right), \quad D_x\nu_{i+1/2,j} := \frac{1}{h}\left(\nu_{i+1,j}-\nu_{i,j}\right),$$
$$A_y\nu_{i,j+1/2} := \frac{1}{2}\left(\nu_{i,j+1}+\nu_{i,j}\right), \quad D_y\nu_{i,j+1/2} := \frac{1}{h}\left(\nu_{i,j+1}-\nu_{i,j}\right),$$

with $A_x, D_x : \mathcal{C}_{\rm per} \to \mathcal{E}_{\rm per}^{\rm x}$, $A_y, D_y : \mathcal{C}_{\rm per} \to \mathcal{E}_{\rm per}^{\rm y}$. Likewise,

$$a_x\nu_{i,j} := \frac{1}{2}\left(\nu_{i+1/2,j}+\nu_{i-1/2,j}\right), \quad d_x\nu_{i,j} := \frac{1}{h}\left(\nu_{i+1/2,j}-\nu_{i-1/2,j}\right),$$
$$a_y\nu_{i,j} := \frac{1}{2}\left(\nu_{i,j+1/2}+\nu_{i,j-1/2}\right), \quad d_y\nu_{i,j} := \frac{1}{h}\left(\nu_{i,j+1/2}-\nu_{i,j-1/2}\right),$$

with $a_x, d_x : \mathcal{E}_{\rm per}^{\rm x} \to \mathcal{C}_{\rm per}$, $a_y, d_y : \mathcal{E}_{\rm per}^{\rm y} \to \mathcal{C}_{\rm per}$. The discrete gradient gradient $\nabla_h : \mathcal{C}_{\rm per} \to \vec{\mathcal{E}}_{\rm per}$ is given by

$$\nabla_h\nu_{i,j} = \left(D_x\nu_{i+1/2,j}, D_y\nu_{i,j+1/2}\right),$$

and the discrete divergence $\nabla_h\cdot : \vec{\mathcal{E}}_{\rm per} \to \mathcal{C}_{\rm per}$ is defined via

$$\nabla_h\cdot\vec{f}_{i,j} = d_x f^x_{i,j} + d_y f^y_{i,j},$$

where $\vec{f} = (f^x, f^y) \in \vec{\mathcal{E}}_{\rm per}$. The standard 2-D discrete Laplacian, $\Delta_h : \mathcal{C}_{\rm per} \to \mathcal{C}_{\rm per}$, becomes

$$\begin{aligned}\Delta_h\nu_{i,j} :=& d_x(D_x\nu)_{i,j} + d_y(D_y\nu)_{i,j}\\ =& \frac{1}{h^2}\left(\nu_{i+1,j}+\nu_{i-1,j}+\nu_{i,j+1}+\nu_{i,j-1}-4\nu_{i,j}\right).\end{aligned}$$

More generally, if $\mathcal{D}$ is a periodic *scalar* function that is defined at all of the edge center points and $\vec{f} \in \vec{\mathcal{E}}_{\rm per}$, then $\mathcal{D}\vec{f} \in \vec{\mathcal{E}}_{\rm per}$, assuming point-wise multiplication, and we may define

$$\nabla_h\cdot\left(\mathcal{D}\vec{f}\right)_{i,j} = d_x\left(\mathcal{D}f^x\right)_{i,j} + d_y\left(\mathcal{D}f^y\right)_{i,j}.$$

Specifically, if $\nu \in \mathcal{C}_{\rm per}$, then $\nabla_h\cdot(\mathcal{D}\nabla_h \quad) : \mathcal{C}_{\rm per} \to \mathcal{C}_{\rm per}$ is defined point-wise via

$$\nabla_h\cdot\left(\mathcal{D}\nabla_h\nu\right)_{i,j} = d_x\left(\mathcal{D}D_x\nu\right)_{i,j} + d_y\left(\mathcal{D}D_y\nu\right)_{i,j}.$$

Now we are ready to define the following grid inner products:

$$\langle\nu,\xi\rangle_\Omega := h^2\sum_{i,j=1}^{N}\nu_{i,j}\xi_{i,j}, \quad \nu,\xi \in \mathcal{C}_{\rm per}, \qquad [\nu,\xi]_{\rm x} := \langle a_x(\nu\xi), 1\rangle_\Omega, \quad \nu,\xi \in \mathcal{E}_{\rm per}^{\rm x},$$
$$[\nu,\xi]_{\rm y} := \langle a_y(\nu\xi), 1\rangle_\Omega, \quad \nu,\xi \in \mathcal{E}_{\rm per}^{\rm y}.$$

$$\left[\vec{f}_1, \vec{f}_2\right]_\Omega := [f_1^x, f_2^x]_{\rm x} + [f_1^y, f_2^y]_{\rm y}, \quad \vec{f}_i = (f_i^x, f_i^y) \in \vec{\mathcal{E}}_{\rm per}, \ i = 1,2.$$

In turn, the following norms could be appropriately introduced for cell-centered functions. If $\nu \in \mathcal{C}_{\rm per}$, then $\|\nu\|_2^2 := \langle\nu,\nu\rangle_\Omega$; $\|\nu\|_p^p := \langle|\nu|^p, 1\rangle_\Omega$, for $1 \le p < \infty$, and $\|\nu\|_\infty := \max_{1\le i,j\le N}|\nu_{i,j}|$. We define norms of the gradient as follows: for $\nu \in \mathcal{C}_{\rm per}$,

$$\|\nabla_h\nu\|_2^2 := [\nabla_h\nu, \nabla_h\nu]_\Omega = [D_x\nu, D_x\nu]_{\rm x} + [D_y\nu, D_y\nu]_{\rm y},$$

and, more generally, for $1 \le p < \infty$,

$$\|\nabla_h \nu\|_p := \left([|D_x \nu|^p, 1]_{\mathrm{x}} + [|D_y \nu|^p, 1]_{\mathrm{y}} \right)^{\frac{1}{p}}. \tag{3.1}$$

Higher order norms can be similarly formulated. For example,

$$\|\nu\|_{H_h^1}^2 := \|\nu\|_2^2 + \|\nabla_h \nu\|_2^2, \quad \|\nu\|_{H_h^2}^2 := \|\nu\|_{H_h^1}^2 + \|\Delta_h \nu\|_2^2.$$

LEMMA 3.1. *Let $\mathcal{D}$ be an arbitrary periodic, scalar function defined on all of the edge center points. For any $\psi, \nu \in \mathcal{C}_{\mathrm{per}}$ and any $\vec{f} \in \vec{\mathcal{E}}_{\mathrm{per}}$, the following summation by parts formulas are valid:*

$$\left\langle \psi, \nabla_h \cdot \vec{f} \right\rangle_\Omega = -\left[\nabla_h \psi, \vec{f} \right]_\Omega, \quad \langle \psi, \nabla_h \cdot (\mathcal{D} \nabla_h \nu) \rangle_\Omega = -[\nabla_h \psi, \mathcal{D} \nabla_h \nu]_\Omega. \tag{3.2}$$

