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# NUMERICAL APPROXIMATIONS OF ALLEN-CAHN AND CAHN-HILLIARD EQUATIONS

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ABSTRACT. Stability analyses and error estimates are carried out for a number of commonly used numerical schemes for the Allen-Cahn and Cahn-Hilliard equations. It is shown that all the schemes we considered are either unconditionally energy stable, or conditionally energy stable with reasonable stability conditions in the semi-discretized versions. Error estimates for selected schemes with a spectral-Galerkin approximation are also derived. The stability analyses and error estimates are based on a weak formulation thus the results can be easily extended to other spatial discretizations, such as Galerkin finite element methods, which are based on a weak formulation.

1. **Introduction.** We consider in this paper numerical schemes for solving the Allen-Cahn equation

$$\begin{cases} u_t - \Delta u + \frac{1}{\varepsilon^2} f(u) = 0, \quad (x,t) \in \Omega \times (0,T], \\ \partial_n u|_{\partial\Omega} = 0, \\ u|_{t=0} = u_0; \end{cases}$$
(1.1)

and the Cahn-Hilliard equation

$$\begin{cases} u_t - \Delta(-\Delta u + \frac{1}{\varepsilon^2}f(u)) = 0, \quad (x,t) \in \Omega \times (0,T], \\ \partial_n u|_{\partial\Omega} = 0, \quad \partial_n (\Delta u - \frac{1}{\varepsilon^2}f(u))|_{\partial\Omega} = 0, \\ u|_{t=0} = u_0. \end{cases}$$
(1.2)

In the above,  $\Omega \subset \mathbb{R}^d$  (d = 2, 3) is a bounded domain, n is the outward normal, f(u) = F'(u) with F(u) being a given energy potential. An important feature of the

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Allen-Cahn and Cahn-Hilliard equations is that they can be viewed as the gradient flow of the Liapunov energy functional

$$E(u) := \int_{\Omega} \left( \frac{1}{2} |\nabla u|^2 + \frac{1}{\varepsilon^2} F(u) \right) dx \tag{1.3}$$

in  $L^2$  and  $H^{-1}$ , respectively. More precisely, by taking the inner product of (1.1) with  $-\Delta u + \frac{1}{\varepsilon^2} f(u)$ , we immediately find the following energy law for (1.1):

$$\frac{\partial}{\partial t}E(u(t)) = -\int_{\Omega} |-\Delta u + \frac{1}{\varepsilon^2}f(u)|^2 dx; \qquad (1.4)$$

and similarly, the energy law for (1.2) is

$$\frac{\partial}{\partial t}E(u(t)) = -\int_{\Omega} |\nabla(-\Delta u + \frac{1}{\varepsilon^2}f(u))|^2 dx.$$
(1.5)

The Allen-Cahn equation was originally introduced by Allen and Cahn in [1] to describe the motion of anti-phase boundaries in crystalline solids. In this context, u represents the concentration of one of the two metallic components of the alloy and the parameter  $\varepsilon$  represents the interfacial width, which is small compared to the characteristic length of the laboratory scale. The homogenous Neumann boundary condition implies that no mass loss occurs across the boundary walls. On the other hand, the Cahn-Hilliard equation was introduced by Cahn and Hilliard in [4] to describe the complicated phase separation and coarsening phenomena in a solid. The two boundary conditions also imply that none of the mixture can pass through the boundary walls.

Nowadays, the Allen-Cahn and Cahn-Hilliard equations have been widely used in many complicated moving interface problems in materials science and fluid dynamics through a phase-field approach (cf., for instance, [19, 7, 2, 6, 17, 27, 25, 9]). Therefore, it is very important to develop accurate and efficient numerical schemes to solve the Allen-Cahn and Cahn-Hilliard equations. Since an essential feature of the Allen-Cahn and Cahn-Hilliard equations are that they satisfy the energy laws (1.4) and (1.5) respectively, it is important to design efficient and accurate numerical schemes that satisfy a corresponding discrete energy law, or in other words, energy stable.

In this paper, we shall restrict our attention to potential function F(u) whose derivative f(u) = F'(u) satisfies the following condition: there exists a constant L such that

$$\max_{u \in \mathbb{R}} |f'(u)| \le L. \tag{1.6}$$

We note that this condition is satisfied by many physically relevant potentials by restricting the growth of F(u) to be quadratic for  $|u| \ge M$ . Consider, for example, the Ginzburg-Landau double-well potential  $F(u) = \frac{1}{4}(u^2-1)^2$  which has been widely used. However, its quartic growth at infinity introduces various technical difficulties in the analysis and approximation of Allen-Cahn and Cahn-Hilliard equations. Since it is well-known that the Allen-Cahn equation satisfies the maximum principle, we can truncate F(u) to quadratic growth outside of the interval [-M, M] without affecting the solution if the maximum norm of the initial condition  $u_0$  is bounded by M. While the Cahn-Hilliard equation does not satisfy the maximum principle, it has been shown that in [3] that for a truncated potential F(u) with quadratic growth at infinities, the maximum norm of the solution for the Cahn-Hilliard equation is bounded. Therefore, it has been a common practice (cf. [15, 8]) to consider the

Allen-Cahn and Cahn-Hilliard equations with a truncated double-well potential F(u). More precisely, for a given M, we can replace  $F(u) = \frac{1}{4}(u^2 - 1)^2$  by

$$\tilde{F}(u) = \begin{cases} \frac{3M^2 - 1}{2}u^2 - 2M^3u + \frac{1}{4}(3M^4 + 1), & u > M\\ \frac{1}{4}(u^2 - 1)^2, & u \in [-M, M],\\ \frac{3M^2 - 1}{2}u^2 + 2M^3u + \frac{1}{4}(3M^4 + 1), & u < -M \end{cases}$$
(1.7)

and replace  $f(u) = (u^2 - 1)u$  by  $\tilde{F}'(u)$  which is

$$\tilde{f}(u) = \tilde{F}'(u) = \begin{cases} (3M^2 - 1)u - 2M^3, & u > M\\ (u^2 - 1)u, & u \in [-M, M] \\ (3M^2 - 1)u + 2M^3, & u < -M \end{cases}$$
(1.8)

It is then obvious that there exists L such that (1.6) is satisfied with f replaced by  $\tilde{f}$ .

It is well known that explicit schemes usually lead to very severe time step restrictions and do not satisfy a discrete energy law. So we shall focus our attention on semi-implicit (or linearly implicit) and fully implicit schemes. The advantage of semi-implicit schemes are that only an elliptic equation with constant coefficients needs to be solved at each time step, making it easy to implement and remarkably efficient when fast elliptic solvers are available. However, the semi-implicit schemes usually have larger truncation errors and require smaller time steps than fully implicit schemes. On the other hand, one can easily design an implicit scheme that satisfies an energy law, has smaller truncation errors and better stability property. But it requires solving a nonlinear equation at each time step. Our first objective is to design stabilized semi-implicit schemes that satisfy an energy law, and fully or partially alleviate the restriction on time steps.

There have been a large body of work on numerical analysis of Allen-Cahn and Cahn-Hilliard equations (cf. [10, 11, 12, 26, 13, 15, 28, 8] and the references therein). Most of the analysis are for finite element/finite difference methods or Fourier-spectral method with periodic boundary conditions. Very few work has been devoted to the analysis of non-periodic spectral methods, even though they have been widely used in practice. This is partly due to some technical difficulties related to the "non-optimal" inverse inequalities of the spectral methods, making it difficult to handle nonlinear terms optimally. However, thanks to the Lipschitz property of the modified potential. The nonlinear terms can now be easily handled. Thus, the second purpose of this paper is to derive optimal error estimates for fully discretized schemes with a spectral-Galerkin method in space. We shall also demonstrate, through error estimates, why spectral methods are particularly suitable for interface problems governed by Allen-Cahn and Cahn-Hilliard equations.