To facilitate the convergence analysis, we need to introduce a discrete analogue of the space $H_{per}^{-1}(\Omega)$, as outlined in [38]. Suppose that $\mathcal{D}$ is a positive, periodic scalar function defined at all of face center points. For any $\phi \in \mathcal{C}_{\mathrm{per}}$, there exists a unique $\psi \in \mathring{\mathcal{C}}_{\mathrm{per}}$ that solves

$$\mathcal{L}_{\mathcal{D}}(\psi) := -\nabla_h \cdot (\mathcal{D} \nabla_h \psi) = \phi - \overline{\phi}, \tag{3.3}$$

where $\overline{\phi} := |\Omega|^{-1} \langle \phi, 1 \rangle_\Omega$. We equip this space with a bilinear form: for any $\phi_1, \phi_2 \in \mathring{\mathcal{C}}_{\mathrm{per}}$, define

$$\langle \phi_1, \phi_2 \rangle_{\mathcal{L}_{\mathcal{D}}^{-1}} := [\mathcal{D} \nabla_h \psi_1, \nabla_h \psi_2]_\Omega, \tag{3.4}$$

where $\psi_i \in \mathring{\mathcal{C}}_{\mathrm{per}}$ is the unique solution to

$$\mathcal{L}_{\mathcal{D}}(\psi_i) := -\nabla_h \cdot (\mathcal{D} \nabla_h \psi_i) = \phi_i, \quad i = 1, 2. \tag{3.5}$$

The following identity [38] is easy to prove via summation-by-parts:

$$\langle \phi_1, \phi_2 \rangle_{\mathcal{L}_{\mathcal{D}}^{-1}} = \left\langle \phi_1, \mathcal{L}_{\mathcal{D}}^{-1}(\phi_2) \right\rangle_\Omega = \left\langle \mathcal{L}_{\mathcal{D}}^{-1}(\phi_1), \phi_2 \right\rangle_\Omega, \tag{3.6}$$

and since $\mathcal{L}_{\mathcal{D}}$ is symmetric positive definite, $\langle \cdot , \cdot \rangle_{\mathcal{L}_{\mathcal{D}}^{-1}}$ is an inner product on $\mathring{\mathcal{C}}_{\mathrm{per}}$ [38]. When $\mathcal{D} \equiv 1$, we drop the subscript and write $\mathcal{L}_1 = \mathcal{L}$, and in this case we usually write $\langle \cdot , \cdot \rangle_{\mathcal{L}_{\mathcal{D}}^{-1}} =: \langle \cdot , \cdot \rangle_{-1,h}$. In the gerneral setting, the norm associated to this inner product is denoted $\|\phi\|_{\mathcal{L}_{\mathcal{D}}^{-1}} := \sqrt{\langle \phi, \phi \rangle_{\mathcal{L}_{\mathcal{D}}^{-1}}}$, for all $\phi \in \mathring{\mathcal{C}}_{\mathrm{per}}$, but, if $\mathcal{D} \equiv 1$, we write $\|\cdot\|_{\mathcal{L}_{\mathcal{D}}^{-1}} =: \|\cdot\|_{-1,h}$.

The following preliminary results are associated with the existence of a convex splitting.

PROPOSITION 3.1.
(1) S and -H are both convex in $(0, 1/\rho)$, where S and H are defined by (2.2);
(2) $K(u,v) := \kappa(u) v^2$ is convex in $(0, 1/\rho) \times \mathbb{R}$, where κ is defined by (2.3);
(3) $K_1(u,v) := \left(\kappa(u) - \frac{1}{36} \right) v^2$ and $K_2(v) := \frac{1}{36} v^2$ are both convex in $(0, 1/\rho) \times \mathbb{R}$ and $\mathbb{R}$, respectively.

Proof. For S, H, K_2, differentiating S, H, K_2 twice, we obtain

$$S''(\phi) = \left(\frac{1}{\tau} + \frac{1}{N_1} \right) \frac{1}{\phi} + \frac{\rho^2}{1 - \rho\phi}, \quad H''(\phi) = -2\chi\rho, \quad K_2''(v) = \frac{1}{18} > 0.$$

When $\phi \in (0, 1/\rho)$, we have $S''(\phi) > 0$ and $H''(\phi) < 0$.

For $K(u,v) := \kappa(u)v^2$, by some careful calculations, we obtain the Hessian matrix of K:

$$\nabla^2 K = \begin{pmatrix} \frac{(3u^2-3u+1)v^2}{18u^3(1-u)^3} & \frac{(2u-1)v}{18u^2(1-u)^2} \\ \frac{(2u-1)v}{18u^2(1-u)^2} & \frac{1}{18u(1-u)} \end{pmatrix}.$$

The first-order principal minors of the matrix $\nabla^2 K$ are

$$D_1 = \frac{(3u^2-3u+1)v^2}{18u^3(1-u)^3}, \quad D_2 = \frac{1}{18u(1-u)}.$$

The second-order principal minor is

$$D_{12} = det(\nabla^2 K) = \frac{v^2}{18^2 u^3 (1-u)^3}.$$

These principal minors are all non-negative when $u \in (0, 1/\rho)$ and $v \in \mathbb{R}$. The Hessian matrix $\nabla^2 K$ is positive semi-definite and thus K is convex in $(0, 1/\rho) \times \mathbb{R}$.

For $K_1(u,v) := \left(\kappa(u) - \frac{1}{36}\right) v^2$, by some careful calculations, we obtain the Hessian matrix of K_1:

$$\nabla^2 K_1 = \begin{pmatrix} \frac{(3u^2-3u+1)v^2}{18u^3(1-u)^3} & \frac{(2u-1)v}{18u^2(1-u)^2} \\ \frac{(2u-1)v}{18u^2(1-u)^2} & \frac{u^2-u+1}{18u(1-u)} \end{pmatrix}.$$

The first-order principal minors of the matrix $\nabla^2 K_1$ are

$$D_1 = \frac{(3u^2-3u+1)v^2}{18u^3(1-u)^3}, \quad D_2 = \frac{u^2-u+1}{18u(1-u)}.$$

The second-order principal minor is

$$D_{12} = det(\nabla^2 K_1) = \frac{3}{18^2 u^2 (1-u)^2}.$$

These principal minors are all non-negative when $u \in (0, 1/\rho)$ and $v \in \mathbb{R}$. The Hessian matrix $\nabla^2 K_1$ is positive semi-definite and thus K_1 is convex in $(0, 1/\rho) \times \mathbb{R}$. $\square$

Define the discrete energy $F : \mathcal{C}_{\mathrm{per}} \to \mathbb{R}$ as

$$\begin{aligned} F(\phi) &= h^2 \sum_{i,j=1}^{N} \left(S(\phi_{i,j}) + H(\phi_{i,j}) + \kappa(\phi_{i,j})(a_x((D_x\phi)^2)_{i,j} + a_y((D_y\phi)^2)_{i,j}) \right) \\ &= h^2 \sum_{i,j=1}^{N} \left(S(\phi_{i,j}) + H(\phi_{i,j}) + (\kappa(\phi_{i,j}) - \frac{1}{36})(a_x((D_x\phi)^2)_{i,j} + a_y((D_y\phi)^2)_{i,j}) \right) \\ &\quad + \frac{1}{36} \|\nabla_h \phi\|_2^2. \end{aligned} \tag{3.7}$$

LEMMA 3.2 (Existence of a convex splitting). *Assume that* $\phi \in \mathcal{C}_{\mathrm{per}}$. *Defining*

$$F_S(\phi) = h^2 \sum_{i,j=1}^{N} S(\phi_{i,j}), \quad F_e(\phi) = F_H(\phi) = -h^2 \sum_{i,j=1}^{N} H(\phi_{i,j}),$$

$$F_{K_1}(\phi) = h^2 \sum_{i,j=1}^{N} (\kappa(\phi_{i,j}) - \frac{1}{36})(a_x((D_x\phi)^2)_{i,j} + a_y((D_y\phi)^2)_{i,j}),$$

$$F_{K_2}(\phi) = h^2 \sum_{i,j=1}^{N} \frac{1}{36}(a_x((D_x\phi)^2)_{i,j} + a_y((D_y\phi)^2)_{i,j}) = \frac{1}{36}\|\nabla_h \phi\|_2^2,$$

$$F_c(\phi) = F_S(\phi) + F_{K_1}(\phi) + F_{K_2}(\phi).$$

We have

$$F(\phi) = F_c(\phi) - F_e(\phi) = F_S(\phi) + F_{K_1}(\phi) + F_{K_2}(\phi) - F_H(\phi),$$

where $F_c(\phi), F_e(\phi), F_S(\phi), F_{K_1}(\phi), F_{K_2}(\phi)$ and $F_H(\phi)$ are convex.

3.2. The fully discrete numerical scheme and the main theoretical results We follow the idea of convexity splitting and consider the following semi-implicit, fully discrete schemes: given $\phi^n \in \mathcal{C}_{\text{per}}$, find $\phi^{n+1}, \mu^{n+1} \in \mathcal{C}_{\text{per}}$, such that

$$\begin{aligned}
\phi^{n+1} - \phi^n &= \Delta t \Delta_h \mu^{n+1}, && (3.8)\\
\mu^{n+1} &= \delta_\phi F_c(\phi^{n+1}) - \delta_\phi F_e(\phi^n)\\
&= \delta_\phi F_S(\phi^{n+1}) + \delta_\phi F_{K_1}(\phi^{n+1}) + \delta_\phi F_{K_2}(\phi^{n+1}) - \delta_\phi F_H(\phi^n)\\
&= S'(\phi^{n+1}) + \kappa'(\phi^{n+1})\left(a_x((D_x\phi^{n+1})^2) + a_y((D_y\phi^{n+1})^2)\right)\\
&\quad - 2d_x(A_x\kappa(\phi^{n+1})D_x\phi^{n+1}) - 2d_y(A_y\kappa(\phi^{n+1})D_y\phi^{n+1})\\
&\quad + H'(\phi^n), && (3.9)
\end{aligned}$$

where

$$S'(\phi) = (\frac{1}{\tau} + \frac{1}{N_1})\ln\phi - \rho\ln(1-\rho\phi), \quad H'(\phi) = -2\chi\rho\phi, \quad \kappa'(\phi) = \frac{2\phi - 1}{36\phi^2(1-\phi)^2}.$$

Since μ follows the Laplacian Δ_h, we omit the constants in the expressions $S'(\phi)$ and $H'(\phi)$ above.

If solutions to the scheme (3.8)-(3.9) exist, it is clear that, for any $n \in \mathbb{N}$,

$$\overline{\phi}_0 := |\Omega|^{-1}\langle \phi^0, 1\rangle_\Omega = |\Omega|^{-1}\langle \phi^1, 1\rangle_\Omega = \cdots = |\Omega|^{-1}\langle \phi^n, 1\rangle_\Omega = \overline{\phi^n},$$

with $|\overline{\phi^n}| < 1$. Thus we get $\langle \phi^n - \overline{\phi}_0, 1\rangle_\Omega = 0$.

The following result concerning the unconditional energy stability was similar to the work by Li, Qiao and Zhang [25].

THEOREM 3.1. *The scheme (3.8)-(3.9) is unconditionally energy-stable, i.e., for any time step $\Delta t > 0$, we always have*

$$F(\phi^{k+1}) + \Delta t \left\|\nabla_h \mu^{k+1}\right\|_2^2 \le F(\phi^k),$$

in other words,

$$F(\phi^{k+1}) + \Delta t \left\| \frac{\phi^{k+1} - \phi^k}{\Delta t} \right\|_{-1,h}^2 \le F(\phi^k).$$

Proof. The following estimate is always valid:

$$\begin{aligned}
F(\phi^{k+1})-F(\phi^k) &= F_c(\phi^{k+1})-F_e(\phi^{k+1})-F_c(\phi^k)+F_e(\phi^k)\\
&= F_c(\phi^{k+1})-F_c(\phi^k)-(F_e(\phi^{k+1})-F_e(\phi^k))\\
&\le \langle \delta_\phi F_c(\phi^{k+1}),\phi^{k+1}-\phi^k\rangle_\Omega-\langle \delta_\phi F_e(\phi^k),\phi^{k+1}-\phi^k\rangle_\Omega\\
&= \langle \delta_\phi F_c(\phi^{k+1})-\delta_\phi F_e(\phi^k),\phi^{k+1}-\phi^k\rangle_\Omega\\
&= \langle \mu^{k+1},\phi^{k+1}-\phi^k\rangle_\Omega\\
&= \Delta t\langle \mu^{k+1},\Delta_h\mu^{k+1}\rangle_\Omega=-\frac{1}{\Delta t}\langle(-\Delta_h)^{-1}(\phi^{k+1}-\phi^k),\phi^{k+1}-\phi^k\rangle_\Omega\\
&= -\Delta t\|\nabla_h\mu^{k+1}\|_2^2=-\Delta t\left\|\frac{\phi^{k+1}-\phi^k}{\Delta t}\right\|_{-1,h}^2\\
&\le 0.
\end{aligned} \tag{3.10}$$

∎

The proof of the following lemma could be found in [5].

LEMMA 3.3. *Suppose that ϕ_1, $\phi_2\in\mathcal{C}_{\rm per}$, with $\langle\phi_1-\phi_2,1\rangle_\Omega=0$, that is, $\phi_1-\phi_2\in\mathring{\mathcal{C}}_{\rm per}$, and assume that $\|\phi_1\|_\infty<1$, $\|\phi_2\|_\infty\le M$. Then, we have the following estimate:*

$$\left\|\mathcal{L}^{-1}(\phi_1-\phi_2)\right\|_\infty\le C_1, \tag{3.11}$$

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

The proof for the following lemma and theorem will be provided in the next section.

LEMMA 3.4. *Assume that ϕ_1, $\phi_2\in(0,1)$, and κ is defined by (2.3). Then*

$$\frac{1}{2}\kappa'(\phi_1)(\phi_2-\phi_1)\le\kappa(\phi_2). \tag{3.12}$$

THEOREM 3.2. *Let $\phi^n\in\mathcal{C}_{\rm per}$, with $0<\phi^n<M$, for some $M>0$, and $\overline{\phi^n}<1/\rho$, there is a unique solution $\phi^{n+1}\in\mathcal{C}_{\rm per}$ to the scheme (3.8)-(3.9), with $\overline{\phi^{n+1}}=\overline{\phi^n}$ and $0<\phi^{n+1}<1/\rho$.*

4. The detailed proof of the positivity-preserving property

4.1. Proof of Lemma 3.4.

Proof. The proof will be divided into two cases:
Case 1: If $\kappa'(\phi_1)(\phi_2-\phi_1)\le0$, we see that

$$\frac{1}{2}\kappa'(\phi_1)(\phi_2-\phi_1)\le0\le\kappa(\phi_2), \tag{4.1}$$

due to the fact that $\kappa(\phi_2)>0$, for any $0<\phi_2<1$.

Case 2: If $\kappa'(\phi_1)(\phi_2-\phi_1)\ge0$, we have

$$\frac{1}{2}\kappa'(\phi_1)(\phi_2-\phi_1)\le\kappa'(\phi_1)(\phi_2-\phi_1)\le\kappa(\phi_2)-\kappa(\phi_1)\le\kappa(\phi_2), \tag{4.2}$$

in which the second step is based on the convexity of $\kappa(\phi)$ (in terms of ϕ), and the last step comes from the fact that $\kappa(\phi_1)>0$.