The rest of the paper is organized as follows. In Section 2, we consider the Allen-Cahn equation and show that a number of commonly used time discretization schemes are energy stable. We also establish error estimates for two fully discretized schemes with a spectral-Galerkin approximation in space. In section 3, we consider the Cahn-Hilliard equations and carry out the corresponding stability and error analysis. We make a few remarks about the generalization and interpretation of our analysis and present some numerical results in Section 4.

2. Allen-Cahn equation. We consider in this section the numerical analysis of a few commonly used schemes for the Allen-Cahn equation (1.1).

We first introduce some notations which will be used throughout the paper. We use  $H^m(\Omega)$  and  $\|\cdot\|_m$   $(m=0,\pm 1,\cdots)$  to denote the standard Sobolev spaces and their norms, respectively. In particular, the norm and inner product of  $L^2(\Omega) =$  $H^0(\Omega)$  are denoted by  $\|\cdot\|_0$  and  $(\cdot, \cdot)$  respectively. We also denote the  $L^{\infty}(\Omega)$  by  $\|\cdot\|_{\infty}$ .

2.1. Stability analysis. We show in this subsection that several commonly used time discretization schemes are energy stable under reasonable assumptions.

2.1.1. First-order semi-implicit schemes. We consider first the usual first-order semiimplicit method

$$\frac{1}{\delta t}(u^{n+1} - u^n, \psi) + (\nabla u^{n+1}, \nabla \psi) + \frac{1}{\varepsilon^2}(f(u^n), \psi) = 0, \quad \forall \psi \in H^1(\Omega).$$
(2.1)

Lemma 2.1. Under the condition

$$\delta t \le \frac{2\varepsilon^2}{L},\tag{2.2}$$

the following energy law holds

$$E(u^{n+1}) \le E(u^n), \quad \forall n \ge 0.$$

*Proof.* Taking  $\psi = u^{n+1} - u^n$  in (2.1) and using the identity

$$(a - b, 2a) = |a|^2 - |b|^2 + |a - b|^2,$$
(2.3)

we find

$$\frac{1}{\delta t} \|u^{n+1} - u^n\|_0^2 + \frac{1}{2} (\|\nabla u^{n+1}\|_0^2 - \|\nabla u^n\|_0^2 + \|\nabla (u^{n+1} - u^n)\|_0^2) 
+ \frac{1}{\varepsilon^2} (f(u^n), u^{n+1} - u^n) = 0.$$
(2.4)

For the last term in (2.4), we use the Taylor expansion

$$F(u^{n+1}) - F(u^n) = f(u^n)(u^{n+1} - u^n) + \frac{f'(\xi^n)}{2}(u^{n+1} - u^n)^2.$$
(2.5)

Therefore, by using (1.6), we find

$$\begin{split} \frac{1}{\delta t} \| u^{n+1} - u^n \|_0^2 &+ \frac{1}{2} (\| \nabla u^{n+1} \|_0^2 - \| \nabla u^n \|_0^2 + \| \nabla (u^{n+1} - u^n) \|_0^2) \\ &+ \frac{1}{\varepsilon^2} (F(u^{n+1}) - F(u^n), 1) \\ &= \frac{1}{2\varepsilon^2} (f'(\xi^n) (u^{n+1} - u^n), u^{n+1} - u^n) \le \frac{L}{2\varepsilon^2} \| u^{n+1} - u^n \|_0^2, \end{split}$$
ch implies the desired results.

which implies the desired results.

The above lemma indicates that the first-order semi-implicit scheme satisfies a discrete energy law under the condition (2.2). While the condition (2.2) appears to be quite restrictive when  $\varepsilon \ll 1$ , a condition such as  $\delta t \sim \varepsilon^2$  is in fact needed for any scheme to be convergent. Nevertheless, This condition can be removed by introducing a stabilizing term as we show below.

The stabilized first-order semi-implicit method reads

$$\left(\frac{1}{\delta t} + \frac{S}{\varepsilon^2}\right)\left(u^{n+1} - u^n, \psi\right) + \left(\nabla u^{n+1}, \nabla \psi\right) + \frac{1}{\varepsilon^2}\left(f(u^n), \psi\right) = 0, \quad \forall \psi \in H^1(\Omega), \ (2.6)$$

where S is a stabilizing parameter to be specified.

The stabilizing term  $\frac{S}{\varepsilon^2}(u^{n+1}-u^n)$  introduces an extra consistency error of order  $\frac{S\delta t}{\varepsilon^2}u_t(\xi_n)$ . We note that this error is of the same order as the error introduced by the explicit treatment of the nonlinear term which is,  $\frac{1}{\varepsilon^2}(f(u(t^{n+1})) - f(u(t^n))) = \frac{\delta t}{\varepsilon^2}u_t(\eta_n)$ . Therefore, the stabilized semi-implicit scheme (2.6) is of the same order of accuracy, in terms of  $\delta t$  and  $\varepsilon$ , as the semi-implicit scheme (2.1). However, we have the following result for the stabilized scheme.

**Lemma 2.2.** For  $S \ge \frac{L}{2}$ , the stabilized scheme (2.6) is unconditionally stable and the following energy law holds for any  $\delta t$ :

$$E(u^{n+1}) \le E(u^n), \quad \forall n \ge 0.$$

$$(2.7)$$

*Proof.* Taking  $\psi = u^{n+1} - u^n$  in (2.6), we obtain

$$\begin{aligned} (\frac{1}{\delta t} + \frac{S}{\varepsilon^2}) \|u^{n+1} - u^n\|_0^2 + \frac{1}{2} (\|\nabla u^{n+1}\|_0^2 - \|\nabla u^n\|_0^2 + \|\nabla u^{n+1} - \nabla u^n\|_0^2) \\ &+ \frac{1}{\varepsilon^2} (f(u^n), u^{n+1} - u^n) = 0. \end{aligned}$$
(2.8)

Using again the Taylor expansion (2.5) and (1.6), we find

$$(f(u^n), u^{n+1} - u^n) \ge (F(u^{n+1}) - F(u^n), 1) - \frac{L}{2}(u^{n+1} - u^n, u^{n+1} - u^n).$$
(2.9)

We can then conclude from (2.8) and (2.9).

Remark 2.1. The scheme (2.6) can also be viewed as a linearized convex splitting scheme (cf. [11]). One can also design other unconditionally stable schemes with energy law by using the convex splitting approach (cf. [11, 22, 14]). Note that the stabilizing technique has also been considered in [23] for an epitaxial growth model. However, their stability proof is based on assuming the boundedness of the numerical solution which can not be verified *a priori*. In fact, by using a similar argument as above (see also Lemma 3.2 for the Cahn-Hilliard equation below), we can prove that the stabilized scheme for the epitaxial growth model consider in [23] satisfies an energy law and is also unconditionally stable.

2.1.2. Second-order semi-implicit and implicit schemes. A second-order semi-implicit scheme based on the second-order BDF and Adam-Bashforth is as follows:

$$\frac{1}{2\delta t}(3u^{n+1} - 4u^n + u^{n-1}, \psi) + (\nabla u^{n+1}, \nabla \psi) + \frac{1}{\varepsilon^2}(2f(u^n) - f(u^{n-1}), \psi) = 0, \quad \forall \psi \in H^1(\Omega).$$
(2.10)

Its stabilized version reads:

$$\frac{1}{2\delta t}(3u^{n+1} - 4u^n + u^{n-1}, \psi) + \frac{S}{\varepsilon^2}(u^{n+1} - 2u^n + u^{n-1}, \psi) + (\nabla u^{n+1}, \nabla \psi) + \frac{1}{\varepsilon^2}(2f(u^n) - f(u^{n-1}), \psi) = 0, \quad \forall \psi \in H^1(\Omega).$$
(2.11)

The stabilizing term  $\frac{S}{\varepsilon^2}(u^{n+1}-2u^n+u^{n-1})$  introduces an extra consistency error of order  $\frac{S\delta t^2}{\varepsilon^2}u_{tt}(\xi_n)$  which is of the same order as the error introduced by replacing  $f(u^{n+1})$  with  $2f(u^n) - f(u^{n-1})$ . Therefore, the stabilized semi-implicit scheme

(2.11) is of the same order of accuracy, in terms of  $\delta t$  and  $\varepsilon$ , as the semi-implicit scheme (2.10).

The stability results for the scheme (2.10) and its stabilized version (2.11) are shown below.

Lemma 2.3. Under the condition

$$\delta t \le \frac{2\varepsilon^2}{3L},\tag{2.12}$$

the solution of the scheme (2.11) with  $S \ge 0$  satisfies

$$E(u^{n+1}) + \left(\frac{1}{4\delta t} + \frac{S+L}{2\varepsilon^2}\right) \|u^{n+1} - u^n\|_0^2$$
  
$$\leq E(u^n) + \left(\frac{1}{4\delta t} + \frac{S+L}{2\varepsilon^2}\right) \|u^n - u^{n-1}\|_0^2, \quad \forall n \ge 1.$$
(2.13)

*Proof.* To simplify the notation, we denote  $\delta u^{n+1} = u^{n+1} - u^n$  and  $\delta^2 u^{n+1} = u^{n+1} - 2u^n + u^{n-1}$ .

Taking  $\psi = 2\delta t(u^{n+1} - u^n)$  in (2.11), we compute each term in the resultant equation as follows:

$$\begin{aligned} (3u^{n+1} - 4u^n + u^{n-1}, u^{n+1} - u^n) &= (2(u^{n+1} - u^n) + \delta^2 u^{n+1}, u^{n+1} - u^n) \\ &= 2\|u^{n+1} - u^n\|_0^2 + \frac{1}{2}(\|u^{n+1} - u^n\|_0^2 - \|u^n - u^{n-1}\|_0^2 + \|\delta^2 u^{n+1}\|_0^2). \end{aligned} \tag{2.14}$$

$$\begin{aligned} \frac{2S\delta t}{\varepsilon^2}(u^{n+1} - 2u^n + u^{n-1}, u^{n+1} - u^n) &= \frac{S\delta t}{\varepsilon^2}(\|u^{n+1} - u^n\|_0^2 - \|u^n - u^{n-1}\|_0^2 + \|\delta^2 u^{n+1}\|_0^2). \end{aligned} \tag{2.15}$$

From the Taylor expansion (2.5),

$$\frac{2\delta t}{\varepsilon^2}(f(u^n), u^{n+1} - u^n) = \frac{2\delta t}{\varepsilon^2}(F(u^{n+1}) - F(u^n), 1) + \frac{\delta t}{\varepsilon^2}(f'(\xi^n)(u^{n+1} - u^n), u^{n+1} - u^n);$$
(2.16)

On the other hand,

$$\frac{2\delta t}{\varepsilon^2}(f(u^n) - f(u^{n-1}), u^{n+1} - u^n) = \frac{2\delta t}{\varepsilon^2}(f'(\xi^{n-1})(u^n - u^{n-1}), u^{n+1} - u^n).$$
(2.17)

Combining the above relations together and using (1.6), we arrive at

$$2\|u^{n+1} - u^n\|_0^2 + (\frac{1}{2} + \frac{S\delta t}{\varepsilon^2})(\|u^{n+1} - u^n\|_0^2 - \|u^n - u^{n-1}\|_0^2 + \|\delta^2 u^{n+1}\|_0^2) + \frac{2\delta t}{\varepsilon^2}(F(u^{n+1}) - F(u^n), 1) + \delta t(\|\nabla u^{n+1}\|_0^2 - \|\nabla u^n\|_0^2 + \|\nabla (u^{n+1} - u^n)\|_0^2) \leq \frac{L\delta t}{\varepsilon^2}(\|u^{n+1} - u^n\|_0^2 + 2\|u^{n+1} - u^n\|_0\|u^n - u^{n-1}\|_0) \leq \frac{L\delta t}{\varepsilon^2}(2\|u^{n+1} - u^n\|_0^2 + \|u^n - u^{n-1}\|_0^2)$$

$$(2.18)$$

Under the condition (2.12), we have  $2 - \frac{2L\delta t}{\varepsilon^2} \ge \frac{L\delta t}{\varepsilon^2}$ . Therefore, after dropping some unnecessary terms, we can rearrange the above relation to

$$\left(\frac{1}{2} + \frac{(S+L)\delta t}{\varepsilon^2}\right)\left(\|u^{n+1} - u^n\|_0^2 - \|u^n - u^{n-1}\|_0^2\right) + 2\delta t(E(u^{n+1}) - E(u^n)) \le 0,$$

which implies (2.13).

Remark 2.2. The above lemma is valid for all  $S \ge 0$  which include in particular the usual second-order semi-implicit scheme (S = 0). The stability condition (2.12) is only slightly more restrictive than the condition (2.2) for the first-order semi-implicit scheme (2.1).

Unlike in the first-order case, we were unable to show theoretically that the stabilized scheme (2.11) with S > 0 has better stability than (2.10), which is (2.11) with S = 0. However, ample numerical evidences indicate that the stabilized version (2.11) with a suitable S allows much large time steps than that is allowed by the unstabilized version (2.10) (cf. [18]).

Next, we shall consider a second-order implicit scheme.

It is well-known that the usual second-order implicit Crank-Nicolson scheme does not satisfy an energy law. In order to construct a second-order implicit scheme which satisfies an energy law, we follow the idea in [10] (see also [8]) to introduce the following approximation to f(u):

$$\tilde{f}(u,v) = \begin{cases} \frac{F(u) - F(v)}{u - v} & \text{if } u \neq v \\ f(u) & \text{if } u = v \end{cases},$$
(2.19)

and consider the following (modified) Crank-Nicolson scheme

$$(\frac{u^{n+1} - u^n}{\delta t}, \psi) + (\nabla \frac{u^{n+1} + u^n}{2}, \nabla \psi) + \frac{1}{\varepsilon^2} (\tilde{f}(u^{n+1}, u^n), \psi) = 0, \quad \forall \psi \in H^1(\Omega)(2.20)$$

It is clear that the above scheme is of second-order accurate, but it can also be easily seen that its dominate truncation error is of order  $\frac{S\delta t^2}{\varepsilon^2}u_{tt}(\xi_n)$ , which is of the same order, in terms of  $\delta t$  and  $\varepsilon$ , as that of (2.11). Taking  $\psi = u^{n+1} - u^n$ , one immediately obtains the following result:

**Lemma 2.4.** The scheme (2.20) is unconditionally stable and its solution satisfies  $E(u^{n+1}) \le E(u^n), \quad \forall n \ge 0. \tag{2.21}$ 

While the scheme is unconditionally stable, but at each time step, one has to solve a nonlinear system for which the existence and uniqueness of the solution can only be proved under a condition  $\delta t \leq C\varepsilon^2$  for certain constant C > 0. This latter result can be proved by using a similar approach as in [8]. We leave the detail to the interested reader.