A combination of these two cases yields the desired result. ∎

4.2. Proof of Theorem 3.2.

Proof. The numerical solution of (3.8) is a minimizer of the following discrete energy functional:

$$\mathcal{J}^n(\phi):=\frac{1}{2\Delta t}\|\phi-\phi^n\|_{-1,h}^2+\frac{1}{\tau}\left\langle\phi,\ln\frac{\alpha\phi}{\tau}\right\rangle_\Omega+\frac{1}{N_1}\left\langle\phi,\ln\frac{\beta\phi}{\tau}\right\rangle_\Omega+\langle 1-\rho\phi,\ln(1-\rho\phi)\rangle_\Omega$$
$$+\left\langle\kappa(\phi),a_x((D_x\phi)^2)+a_y((D_y\phi)^2)\right\rangle_\Omega-2\rho\chi\langle\phi,\phi^n\rangle_\Omega, \tag{4.3}$$

over the admissible set

$$A_h:=\left\{\phi\in\mathcal{C}_{\rm per}\;\middle|\;0\le\phi\le 1/\rho,\quad\langle\phi-\overline{\phi}_0,1\rangle_\Omega=0\right\}\subset\mathbb{R}^{N^2}.$$

It is easy to see that $\mathcal{J}^n$ is a strictly convex function over this domain.

Equivalently, we consider the following functional

$$\mathcal{F}^n(\varphi):=\mathcal{J}^n(\varphi+\overline{\phi}_0)$$
$$=\frac{1}{2\Delta t}\|\varphi+\overline{\phi}_0-\phi^n\|_{-1,h}^2+\frac{1}{\tau}\left\langle\varphi+\overline{\phi}_0,\ln\frac{\alpha(\varphi+\overline{\phi}_0)}{\tau}\right\rangle_\Omega \tag{4.4}$$
$$+\frac{1}{N_1}\left\langle\varphi+\overline{\phi}_0,\ln\frac{\beta(\varphi+\overline{\phi}_0)}{\tau}\right\rangle_\Omega$$
$$+\left\langle 1-\rho(\varphi+\overline{\phi}_0),\ln(1-\rho(\varphi+\overline{\phi}_0))\right\rangle_\Omega \tag{4.5}$$
$$+\left\langle\kappa(\varphi+\overline{\phi}_0),a_x((D_x\varphi)^2)+a_y((D_y\varphi)^2)\right\rangle_\Omega$$
$$-2\rho\chi\left\langle\varphi+\overline{\phi}_0,\phi^n\right\rangle_\Omega, \tag{4.6}$$

defined on the set

$$\mathring{A}_h:=\left\{\varphi\in\mathring{\mathcal{C}}_{\rm per}\;\middle|\;-\overline{\phi}_0\le\varphi\le 1/\rho-\overline{\phi}_0\right\}\subset\mathbb{R}^{N^2}.$$

If $\varphi\in\mathring{A}_h$ minimizes $\mathcal{F}^n$, then $\phi:=\varphi+\overline{\phi}_0\in A_h$ minimizes $\mathcal{J}^n$, and *vice versa*. Next, we prove that there exists a minimizer of $\mathcal{F}^n$ over the domain $\mathring{A}_h$.We consider the following closed domain: for $\delta\in(0,1/2)$,

$$\mathring{A}_{h,\delta}:=\left\{\varphi\in\mathring{\mathcal{C}}_{\rm per}\;\middle|\;\delta-\overline{\phi}_0\le\varphi\le 1/\rho-\delta-\overline{\phi}_0\right\}\subset\mathbb{R}^{N^2}. \tag{4.7}$$

Since $\mathring{A}_{h,\delta}$ is a bounded, compact, and convex set in the subspace $\mathring{\mathcal{C}}_{\rm per}$, 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 get a contradiction, suppose that the minimizer of $\mathcal{F}^n$, call it $\varphi^\star$, occurs at a boundary point of $\mathring{A}_{h,\delta}$ and there is at least one grid point $\vec{\alpha}_0=(i_0,j_0)$ such that $\varphi^\star_{\vec{\alpha}_0}+\overline{\phi}_0=\delta$. Then the grid function $\varphi^\star$ has a global minimum at $\vec{\alpha}_0$. Suppose that $\vec{\alpha}_1=(i_1,j_1)$ is a grid point at which $\varphi^\star$ achieves its maximum. By the fact that $\overline{\varphi^\star}=0$, it is obvious that

$$1/\rho-\delta\ge\varphi^\star_{\vec{\alpha}_1}+\overline{\phi}_0\ge\overline{\phi}_0.$$

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

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

$$
\begin{aligned}
&= \left\langle \frac{1}{\tau}\ln\frac{\alpha(\varphi^\star+\overline{\phi}_0)}{\tau}+\frac{1}{N_1}\ln\frac{\beta(\varphi^\star+\overline{\phi}_0)}{\tau}-\rho\ln(1-\rho(\varphi^\star+\overline{\phi}_0)),\psi\right\rangle_\Omega \\
&\quad+\left\langle \frac{1}{\tau}+\frac{1}{N_1}-\rho,\psi\right\rangle_\Omega-\langle 2\rho\chi\phi^n,\psi\rangle_\Omega+\frac{1}{\Delta t}\left\langle \mathcal{L}^{-1}\left(\varphi^\star-\phi^n+\overline{\phi}_0\right),\psi\right\rangle_\Omega \\
&\quad+\left\langle \kappa'(\varphi^\star+\overline{\phi}_0)(a_x((D_x\varphi^\star)^2)+a_y((D_y\varphi^\star)^2)),\psi\right\rangle_\Omega-\left\langle \kappa(\varphi^\star+\overline{\phi}_0)\Delta_h\varphi^\star,\psi\right\rangle_\Omega \\
&\quad+h\sum_{i,j=1}^{N}\kappa(\varphi^\star_{i,j}+\overline{\phi}_0)\left(D_x\varphi^\star_{i+1/2,j}\psi_{i+1,j}-D_x\varphi^\star_{i-1/2,j}\psi_{i-1,j}\right) \\
&\quad+h\sum_{i,j=1}^{N}\kappa(\varphi^\star_{i,j}+\overline{\phi}_0)\left(D_y\varphi^\star_{i,j+1/2}\psi_{i,j+1}-D_y\varphi^\star_{i,j-1/2}\psi_{i,j-1}\right).
\end{aligned}
$$

This time, let us pick the direction $\psi\in\mathring{\mathcal{C}}_{\rm per}$, such that

$$\psi_{i,j}=\delta_{i,i_0}\delta_{j,j_0}-\delta_{i,i_1}\delta_{j,j_1},$$

here $\delta_{i,j}$ is the Dirac delta function. Then the derivative may be expressed as