2.2. Error analysis. In this subsection, we shall adopt a spectral-Galerkin approximation for the spacial variables, and establish error estimates for the fully discrete versions of the first-order stabilized scheme and second-order implicit scheme.

We now introduce some notations and basic approximation results for the spectral approximations. We denote by  $Y_N$  the space of polynomials of degree  $\leq N$  in each direction, and by  $\Pi_N$  the usual  $L^2$ -projection operator in  $Y_N$ , namely

$$(\Pi_N v - v, \psi) = 0, \forall \psi \in Y_N, \tag{2.22}$$

and we define a projection operator  $\Pi^1_N : H^1(\Omega) \to Y_N$  by

$$(\nabla(\Pi_N^1 v - v), \nabla\psi) = 0, \quad (\Pi_N^1 v - v, 1) = 0, \quad \forall \psi \in Y_N.$$
(2.23)

It is well known (cf. [16, 5]) that the following estimates hold:

$$||u - \Pi_N u||_0 \lesssim N^{-m} ||u||_m \quad \forall u \in H^m(\Omega), \quad m \ge 0;$$
 (2.24)

$$||u - \Pi_N^1 u||_k \lesssim N^{k-m} ||u||_m, \quad k = 0, 1; \quad \forall u \in H^m(\Omega), \quad m \ge 1.$$
 (2.25)

2.2.1. First-order stabilized scheme. The spectral-Galerkin method for the first-order stabilized scheme (2.6) reads: Given  $u_N^0 = \prod_N u_0$ , for  $n \ge 0$ , find  $u_N^{n+1} \in Y_N$  such that

$$\left(\frac{1}{\delta t} + \frac{S}{\varepsilon^2}\right)\left(u_N^{n+1} - u_N^n, \psi_N\right) + \left(\nabla u_N^{n+1}, \nabla \psi_N\right) + \frac{1}{\varepsilon^2}\left(f(u_N^n), \psi_N\right) = 0, \quad \forall \psi_N \in Y_N.$$
(2.26)

Let us denote

$$\tilde{e}_N^{n+1} = \Pi_N^1 u(t^{n+1}) - u_N^{n+1}, \ \hat{e}_N^{n+1} = u(t^{n+1}) - \Pi_N^1 u(t^{n+1}), 
e_N^{n+1} = u(t^{n+1}) - u_N^{n+1} = \tilde{e}_N^{n+1} + \hat{e}_N^{n+1}.$$
(2.27)

We also denote

$$R^{n+1} := \frac{u(t^{n+1}) - u(t^n)}{\delta t} - u_t(t^{n+1}).$$
(2.28)

By using the Taylor expansion with integral residuals and the Cauchy-Schwarz inequality, we derive easily

$$\|R^{n+1}\|_{s}^{2} \leq \frac{1}{\delta t^{2}} \|\int_{t^{n}}^{t^{n+1}} (t-t^{n}) u_{tt}(t) dt\|_{s}^{2} \leq \frac{\delta t}{3} \int_{t^{n}}^{t^{n+1}} \|u_{tt}(t)\|_{s}^{2} dt, \quad s = -1, 0.$$
(2.29)

**Theorem 2.1.** Given T > 0. We assume that, for some  $m \ge 1$ ,  $u \in C(0,T; H^m(\Omega))$ ,  $u_t \in L^2(0,T; H^m(\Omega))$  and  $u_{tt} \in L^2(0,T; H^{-1}(\Omega))$ . Then, for  $S > \frac{L}{2}$ , the solution of (2.26) satisfies

$$E(u_N^{n+1}) \le E(u_N^n) \tag{2.30}$$

and the following error estimate holds:

$$\|u(t_{k}) - u_{N}^{k}\|_{0}$$

$$\leq C(\varepsilon, T)(K_{1}(u, \varepsilon)\delta t + K_{2}(u, \varepsilon)N^{-m}), \quad \forall 0 \leq k \leq \frac{T}{\delta t},$$

$$\left(\delta t \sum_{n=0}^{k} \|u(t_{n+1}) - u_{N}^{n+1}\|_{0}^{2}\right)^{\frac{1}{2}}$$

$$\leq C(\varepsilon, T)(K_{1}(u, \varepsilon)\delta t + K_{2}(u, \varepsilon)N^{1-m}), \quad \forall 0 \leq k \leq \frac{T}{\delta t},$$

$$(2.31)$$

where

$$C(\varepsilon, T) \sim \exp(T/\varepsilon^{2});$$
  

$$K_{1}(u, \varepsilon) = \|u_{tt}\|_{L^{2}(0,T;H^{-1})} + \frac{1}{\varepsilon} \|u_{t}\|_{L^{2}(0,T;L^{2})};$$
  

$$K_{2}(u, \varepsilon) = \|u_{0}\|_{m} + (\varepsilon + \frac{\delta t}{\varepsilon}) \|u_{t}\|_{L^{2}(0,T;H^{m})} + \frac{1}{\varepsilon} \|u\|_{C(0,T;H^{m})}$$

*Proof.* It is clear that the proof of Lemma 2.2 is also valid for the fully discrete scheme (2.26). Thus (2.30) holds for  $S > \frac{L}{2}$ . Next we proceed to error estimates.

Subtracting (2.26) from (1.1) at  $t^{n+1}$ , we find

$$((\frac{1}{\delta t} + \frac{S}{\varepsilon^2})(\tilde{e}_N^{n+1} - \tilde{e}_N^n), \psi_N) + (\nabla \tilde{e}_N^{n+1}, \nabla \psi_N)$$
  
=  $(R^{n+1}, \psi_N) + (\frac{1}{\delta t} + \frac{S}{\varepsilon^2}) ((\Pi_N^1 - I)(u(t^{n+1}) - u(t^n)), \psi_N)$ (2.32)  
+  $\frac{S}{\varepsilon^2}(u(t^{n+1}) - u(t^n), \psi_N) + \frac{1}{\varepsilon^2}(f(u_N^n) - f(u(t^{n+1})), \psi_N).$ 

Taking  $\psi = 2\delta t \tilde{e}_N^{n+1}$ , we derive  $S\delta t$ 

$$(1 + \frac{S\delta t}{\varepsilon^{2}})(\|\tilde{e}_{N}^{n+1}\|_{0}^{2} - \|\tilde{e}_{N}^{n+1}\|_{0}^{2} + \|\tilde{e}_{N}^{n+1} - \tilde{e}_{N}^{n}\|_{0}^{2}) + 2\delta t \|\nabla \tilde{e}_{N}^{n+1}\|_{0}^{2}$$

$$\leq 2\delta t \|R^{n+1}\|_{-1} \|\tilde{e}_{N}^{n+1}\|_{1}$$

$$+ (2 + \frac{2S\delta t}{\varepsilon^{2}})\|(I - \Pi_{N}^{1})(u(t^{n+1}) - u(t^{n}))\|_{0}\|\tilde{e}_{N}^{n+1}\|_{0}$$

$$+ \frac{2S\delta t}{\varepsilon^{2}}\|u(t^{n+1}) - u(t^{n})\|_{0}\|\tilde{e}_{N}^{n+1}\|_{0}$$

$$+ \frac{2\delta t}{\varepsilon^{2}}\|f(u_{N}^{n}) - f(u(t^{n+1}))\|_{0}\|\tilde{e}_{N}^{n+1}\|_{0} := \mathbf{I} + \mathbf{II} + \mathbf{III} + \mathbf{IV}.$$
(2.33)

Using the Cauchy-Schwarz inequality and Young's inequality, the first three terms can be easily estimated as follows:

$$\begin{split} \mathbf{I} &\leq C_0 \delta t \|R^{n+1}\|_{-1}^2 + \delta t \|\nabla \tilde{e}_N^{n+1}\|_0^2;\\ \mathbf{II} &\leq (\varepsilon^2 + \frac{S^2 \delta t^2}{\varepsilon^2}) \int_{t^n}^{t^{n+1}} \|(I - \Pi_N^1) u_t(t)\|_0^2 dt + \frac{2\delta t}{\varepsilon^2} \|\tilde{e}_N^{n+1}\|_0^2;\\ \mathbf{III} &\leq \frac{S^2 \delta t^2}{\varepsilon^2} \int_{t^n}^{t^{n+1}} \|u_t(t)\|_0^2 dt + \frac{\delta t}{\varepsilon^2} \|\tilde{e}_N^{n+1}\|_0^2. \end{split}$$

For the fourth term IV, we use (1.6) to derive

$$\begin{aligned} \|f(u_N^n) - f(u(t^{n+1}))\|_0 &\leq \|f(u_N^n) - f(u_N^{n+1})\|_0 + \|f(u_N^{n+1}) - f(u(t^{n+1}))\|_0 \\ &\leq L \|u_N^n - u_N^{n+1}\|_0 + L(\|\tilde{e}_N^{n+1}\|_0 + \|\hat{e}_N^{n+1}\|_0) \\ &\leq L(\|\tilde{e}_N^{n+1} - \tilde{e}_N^n\|_0 + \|(I - \Pi_N^1)(u(t^{n+1}) - u(t^n))\|_0 \\ &+ \|u(t^{n+1}) - u(t^n)\|_0) + L(\|\tilde{e}_N^{n+1}\|_0 + \|\hat{e}_N^{n+1}\|_0). \end{aligned}$$

$$(2.34)$$

Therefore,

$$\mathbf{IV} \leq \frac{L\delta t}{\varepsilon^2} \|\tilde{e}_N^{n+1} - \tilde{e}_N^n\|_0^2 + \frac{L\delta t^2}{\varepsilon^2} \int_{t^n}^{t^{n+1}} \|(I - \Pi_N^1)u_t(t)\|_0^2 dt + \frac{L\delta t^2}{\varepsilon^2} \int_{t^n}^{t^{n+1}} \|u_t(t)\|_0^2 dt + \frac{L\delta t}{\varepsilon^2} (\|\hat{e}_N^{n+1}\|_0^2 + C_1 \|\tilde{e}_N^{n+1}\|_0^2).$$
(2.35)

Combining the above inequalities into (2.33), we arrive at

$$\begin{split} \|\tilde{e}_{N}^{n+1}\|_{0}^{2} &- \|\tilde{e}_{N}^{n+1}\|_{0}^{2} + \|\tilde{e}_{N}^{n+1} - \tilde{e}_{N}^{n}\|_{0}^{2} + \delta t \|\nabla \tilde{e}_{N}^{n+1}\|_{0}^{2} \\ &\leq C_{0}\delta t \|R^{n+1}\|_{-1}^{2} + \frac{C_{2}\delta t}{\varepsilon^{2}} \|\tilde{e}_{N}^{n+1}\|_{0}^{2} + \frac{L\delta t}{\varepsilon^{2}} \|\hat{e}_{N}^{n+1}\|_{0}^{2} \\ &+ (\varepsilon^{2} + \frac{C_{3}\delta t^{2}}{\varepsilon^{2}}) \int_{t^{n}}^{t^{n+1}} \|(I - \Pi_{N}^{1})u_{t}(t)\|_{0}^{2} dt + \frac{C_{3}\delta t^{2}}{\varepsilon^{2}} \int_{t^{n}}^{t^{n+1}} \|u_{t}(t)\|_{0}^{2} dt. \end{split}$$

Summing up the above inequality for  $n = 0, 1, \dots, k$   $(k \leq \frac{T}{\delta t} + 1)$ , dropping some unnecessary terms and observing (2.29)), we find

$$\begin{split} \|\tilde{e}_{N}^{k+1}\|_{0}^{2} &- \|\tilde{e}_{N}^{0}\|_{0}^{2} + \delta t \sum_{n=0}^{k} \|\nabla \tilde{e}_{N}^{n+1}\|_{0}^{2} \\ \leq & \delta t^{2} \left( \|u_{tt}\|_{L^{2}(0,T;H^{-1})}^{2} + \frac{C_{3}}{\varepsilon^{2}} \|u_{t}\|_{L^{2}(0,T;L^{2})}^{2} \right) \\ &+ (\varepsilon^{2} + \frac{C_{3}\delta t^{2}}{\varepsilon^{2}}) \|(I - \Pi_{N}^{1})u_{t}\|_{L^{2}(0,T;L^{2})}^{2} + \frac{L}{\varepsilon^{2}} \|(I - \Pi_{N}^{1})u\|_{C(0,T;L^{2})}^{2} \\ &+ \frac{C_{2}\delta t}{\varepsilon^{2}} \sum_{n=0}^{k} \|\tilde{e}_{N}^{k+1}\|_{0}^{2}. \end{split}$$

Applying the discrete Gronwall lemma to the above inequality, We can then conclude by using the triangular inequality  $||u(t_n) - u_N^n||_i \leq ||\tilde{e}_N^n||_i + ||\hat{e}_N^n||_i \ (i = 0, 1)$ , and the approximation results (2.24) and (2.25).

Remark 2.3. We note that the bound on constant  $C(\varepsilon, T)$  results from the discrete Gronwall lemma. While it is possible to improve this bound to polynomial order in terms of  $\varepsilon^{-1}$  as is done in [12, 13, 15] and [24], this process is very technical so we decided not to carry it out as our main purpose in this paper is to study the stability properties of various schemes and to demonstrate that optimal error estimates with spectral-Galerkin approximation in space can be derived.

2.2.2. Second-order implicit scheme. The spectral-Galerkin method for the second-order implicit scheme (2.20) reads: Given  $u_N^0 = \prod_N^1 u_0$ . for  $n \ge 0$ , find  $u_N^{n+1} \in Y_N$  such that

$$\left(\frac{u_N^{n+1} - u_N^n}{\delta t}, \psi_N\right) + \left(\nabla \frac{u_N^{n+1} + u_N^n}{2}, \nabla \psi_N\right) \\ + \frac{1}{\varepsilon^2} (\tilde{f}(u_N^{n+1}, u_N^n), \psi_N) = 0, \quad \forall \psi_N \in Y_N.$$
(2.36)

In order to carry out an error analysis, we need to first establish the Lipschitz property for  $\tilde{f}(u, v)$ . Using the definition of (2.19), we derive that for u > v,

$$\frac{\partial \tilde{f}(u,v)}{\partial u} = \frac{F'(u)(u-v) - (F(u) - F(v))}{(u-v)^2}$$
$$= \frac{1}{(u-v)^2} \int_v^u (F'(u) - F'(z))dz$$
$$= \frac{1}{(u-v)^2} \int_v^u \int_z^u f'(y)dydz \le \|f'\|_\infty \le L.$$
(2.37)

Similarly we can show that the above is true for u < v. Thus,

$$|\tilde{f}(u_1, v) - \tilde{f}(u_2, v)| \le L|u_1 - u_2|.$$
(2.38)