$$
\begin{aligned}
&\frac{1}{h^2}d_s\mathcal{F}^n(\varphi^\star+s\psi)|_{s=0} \\
&=\left(\frac{1}{\tau}\ln\frac{\alpha(\varphi^\star_{\vec{\alpha}_0}+\overline{\phi}_0)}{\tau}+\frac{1}{N_1}\ln\frac{\beta(\varphi^\star_{\vec{\alpha}_0}+\overline{\phi}_0)}{\tau}-\rho\ln(1-\rho(\varphi^\star_{\vec{\alpha}_0}+\overline{\phi}_0))\right) \\
&\quad-\left(\frac{1}{\tau}\ln\frac{\alpha(\varphi^\star_{\vec{\alpha}_1}+\overline{\phi}_0)}{\tau}+\frac{1}{N_1}\ln\frac{\beta(\varphi^\star_{\vec{\alpha}_1}+\overline{\phi}_0)}{\tau}-\rho\ln(1-\rho(\varphi^\star_{\vec{\alpha}_1}+\overline{\phi}_0))\right) \\
&\quad-2\rho\chi(\phi^n_{\vec{\alpha}_0}-\phi^n_{\vec{\alpha}_1})-\left(\kappa(\varphi^\star_{\vec{\alpha}_0}+\overline{\phi}_0)\Delta_h\varphi^\star_{\vec{\alpha}_0}-\kappa(\varphi^\star_{\vec{\alpha}_1}+\overline{\phi}_0)\Delta_h\varphi^\star_{\vec{\alpha}_1}\right) \\
&\quad+\left(\frac{1}{\Delta t}\mathcal{L}^{-1}(\varphi^\star-\phi^n+\overline{\phi}_0)_{\vec{\alpha}_0}-\frac{1}{\Delta t}\mathcal{L}^{-1}(\varphi^\star-\phi^n+\overline{\phi}_0)_{\vec{\alpha}_1}\right) \\
&\quad+\kappa'(\varphi^\star_{\vec{\alpha}_0}+\overline{\phi}_0)(a_x((D_x\varphi^\star_{\vec{\alpha}_0})^2)+a_y((D_y\varphi^\star_{\vec{\alpha}_0})^2)) \\
&\quad-\kappa'(\varphi^\star_{\vec{\alpha}_1}+\overline{\phi}_0)(a_x((D_x\varphi^\star_{\vec{\alpha}_1})^2)+a_y((D_y\varphi^\star_{\vec{\alpha}_1})^2)) \\
&\quad+\frac{1}{h}\left(\kappa(\varphi^\star_{i_0-1,j_0}+\overline{\phi}_0)D_x\varphi^\star_{i_0-1/2,j_0}-\kappa(\varphi^\star_{i_0+1,j_0}+\overline{\phi}_0)D_x\varphi^\star_{i_0+1/2,j_0}\right) \\
&\quad+\frac{1}{h}\left(\kappa(\varphi^\star_{i_0,j_0-1}+\overline{\phi}_0)D_y\varphi^\star_{i_0,j_0-1/2}-\kappa(\varphi^\star_{i_0,j_0+1}+\overline{\phi}_0)D_y\varphi^\star_{i_0,j_0+1/2}\right) \\
&\quad-\frac{1}{h}\left(\kappa(\varphi^\star_{i_1-1,j_1}+\overline{\phi}_0)D_x\varphi^\star_{i_1-1/2,j_1}-\kappa(\varphi^\star_{i_1+1,j_1}+\overline{\phi}_0)D_x\varphi^\star_{i_1+1/2,j_1}\right) \\
&\quad-\frac{1}{h}\left(\kappa(\varphi^\star_{i_1,j_1-1}+\overline{\phi}_0)D_y\varphi^\star_{i_1,j_1-1/2}-\kappa(\varphi^\star_{i_1,j_1+1}+\overline{\phi}_0)D_y\varphi^\star_{i_1,j_1+1/2}\right). \qquad (4.8)
\end{aligned}
$$

For simplicity, now let us write $\phi^\star:=\varphi^\star+\overline{\phi}_0$. Since $\phi^\star_{\vec{\alpha}_0}=\delta$ and $\phi^\star_{\vec{\alpha}_1}\geq\overline{\phi}_0$, we have

$$\frac{1}{\tau}\ln\frac{\alpha\phi^\star_{\vec{\alpha}_0}}{\tau}+\frac{1}{N_1}\ln\frac{\beta\phi^\star_{\vec{\alpha}_0}}{\tau}-\rho\ln(1-\rho\phi^\star_{\vec{\alpha}_0})=\frac{1}{\tau}\ln\frac{\alpha\delta}{\tau}+\frac{1}{N_1}\ln\frac{\beta\delta}{\tau}-\rho\ln(1-\rho\delta), \qquad (4.9)$$

$$\frac{1}{\tau}\ln\frac{\alpha\phi^\star_{\vec{\alpha}_1}}{\tau}+\frac{1}{N_1}\ln\frac{\beta\phi^\star_{\vec{\alpha}_1}}{\tau}-\rho\ln(1-\rho\phi^\star_{\vec{\alpha}_1})\geq\frac{1}{\tau}\ln\frac{\alpha\overline{\phi}_0}{\tau}+\frac{1}{N_1}\ln\frac{\beta\overline{\phi}_0}{\tau}-\rho\ln(1-\rho\overline{\phi}_0). \qquad (4.10)$$

Since $\phi^\star$ takes a minimum at the grid point $\vec{\alpha}_0$, with $\phi^\star_{\vec{\alpha}_0}=\delta\leq\phi^\star_{i,j}$, for any (i,j), and a maximum at the grid point $\vec{\alpha}_1$, with $\phi^\star_{\vec{\alpha}_1}\geq\phi^\star_{i,j}$, for any (i,j),

$$\Delta_h\phi^\star_{\vec{\alpha}_0}\geq 0,\quad \Delta_h\phi^\star_{\vec{\alpha}_1}\leq 0. \qquad (4.11)$$

For the numerical solution ϕ^n at the previous time step, the *a priori* assumption $\|\phi^n\|_\infty \le M$ indicates that

$$-2M \le \phi^n_{\vec{\alpha}_0} - \phi^n_{\vec{\alpha}_1} \le 2M. \tag{4.12}$$

For the fifth term appearing in (4.8), we apply Lemma 3.3 and obtain

$$-2C_1 \le \mathcal{L}^{-1}(\phi^\star - \phi^n)_{\vec{\alpha}_0} - \mathcal{L}^{-1}(\phi^\star - \phi^n)_{\vec{\alpha}_1} \le 2C_1. \tag{4.13}$$

The sixth, eighth and ninth terms appearing in (4.8) are non-positive:

$$\kappa'(\varphi^\star_{\vec{\alpha}_0} + \overline{\phi}_0)(a_x((D_x\varphi^\star_{\vec{\alpha}_0})^2) + a_y((D_y\varphi^\star_{\vec{\alpha}_0})^2)) \le 0, \tag{4.14}$$

$$\kappa(\varphi^\star_{i_0-1,j_0} + \overline{\phi}_0)D_x\varphi^\star_{i_0-1/2,j_0} \le 0, \quad \kappa(\varphi^\star_{i_0+1,j_0} + \overline{\phi}_0)D_x\varphi^\star_{i_0+1/2,j_0} \ge 0, \tag{4.15}$$

$$\kappa(\varphi^\star_{i_0,j_0-1} + \overline{\phi}_0)D_y\varphi^\star_{i_0,j_0-1/2} \le 0, \quad \kappa(\varphi^\star_{i_0,j_0+1} + \overline{\phi}_0)D_y\varphi^\star_{i_0,j_0+1/2} \ge 0. \tag{4.16}$$