Likewise, we can prove

$$|\tilde{f}(u,v_1) - \tilde{f}(u,v_2)| \le L|v_1 - v_2|.$$
(2.39)

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Next, we define the truncation error  $R^{n+1/2} = R_1^{n+1/2} + R_2^{n+1/2}$ , where

$$R_1^{n+1/2} := \left(\frac{u(t^{n+1}) - u(t^n)}{\delta t} - u_t(t^{n+1/2})\right), \tag{2.40}$$

$$R_2^{n+1/2} := -\Delta\left(\frac{u(t^{n+1}) + u(t^n)}{2} - u(t^{n+1/2})\right).$$
(2.41)

By using the Taylor expansion with integral residual, it is easy to show (cf. [21]) that

$$\|R_1^{n+1/2}\|_s^2 \le \delta t^3 \int_{t^n}^{t^{n+1}} \|u_{ttt}(t)\|_s^2 dt, s = -1, 0,$$
(2.42)

$$\|R_2^{n+1/2}\|_s^2 \le \delta t^3 \int_{t^n}^{t^{n+1}} \|u_{tt}(t)\|_{s+2}^2 dt, s = -1, 0.$$
(2.43)

We are now ready for the error analysis.

**Theorem 2.2.** Given T > 0. we assume that for some  $m \ge 1$ ,  $u \in C(0, T; H^m(\Omega))$ ,  $u_t \in L^2(0, T; H^m(\Omega)) \cap L^2(0, T; L^4(\Omega))$ ,  $u_{tt} \in L^2(0, T; H^1(\Omega))$  and  $u_{ttt} \in L^2(0, T; H^{-1}(\Omega))$ . Then, the solution of (2.36) satisfies

$$E(u_N^{n+1}) \le E(u_N^n), \tag{2.44}$$

and the following error estimate holds for  $0 \le k \le \frac{T}{\delta t}$ :

$$\begin{aligned} &\|u(t_{k}) - u_{N}^{k}\|_{0} \\ \leq C(\varepsilon, T)(K_{3}(u, \varepsilon)\delta t^{2} + K_{4}(u, \varepsilon)N^{-m}), \\ &\left(\delta t\sum_{n=0}^{k}\|\nabla(u(t_{n+\frac{1}{2}}) - \frac{1}{2}(u_{N}^{n+1} + u_{N}^{n})\|_{0}^{2}\right)^{\frac{1}{2}} \\ \leq C(\varepsilon, T)(K_{3}(u, \varepsilon)\delta t^{2} + K_{4}(u, \varepsilon)N^{1-m}), \end{aligned}$$

where

 $C(\varepsilon, T) \sim \exp(T/\varepsilon^2);$ 

 $K_{3}(u,\varepsilon) = \|u_{ttt}\|_{L^{2}(0,T;H^{-1})} + \|u_{tt}\|_{L^{2}(0,T;H^{1})} + \frac{1}{\varepsilon}(\|u_{t}\|_{L^{2}(0,T;L^{4})} + \|u_{tt}\|_{L^{2}(0,T;L^{2})});$  $K_{4}(u,\varepsilon) = \|u_{0}\|_{m} + \varepsilon \|u_{t}\|_{L^{2}(0,T;H^{m})} + \frac{1}{\varepsilon} \|u\|_{C(0,T;H^{m})}.$ 

*Proof.* Taking  $\psi_N = u_N^{n+1} - u_N^n$  in (2.36), one derives immediately (2.44). In addition to (2.27), we define

$$\tilde{e}_N^{n+1/2} = \frac{\tilde{e}_N^{n+1} + \tilde{e}_N^n}{2}.$$

Subtracting (2.36) from (1.1) at  $t^{n+1/2}$ , we find

$$(\frac{\tilde{e}_N^{n+1} - \tilde{e}_N^n}{\delta t}, \psi) + (\nabla \tilde{e}_N^{n+1/2}, \nabla \psi) = (R^{n+1/2}, \psi_N) + \frac{1}{\delta t} ((\Pi_N^1 - I)(u(t^{n+1}) - u(t^n)), \psi_N) + \frac{1}{\varepsilon^2} (\tilde{f}(u_N^{n+1}, u_N^n) - f(u(t^{n+1/2})), \psi_N).$$

Taking  $\psi_N = 2\delta t \tilde{e}_N^{n+1/2}$ , we derive

$$\begin{split} \|\tilde{e}_{N}^{n+1}\|_{0} &= \|\tilde{e}_{N}^{n}\|_{0}^{2} + 2\delta t \|\nabla \tilde{e}_{N}^{n+1/2}\|_{0}^{2} \\ \leq & C_{0}\delta t \|R^{n+1/2}\|_{-1}^{2} + \delta t \|\nabla \tilde{e}_{N}^{n+1/2}\|_{0}^{2} \\ &+ \varepsilon^{2} \int_{t^{n}}^{t^{n+1}} \|(I - \Pi_{N}^{1})u_{t}(t)\|_{0}^{2} dt + \frac{\delta t}{\varepsilon^{2}} \|\tilde{e}_{N}^{n+1/2}\|_{0}^{2} \\ &+ \frac{\delta t}{\varepsilon^{2}} \|\tilde{e}_{N}^{n+1/2}\|_{0}^{2} + \frac{\delta t}{\varepsilon^{2}} \|\tilde{f}(u_{N}^{n+1}, u_{N}^{n}) - f(u(t^{n+\frac{1}{2}})\|_{0}^{2}. \end{split}$$

$$(2.45)$$

For the last term, we have

$$\begin{split} \|\tilde{f}(u_{N}^{n+1}, u_{N}^{n}) - f(u(t^{n+1/2}))\|_{0} \\ \leq \|\tilde{f}(u_{N}^{n+1}, u_{N}^{n}) - \tilde{f}(u(t^{n+1}), u_{N}^{n})\|_{0} \\ &+ \|\tilde{f}(u(t^{n+1}), u_{N}^{n}) - \tilde{f}(u(t^{n+1}), u(t^{n}))\|_{0} \\ &+ \|\tilde{f}(u(t^{n+1}), u(t^{n})) - f(\frac{u(t^{n+1}) + u(t^{n})}{2})\|_{0} \\ &+ \|f(\frac{u(t^{n+1}) + u(t^{n})}{2}) - f(u(t^{n+1/2}))\|_{0} \\ &:= \mathbf{I} + \mathbf{II} + \mathbf{III} + \mathbf{IV}. \end{split}$$

$$(2.46)$$

By using the Lipschitz properties (1.6) and (2.38)-(2.39), we find

$$\mathbf{I}^{2} \leq L^{2} \|u_{N}^{n+1} - u(t^{n+1})\|_{0}^{2} \leq L^{2}(\|\tilde{e}_{N}^{n+1}\|_{0}^{2} + \|\hat{e}_{N}^{n+1}\|_{0}^{2});$$

$$\mathbf{II}^{2} \leq L^{2} \|u_{N}^{n} - u(t^{n})\|_{0}^{2} \leq L^{2}(\|\tilde{e}_{N}^{n}\|_{0}^{2} + \|\hat{e}_{N}^{n}\|_{0}^{2});$$

$$\mathbf{IV}^{2} \leq L^{2} \|\frac{u(t^{n+1}) + u(t^{n})}{2} - u(t^{n+1/2})\|_{0}^{2} \leq L^{2}\delta t^{3} \int_{t^{n}}^{t^{n+1}} \|u_{tt}(t)\|_{0}^{2} dt.$$
(2.47)

By using the Taylor expansion and the definitions of f and  $\tilde{f}$ , it is easy to show that

$$|\tilde{f}(u,v) - f(\frac{u+v}{2})| \le \frac{1}{24} \max_{\xi \in [u,v]} |f''(\xi)| |u-v|^2.$$
(2.48)

Therefore, we have

$$\mathbf{III}^{2} \leq C_{4} \| (u(t^{n+1}) - u(t^{n}))^{2} \|_{0}^{2} \leq C_{4} \delta t^{3} \int_{t_{n}}^{t^{n+1}} \| u_{t}^{2}(t) \|_{0}^{2} dt$$

Combining these into (2.45), we arrive at

$$\begin{split} \|\tilde{e}_{N}^{n+1}\|_{0} - \|\tilde{e}_{N}^{n}\|_{0}^{2} + \delta t \|\nabla \tilde{e}_{N}^{n+1/2}\|_{0}^{2} \\ &\leq C_{0} \delta t \|R^{n+1/2}\|_{-1}^{2} + \varepsilon^{2} \int_{t^{n}}^{t^{n+1}} \|(I - \Pi_{N}^{1})u_{t}(t)\|_{0}^{2} dt \\ &+ \frac{C_{5} \delta t}{\varepsilon^{2}} \left(\|\tilde{e}_{N}^{n+1}\|_{0}^{2} + \|\tilde{e}_{N}^{n}\|_{0}^{2} + \|\hat{e}_{N}^{n+1}\|_{0}^{2} + \|\hat{e}_{N}^{n+1}\|_{0}^{2} + \|\hat{e}_{N}^{n+1}\|_{0}^{2} \right) \\ &+ \frac{C_{6} \delta t^{4}}{\varepsilon^{2}} \int_{t_{n}}^{t^{n+1}} (\|u_{t}^{2}(t)\|_{0}^{2} + \|u_{tt}(t)\|_{0}^{2}) dt. \end{split}$$

$$(2.49)$$

Summing up the above inequality for  $n = 0, 1, \dots, k$   $(k \leq \frac{T}{\delta t} - 1)$ , and using (2.25) and (2.42)-(2.43), we obtain

$$\begin{split} \|\tilde{e}_{N}^{k+1}\|_{0} &- \|\tilde{e}_{N}^{0}\|_{0}^{2} + \delta t \sum_{n=0}^{k} \|\nabla \tilde{e}_{N}^{n+1/2}\|_{0}^{2} \\ \leq & C_{0}\delta t^{4}(\|u_{ttt}\|_{L^{2}(0,T;H^{-1})}^{2} + \|u_{tt}\|_{L^{2}(0,T;H^{1})}^{2}) + \varepsilon^{2}N^{-2m}\|u_{t}\|_{L^{2}(0,T;H^{m})}^{2} \\ &+ \frac{C_{5}\delta t}{\varepsilon^{2}} \sum_{n=0}^{k} \left(\|\tilde{e}_{N}^{n+1}\|_{0}^{2} + \|\tilde{e}_{N}^{n}\|_{0}^{2} + \|\hat{e}_{N}^{n+1}\|_{0}^{2} + \|\hat{e}_{N}^{n}\|_{0}^{2} \right) \\ &+ \frac{C_{6}\delta t^{4}}{\varepsilon^{2}}(\|u_{t}\|_{L^{2}(0,T;L^{4})}^{2} + \|u_{tt}\|_{L^{2}(0,T;L^{2})}^{2}). \end{split}$$

We can then conclude by applying the discrete Gronwall lemma to the above inequality, and by using the triangular inequality and (2.25).

3. Cahn-Hilliard equation. We now consider the Cahn-Hilliard equation (1.2) which we rewrite in the following mixed formulation:

$$(u_t, q) + (\nabla w, \nabla q) = 0, \quad \forall q \in H^1(\Omega),$$
  
$$(\nabla u, \nabla \psi) + \frac{1}{\varepsilon^2} (f(u), \psi) = (w, \psi), \quad \forall \psi \in H^1(\Omega).$$
  
(3.1)

As for the Allen-Cahn equation, we shall construct semi-implicit and implicit schemes for (3.1) and carry out stability and error analysis for them.

## 3.1. Stability analysis.

3.1.1. *First-order semi-implicit schemes.* We consider first the usual first-order semi-implicit method

$$\frac{1}{\delta t}(u^{n+1} - u^n, q) + (\nabla w^{n+1}, \nabla q) = 0, \quad \forall q \in H^1(\Omega),$$

$$(\nabla u^{n+1}, \nabla \psi) + \frac{1}{\varepsilon^2}(f(u^n), \psi) = (w^{n+1}, \psi), \quad \forall \psi \in H^1(\Omega).$$
(3.2)

Lemma 3.1. Under the condition

$$\delta t \le \frac{4\varepsilon^4}{L^2},\tag{3.3}$$

the solution of (3.2) satisfies

$$E(u^{n+1}) \le E(u^n), \quad \forall n \ge 0.$$

*Proof.* Taking  $q = \delta t w^{n+1}$  and  $\psi = u^{n+1} - u^n$  in (3.2), and using (2.5), we find

$$(u^{n+1} - u^n, w^{n+1}) + \delta t \|\nabla w^{n+1}\|_0^2 = 0,$$
(3.4)

and

$$\frac{1}{2}(\|\nabla u^{n+1}\|_{0}^{2} - \|\nabla u^{n}\|_{0}^{2} + \|\nabla (u^{n+1} - u^{n})\|_{0}^{2}) + \frac{1}{\varepsilon^{2}}(F(u^{n+1}) - F(u^{n}), 1) + \frac{1}{2\varepsilon^{2}}(f'(\xi^{n})(u^{n+1} - u^{n}), u^{n+1} - u^{n}) = (w^{n+1}, u^{n+1} - u^{n}).$$
(3.5)

On the other hand, taking  $q = \sqrt{\delta t}(u^{n+1} - u^n)$  in (3.2), we obtain

$$\frac{1}{\sqrt{\delta t}} \|u^{n+1} - u^n\|_0^2 = -\sqrt{\delta t} (\nabla w^{n+1}, \nabla (u^{n+1} - u^n))$$
  
$$\leq \frac{\delta t}{2} \|\nabla w^{n+1}\|_0^2 + \frac{1}{2} \|\nabla (u^{n+1} - u^n)\|_0^2.$$
(3.6)

Summing up the above three relations and using (1.6), we arrive at

$$\frac{1}{\sqrt{\delta t}} \|u^{n+1} - u^n\|_0^2 + \frac{\delta t}{2} \|\nabla w^{n+1}\|_0^2 + \frac{1}{2} (\|\nabla u^{n+1}\|_0^2 - \|\nabla u^n\|_0^2) \\
+ \frac{1}{\varepsilon^2} (F(u^{n+1}) - F(u^n), 1) = -\frac{1}{2\varepsilon^2} (f'(\xi^n)(u^{n+1} - u^n), u^{n+1} - u^n) \\
\leq \frac{L}{2\varepsilon^2} \|u^{n+1} - u^n\|_0^2.$$

We then conclude that the desired result holds under the condition (3.3).

Notice that, as expected, the stability condition (3.3) for the Cahn-Hilliard equation is much severe than the condition (2.2) for the Allen-Cahn equation. However, a condition such as  $\delta t \sim \varepsilon^4$  is in fact necessary for the sake of convergence.