Inequality (4.14) comes from the fact that $\kappa'(\varphi^\star_{\vec{\alpha}_0} + \overline{\phi}_0) \le 0$, since $\phi_{i_0,j_0} = \varphi^\star_{\vec{\alpha}_0} + \overline{\phi}_0 \le \frac{1}{2}$ takes a minimum at (i_0, j_0). Similarly, such a fact indicates that

$$D_x\varphi^\star_{i_0-1/2,j_0} \le 0, \quad D_x\varphi^\star_{i_0+1/2,j_0} \ge 0, \quad D_y\varphi^\star_{i_0,j_0-1/2} \le 0, \quad D_y\varphi^\star_{i_0,j_0+1/2} \ge 0, \tag{4.17}$$

which in turn yields the inequalities (4.15), (4.16). For the seventh and the last two terms appearing in (4.8), it is observed that

$$\begin{aligned}
&\kappa'(\varphi^\star_{\vec{\alpha}_1} + \overline{\phi}_0)\cdot a_x((D_x\varphi^\star_{\vec{\alpha}_1})^2) \\
&+\frac{1}{h}\left(\kappa(\varphi^\star_{i_1-1,j_1} + \overline{\phi}_0)D_x\varphi^\star_{i_1-1/2,j_1} - \kappa(\varphi^\star_{i_1+1,j_1} + \overline{\phi}_0)D_x\varphi^\star_{i_1+1/2,j_1}\right) \\
=&\frac{1}{h}\left(\frac{1}{2}\kappa'(\phi_{i_1,j_1})(\phi_{i_1,j_1} - \phi_{i_1-1,j_1}) + \kappa(\phi_{i_1-1,j_1})\right)\cdot D_x\phi_{i_1-1/2,j_1} \\
&-\frac{1}{h}\left(\frac{1}{2}\kappa'(\phi_{i_1,j_1})(\phi_{i_1,j_1} - \phi_{i_1+1,j_1}) + \kappa(\phi_{i_1+1,j_1})\right)\cdot D_x\phi_{i_1+1/2,j_1} \ge 0,
\end{aligned} \tag{4.18}$$

in which the last step is based on an application of Lemma 3.4, as well as the fact that $D_x\phi_{i_1-1/2,j_1} \ge 0$, $D_x\phi_{i_1+1/2,j_1} \le 0$, since ϕ takes a global maximum at (i_1, j_1). A similar inequality could be derived:

$$\begin{aligned}
&\kappa'(\varphi^\star_{\vec{\alpha}_1} + \overline{\phi}_0)\cdot a_y((D_y\varphi^\star_{\vec{\alpha}_1})^2) \\
&+\frac{1}{h}\left(\kappa(\varphi^\star_{i_1,j_1-1} + \overline{\phi}_0)D_y\varphi^\star_{i_1,j_1-1/2} - \kappa(\varphi^\star_{i_1,j_1+1} + \overline{\phi}_0)D_y\varphi^\star_{i_1,j_1+1/2}\right) \ge 0.
\end{aligned} \tag{4.19}$$

Consequently, a substitution of (4.9)-(4.19) into (4.8) yields the following bound on the directional derivative:

$$\begin{aligned}
&\frac{1}{h^2}d_s\mathcal{F}^n(\varphi^\star + s\psi)|_{s=0} \\
\le&\left(\frac{1}{\tau}\ln\frac{\alpha\delta}{\tau} + \frac{1}{N_1}\ln\frac{\beta\delta}{\tau} - \rho\ln(1-\rho\delta)\right) - \left(\frac{1}{\tau}\ln\frac{\alpha\overline{\phi}_0}{\tau} + \frac{1}{N_1}\ln\frac{\beta\overline{\phi}_0}{\tau} - \rho\ln(1-\rho\overline{\phi}_0)\right) \\
&+4M\rho\chi + 2C_1\Delta t^{-1} \\
=&\left((\frac{1}{\tau} + \frac{1}{N_1})\ln\delta - \rho\ln(1-\rho\delta)\right) - \left((\frac{1}{\tau} + \frac{1}{N_1})\ln\overline{\phi}_0 - \rho\ln(1-\rho\overline{\phi}_0)\right) \\
&+4M\rho\chi + 2C_1\Delta t^{-1}.
\end{aligned} \tag{4.20}$$

We denote $C_2 = 4M\rho\chi + 2C_1\Delta t^{-1}$. Note that C_2 is a constant for a fixed Δt, though it becomes singular as $\Delta t \to 0$. However, for any fixed Δt, we may choose $\delta \in (0, 1/2)$ sufficiently small so that

$$\left((\frac{1}{\tau} + \frac{1}{N_1}) \ln \delta - \rho \ln(1 - \rho\delta) \right) - \left((\frac{1}{\tau} + \frac{1}{N_1}) \ln \overline{\phi}_0 - \rho \ln(1 - \rho\overline{\phi}_0) \right) + C_2 < 0. \tag{4.21}$$

This in turn shows that, provided δ satisfies (4.21),

$$\frac{1}{h^2} d_s \mathcal{F}^n(\varphi^\star + s\psi)|_{s=0} < 0. \tag{4.22}$$

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 $(\mathring{A}_{h,\delta})^{\text{o}}$, the interior of $\mathring{A}_{h,\delta}$.

Using 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 $\varphi^\star_{\vec{\alpha}_0} + \overline{\phi}_0 = 1/\rho - \delta$, for some $\vec{\alpha}_0$, so that the grid function $\varphi^\star$ has a global maximum at $\vec{\alpha}_0$. The details are left to the 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 $\varphi \in (\mathring{A}_{h,\delta})^{\text{o}} \subset (\mathring{A}_h)^{\text{o}}$. We conclude that there must be a solution $\phi = \varphi + \overline{\phi}_0 \in A_h$ that minimizes $\mathcal{J}^n$ over A_h, which is equivalent to the numerical solution of (3.8)-(3.9). 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. The proof of Theorem 3.2 is complete. ◻

5. Optimal rate convergence analysis in $\ell^\infty(0,T;H^{-1}) \cap \ell^2(0,T;H^1)$

Now we proceed into the convergence analysis. Let Φ be the exact solution for the Cahn-Hilliard flow (2.4). With sufficiently regular initial data, we could assume that the exact solution has regularity of class $\mathcal{R}$:

$$\Phi \in \mathcal{R} := H^2(0,T; C_{\text{per}}(\Omega)) \cap L^\infty\left(0,T; C^6_{\text{per}}(\Omega)\right). \tag{5.1}$$

Define $\Phi_N(\cdot,t) := \mathcal{P}_N \Phi(\cdot,t)$, the (spatial) Fourier projection of the exact solution into $\mathcal{B}^K$, the space of trigonometric polynomials of degree upto and including K (with $N = 2K+1$). The following projection approximation is standard: if $\Phi \in L^\infty(0,T; H^\ell_{\text{per}}(\Omega))$, for some $\ell \in \mathbb{N}$,

$$\|\Phi_N - \Phi\|_{L^\infty(0,T;H^m)} \le C h^{\ell - k} \|\Phi\|_{L^\infty(0,T;H^\ell)}, \quad \forall\, 0 \le k \le \ell. \tag{5.2}$$

By Φ_N^m, Φ^m we denote $\Phi_N(\cdot,t_m)$ and $\Phi(\cdot,t_m)$, respectively, with $t_m = m \cdot \Delta t$. Since $\Phi_N \in \mathcal{B}^K$, the mass conservative property is available at the discrete level:

$$\overline{\Phi_N^m} = \frac{1}{|\Omega|} \int_\Omega \Phi_N(\cdot,t_m)\, d\mathbf{x} = \frac{1}{|\Omega|} \int_\Omega \Phi_N(\cdot,t_{m-1})\, d\mathbf{x} = \overline{\Phi_N^{m-1}}, \quad \forall\, m \in \mathbb{N}. \tag{5.3}$$

On the other hand, the solution of (3.8)-(3.9) is also mass conservative at the discrete level:

$$\overline{\phi^m} = \overline{\phi^{m-1}}, \quad \forall\, m \in \mathbb{N}. \tag{5.4}$$

As indicated before, we use the mass conservative projection for the initial data: $\phi^0 = \mathcal{P}_h \Phi_N(\cdot, t=0)$, that is

$$\phi^0_{i,j} := \Phi_N(p_i, p_j, t=0). \tag{5.5}$$

The error grid function is defined as

$$\tilde{\phi}^m := \mathcal{P}_h \Phi_N^m - \phi^m, \quad \forall\, m \in \{0,1,2,3,\cdots\}. \tag{5.6}$$

Therefore, it follows that $\overline{\tilde{\phi}^m} = 0$, for any $m \in \{0,1,2,3,\cdots\}$, so that the discrete norm $\|\cdot\|_{-1,h}$ is well defined for the error grid function.

The following theorem is the main result of this section.

THEOREM 5.1. *Given initial data $\Phi(\cdot,t=0) \in C^6_{\rm per}(\Omega)$, suppose the exact solution for Cahn-Hilliard Equation (2.4) is of regularity class $\mathcal{R}$. Then, provided Δt and h are sufficiently small, for all positive integers n, such that $t_n = n\Delta t \le T$, we have*

$$\left\|\tilde{\phi}^n\right\|_{-1,h} + \left(\frac{1}{9}\Delta t \sum_{m=1}^{n} \left\|\nabla_h \tilde{\phi}^m\right\|_2^2\right)^{1/2} \le C(\Delta t + h^2), \tag{5.7}$$

where $C > 0$ is independent of n, Δt, and h.

Proof. A careful consistency analysis indicates the following truncation error estimate:

$$\frac{\Phi_N^{n+1} - \Phi_N^n}{\Delta t} = \Delta_h \left(\delta_\phi F_S(\Phi_N^{n+1}) + \delta_\phi F_{K_1}(\Phi_N^{n+1}) + \delta_\phi F_{K_2}(\Phi_N^{n+1}) - \delta_\phi F_H(\Phi_N^n)\right) + \tau^n, \tag{5.8}$$

with $\|\tau^n\|_{-1,h} \le C(\Delta t + h^2)$. Observe that in Equation (5.8), and from this point forward, we drop the operator $\mathcal{P}_h$, which should appear in front of Φ_N, for simplicity.

Subtracting the numerical scheme (3.8) from (5.8) gives

$$\begin{aligned}\frac{\tilde{\phi}^{n+1} - \tilde{\phi}^n}{\Delta t} = \Delta_h \Big(&(\delta_\phi F_S(\Phi_N^{n+1}) - \delta_\phi F_S(\phi^{n+1})) + (\delta_\phi F_{K_1}(\Phi_N^{n+1}) - \delta_\phi F_{K_1}(\phi^{n+1})) \\ &+ (\delta_\phi F_{K_2}(\Phi_N^{n+1}) - \delta_\phi F_{K_2}(\phi^{n+1})) - (\delta_\phi F_H(\Phi_N^n) - \delta_\phi F_H(\phi^n))\Big) + \tau^n. \end{aligned} \tag{5.9}$$

Since the numerical error function has zero-mean, we see that $(-\Delta_h)^{-1}\tilde{\phi}^m$ is well-defined, for any $m \ge 0$. Taking a discrete inner product with (5.9) by $2(-\Delta_h)^{-1}\tilde{\phi}^{n+1}$ yields

$$\begin{aligned} &\left\|\tilde{\phi}^{n+1}\right\|_{-1,h}^2 - \left\|\tilde{\phi}^n\right\|_{-1,h}^2 + \left\|\tilde{\phi}^{n+1} - \tilde{\phi}^n\right\|_{-1,h}^2 \\ &\quad + 2\Delta t \left\langle \delta_\phi F_S(\Phi_N^{n+1}) - \delta_\phi F_S(\phi^{n+1}), \tilde{\phi}^{n+1} \right\rangle_\Omega \\ &\quad + 2\Delta t \left\langle \delta_\phi F_{K_1}(\Phi_N^{n+1}) - \delta_\phi F_{K_1}(\phi^{n+1}), \tilde{\phi}^{n+1} \right\rangle_\Omega \\ &\quad + 2\Delta t \left\langle \delta_\phi F_{K_2}(\Phi_N^{n+1}) - \delta_\phi F_{K_2}(\phi^{n+1}), \tilde{\phi}^{n+1} \right\rangle_\Omega \\ &= 4\chi\rho\Delta t \left\langle \tilde{\phi}^n, \tilde{\phi}^{n+1} \right\rangle_\Omega + 2\Delta t \left\langle \tau^n, \tilde{\phi}^{n+1} \right\rangle_\Omega. \end{aligned} \tag{5.10}$$

For the F_{K_2} term, it is easy to know that

$$\begin{aligned} &2\Delta t \left\langle \delta_\phi F_{K_2}(\Phi_N^{n+1}) - \delta_\phi F_{K_2}(\phi^{n+1}), \tilde{\phi}^{n+1} \right\rangle_\Omega = 2\Delta t \left\langle -\frac{1}{18}\Delta_h \tilde{\phi}^{n+1}, \tilde{\phi}^{n+1} \right\rangle_\Omega \\ &= \frac{1}{9}\Delta t \|\nabla_h \tilde{\phi}^{n+1}\|_2^2. \end{aligned} \tag{5.11}$$

For the F_S and F_{K_1} terms, we see that both F_S and F_{K_1} are convex, which implies the following result:

$$\left\langle \delta_\phi F_S(\Phi_N^{n+1}) - \delta_\phi F_S(\phi^{n+1}), \tilde{\phi}^{n+1} \right\rangle_\Omega \geq 0, \tag{5.12}$$

$$\left\langle \delta_\phi F_{K_1}(\Phi_N^{n+1}) - \delta_\phi F_{K_1}(\phi^{n+1}), \tilde{\phi}^{n+1} \right\rangle_\Omega \geq 0, \tag{5.13}$$

For the concave part, an application of the Cauchy-Swcharz inequality gives

$$\begin{aligned} 4\chi\rho \left\langle \tilde{\phi}^n, \tilde{\phi}^{n+1} \right\rangle_\Omega &\leq 4\chi\rho \left\| \tilde{\phi}^n \right\|_{-1,h} \left\| \nabla_h \tilde{\phi}^{n+1} \right\|_2 \\ &\leq 8\chi^2\rho^2\varepsilon^{-2} \left\| \tilde{\phi}^n \right\|_{-1,h}^2 + \frac{\varepsilon^2}{2} \left\| \nabla_h \tilde{\phi}^{n+1} \right\|_2. \end{aligned} \tag{5.14}$$

The term associated with the local truncation error can be controlled in a standard way:

$$2\left\langle \tau^n, \mathcal{L}^{-1}\tilde{\phi}^{n+1} \right\rangle_\Omega \leq 2\|\tau^n\|_{-1,h} \left\| \tilde{\phi}^{n+1} \right\|_{-1,h} \leq 2\varepsilon^{-2}\|\tau^n\|_{-1,h}^2 + \frac{\varepsilon^2}{2} \left\| \tilde{\phi}^{n+1} \right\|_{-1,h}^2. \tag{5.15}$$

Then we get

$$\begin{aligned} &\left\| \tilde{\phi}^{n+1} \right\|_{-1,h}^2 - \left\| \tilde{\phi}^n \right\|_{-1,h}^2 + \frac{\Delta t}{9} \left\| \nabla_h \tilde{\phi}^{n+1} \right\|_2^2 \\ \leq &\frac{8\chi^2\rho^2}{\varepsilon^2} \Delta t \left\| \tilde{\phi}^n \right\|_{-1,h}^2 + \frac{\varepsilon^2}{2}\Delta t \left\| \nabla_h \tilde{\phi}^{n+1} \right\|_2^2 + \frac{2}{\varepsilon^2}\Delta t \|\tau^n\|_{-1,h}^2 + \frac{\varepsilon^2}{2}\Delta t \left\| \tilde{\phi}^{n+1} \right\|_{-1,h}^2. \end{aligned}$$

Let $\varepsilon^2 < \frac{2}{9}$, such as $\varepsilon^2 = \frac{1}{9}$. A substitution of (5.11)-(5.15) into (5.10) yields

$$\begin{aligned} &\left\| \tilde{\phi}^{n+1} \right\|_{-1,h}^2 - \left\| \tilde{\phi}^n \right\|_{-1,h}^2 + \frac{\Delta t}{18} \left\| \nabla_h \tilde{\phi}^{n+1} \right\|_2^2 \\ \leq &18 \times 8\chi^2\rho^2 \Delta t \left\| \tilde{\phi}^n \right\|_{-1,h}^2 + 18\Delta t \|\tau^n\|_{-1,h}^2 + \frac{\Delta t}{18} \left\| \tilde{\phi}^{n+1} \right\|_{-1,h}^2. \end{aligned}$$

Finally, let $1 - \frac{\Delta t}{18} \geq \frac{1}{2}$, we get the following estimate by using the discrete Grönwall inequality

$$\left\| \tilde{\phi}^{n+1} \right\|_{-1,h} + \left(\frac{1}{9}\Delta t \sum_{k=0}^{n+1} \left\| \nabla_h \tilde{\phi}^m \right\|_2^2 \right)^{1/2} \leq C(\Delta t + h^2). \tag{5.16}$$

This completes the proof. $\square$

Remark 5.1. The Cahn-Hilliard equation with Flory-Huggins energy potential and constant diffusion coefficient has been studied in a recent work [5]. In this paper, we analyze the Cahn-Hilliard equation with the deGennes diffusive coefficient, $\kappa(\phi) = 1/[36\phi(1-\phi)]$, dependent on the phase variable, so-called MMC-TDGL equation. This diffusion process was proposed by physicist P.G. deGennes [11]. The positivity-preserving analysis for the MMC-TDGL equation follows a similar framework as in [5]. On the other hand, the estimate for the nonlinear diffusion part is much more complicated and challenging than the constant-diffusion-coefficient case. In more details, for the deGennes diffusive coefficient $\kappa(\phi) = 1/[36\phi(1-\phi)]$, we have to find an appropriate inequality, $\frac{1}{2}\kappa'(\phi_1)(\phi_2-\phi_1)\le\kappa(\phi_2),\forall\phi_1,\phi_2\in(0,1)$, which plays an essential role in the analysis of the positivity-preserving property for the numerical solution.

In addition, the convergence analysis for the MMC-TDGL equation, which has remained an open problem due to the highly complicated diffusion term, is provided in this paper. In more details, we make use of the convexity of the logarithmic term and the division of the surface diffusion to estimate the convergent analysis. Furthermore, we treat the three nonlinear logarithmic terms as a whole, and the convexity of the associated nonlinear terms indicates that the corresponding nonlinear error of the inner product is always non-negative. Moreover, we divide the surface diffusion term $\kappa(\phi)|\nabla\phi|^2$ into two convex parts: one term $(\kappa(\phi)-\frac{1}{36})|\nabla\phi|^2$ can be analyzed in a manner similar to the logarithmic term, with the help of its convexity property, and the other term $\frac{1}{36}|\nabla\phi|^2$ can be used to control the explicit error estimate associated with the Huggins interaction.

6. Some numerical results

In this part, we provide numerical simulation results for the two-dimensional scheme (3.8)-(3.9). We use the domain $\Omega=(0,64)\times(0,64)$ and choose the parameters in the model as $\chi=2.37, N_2=0.16, N_1=4.34, T=25$. The space step and time step are given by $h=0.25$ and $\Delta t=10^{-3}$, respectively. And also, the initial data is taken the same as the one given by [25]:

$$\phi_0(x,y)=0.6+r_{i,j}, \tag{6.1}$$

where the $r_{i,j}$ are uniformly distributed random numbers in $[-0.15,0.15]$.

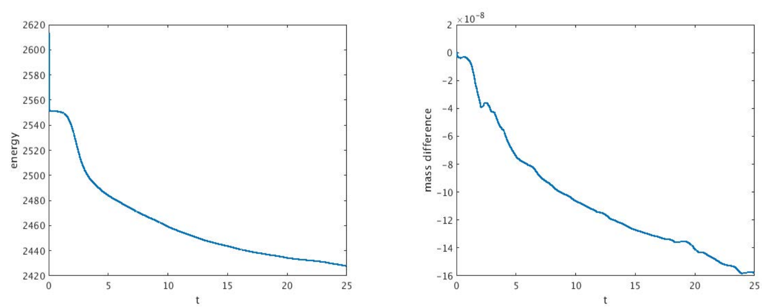

FIG. 6.1. *Left: the energy evolution with time; Right: the error development of the total mass.*

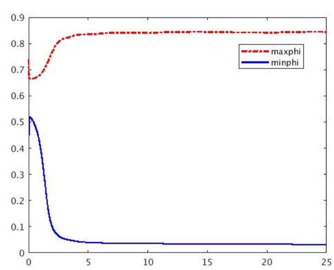

FIG. 6.2. *The maximum and minimum values with time.*

In the left part of the Figure 6.1, we show the energy evolution, and this figure demonstrates the energy decay with time. The total mass error evolution is displayed on the right part, in which the mass conservation is numerically observed.

In Figure 6.2, we present the maximum and minimum values of the numerical solution with time. The positivity-preserving property is clearly observed in the numerical result.

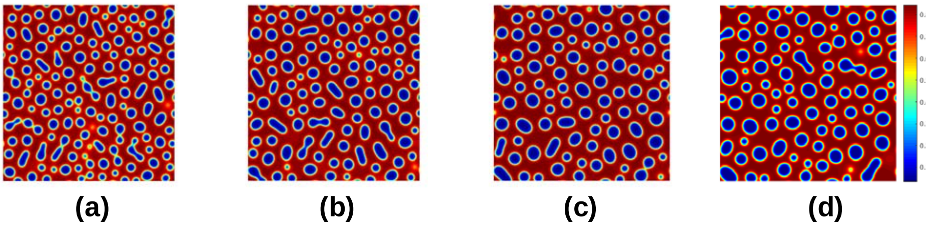

FIG. 6.3. *The snapshot figure of the phase variable at* $t=8,13,19,25$.

In Figure 6.3, we present the evolution of ϕ at different time with the initial data (6.1). The numerical results are similar to the ones shown in [25].

7. Conclusions

In this paper, we have analyzed an unconditional energy-stable finite difference scheme based on the convex splitting of the Flory-Huggins-deGennes energy potential for the MMC-TDGL equation, such as the unique solvability, energy stability, the bound of the numerical solution and an optimal rate convergence analysis. In particular, we have presented detailed theoretical analyses about the positivity-preserving property and the optimal rate of convergence estimate. The positivity-preserving property has been established at a theoretical level, by constructing a strictly convex discrete energy functional and using mass conservation, combined with the following two subtle facts that: first, the singular feature of the logarithmic function guarantees that a minimizer could not occur on a limit value at all; second, a fundamental inequality about the deGennes coefficient: $\frac{1}{2}\kappa'(\phi_1)(\phi_2-\phi_1)\leq\kappa(\phi_2), \forall\phi_1,\phi_2\in(0,1)$. We have also presented a detailed convergence analysis, in which the convexity of the nonlinear potential and some technique of the surface diffusion term with concentration-dependent deGennes type coefficient play an essential role. The numerical simulation results have also verified the positivity-preserving property of the numerical solution.

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