We now consider the following first-order stabilized semi-implicit method:

$$\frac{1}{\delta t}(u^{n+1} - u^n, q) + (\nabla w^{n+1}, \nabla q) = 0, \quad \forall q \in H^1(\Omega), 
(\nabla u^{n+1}, \nabla \psi) + \frac{S}{\varepsilon^2}(u^{n+1} - u^n, \psi) + \frac{1}{\varepsilon^2}(f(u^n), \psi) = (w^{n+1}, \psi), \quad \forall \psi \in H^1(\Omega).$$
(3.7)

As in the Allen-Cahn case, the extra consistency error introduced by the stabilization term is of the same order, in terms of  $\delta t$  and  $\varepsilon$ , as the dominating truncation error in (3.2).

**Lemma 3.2.** For  $S \ge \frac{L}{2}$ , the stabilized scheme (3.7) is unconditionally stable and the following energy law holds for any  $\delta t$ :

$$E(u^{n+1}) \le E(u^n) \quad \forall n \ge 0.$$
(3.8)

*Proof.* As in the proof of Lemma 3.1, taking  $q = \delta t w^{n+1}$  and  $\psi = u^{n+1} - u^n$  in (3.2), we obtain (3.4) and (3.5) with an extra term  $\frac{S}{\varepsilon^2} ||u^{n+1} - u^n||_0^2$  in the left hand side of (3.5). Therefore, summing up (3.4) and and (3.5) with this extra term, we immediately derive the desired result.

3.1.2. *Second-order semi-implicit scheme*. The second-order stabilized semi-implicit scheme reads:

$$\frac{1}{2\delta t}(3u^{n+1} - 4u^n + u^{n-1}, q) + (\nabla w^{n+1}, \nabla q) = 0, \forall q \in H^1(\Omega), 
(\nabla u^{n+1}, \nabla \psi) + \frac{S}{\varepsilon^2}(u^{n+1} - 2u^n + u^{n-1}, \psi) + \frac{1}{\varepsilon^2}(2f(u^n) - f(u^{n-1}, \psi))$$

$$= (w^{n+1}, \psi), \forall \psi \in H^1(\Omega).$$
(3.9)

Since the above scheme is a direct extension of the scheme (2.11) to the Cahn-Hilliard case, we refer to *Remark* 2.1 for its theoretical and numerical stability properties.

3.1.3. Second-order implicit scheme.

$$\frac{1}{\delta t}(u^{n+1} - u^n, q) + (\nabla w^{n+1}, \nabla q) = 0, 
(\frac{\nabla u^{n+1} + \nabla u^n}{2}, \nabla \psi) + \frac{1}{\varepsilon^2}(\tilde{f}(u^n, u^{n+1}), \psi) = (w^{n+1}, \psi).$$
(3.10)

Taking  $q = \delta t w^{n+1}$ ,  $\psi = u^{n+1} - u^n$ , one immediately obtains the following result:

Lemma 3.3. The scheme (3.10) is unconditionally stable and its solution satisfies

$$E(u^{n+1}) \le E(u^n), \quad \forall n \ge 0.$$
(3.11)

Note that while the scheme (3.10) is unconditionally stable, it appears that one can only prove the existence and uniqueness of the solution to (3.10) under a condition similar to (3.3) (cf. [8]).

### 3.2. Error analysis.

3.2.1. First-order stabilized semi-implicit scheme. The spectral-Galerkin method for the first-order stabilized scheme (3.7) reads: Given  $u_N^0 = \prod_N u_0$ , for  $n \ge 0$ , find  $(u_N^{n+1}, w_N^{n+1}) \in Y_N \times Y_N$  such that

$$\frac{1}{\delta t}(u_N^{n+1} - u_N^n, q_N) + (\nabla w_N^{n+1}, \nabla q_N) = 0, \quad \forall q_N \in Y_N 
(\nabla u_N^{n+1}, \nabla \psi_N) + \frac{S}{\varepsilon^2}(u_N^{n+1} - u_N^n, \psi_N) + \frac{1}{\varepsilon^2}(f(u_N^n), \psi_N) = (w_N^{n+1}, \psi_N), \quad \forall \psi_N \in Y_N.$$
(3.12)

We denote

$$\tilde{e}_N^{n+1} = \Pi_N^1 u(t^{n+1}) - u_N^{n+1}, \ \hat{e}_N^{n+1} = u(t^{n+1}) - \Pi_N^1 u(t^{n+1}), 
\bar{e}_N^{n+1} = \Pi_N^1 w(t^{n+1}) - w_N^{n+1}, \\ \tilde{e}_N^{n+1} = w(t^{n+1}) - \Pi_N^1 w(t^{n+1}).$$
(3.13)

**Theorem 3.1.** Given T > 0, we assume that for some  $m \ge 1$ ,  $u, w \in C(0, T; H^m(\Omega))$ ,  $u_t \in L^2(0, T; H^m(\Omega))$  and  $u_{tt} \in L^2(0, T; L^2(\Omega))$ . Then for  $s > \frac{L}{2}$ , the solution of (3.12) satisfies

$$E(u_N^{n+1}) \le E(u_N^n),$$

and the following error estimate holds

$$\begin{aligned} \|u(t^k) - u_N^k\|_0 + \left(\delta t \sum_{n=0}^k \|w(t_{n+1}) - w_N^{n+1}\|_0^2\right)^{\frac{1}{2}} \\ &\leq C(\varepsilon, T)(K_5(u, \varepsilon)\delta t + K_6(u, \varepsilon)N^{-m}), \quad \forall 0 \le k \le \frac{T}{\delta t}, \end{aligned}$$

where

$$C(\varepsilon, T) \sim \exp(T/\varepsilon^4);$$
  

$$K_5(u, \varepsilon) = \varepsilon^2 \|u_{tt}\|_{L^2(0,T;L^2)} + \frac{1}{\varepsilon^2} \|u_t\|_{L^2(0,T;L^2)};$$
  

$$K_6(u, \varepsilon) = \|u_0\|_m + (\varepsilon^2 + \frac{\delta t}{\varepsilon^2}) \|u_t\|_{L^2(0,T;H^m)} + \frac{1}{\varepsilon^2} \|u\|_{C(0,T;H^m)} + \|w\|_{C(0,T;H^m)}.$$

*Proof.* Obviously, the proof of Lemma 3.2 is also valid for the fully discrete scheme 3.12. We now turn to the error estimates. Let  $R^{n+1}$  be defined as in (2.28). Subtracting (3.12) from (3.1), we obtain

$$\frac{1}{\delta t} (\tilde{e}_N^{n+1} - \tilde{e}_N^n, q_N) + (\nabla \bar{e}_N^{n+1}, \nabla q_N) 
= (R^{n+1}, q_N) - \frac{1}{\delta t} ((I - \Pi_N^1)(u(t^{n+1}) - u(t^n)), q_N) 
(\nabla \tilde{e}_N^{n+1}, \nabla \psi_N) + \frac{S}{\varepsilon^2} (\tilde{e}_N^{n+1} - \tilde{e}_N^n, \psi_N) + \frac{1}{\varepsilon^2} (f(u(t^{n+1})) - f(u_N^n), \psi_N) 
= (\bar{e}_N^{n+1} + \check{e}_N^{n+1}, \psi_N) + \frac{S}{\varepsilon^2} (\Pi_N^1 u(t^{n+1}) - \Pi_N^1 u(t^n), \psi_N).$$
(3.14)

Taking  $q_N = 2\delta t \tilde{e}_N^{n+1}$  and  $\psi_N = -2\delta t \bar{e}_N^{n+1}$  and summing up the two identities, we derive

$$\begin{split} \|\tilde{e}_{N}^{n+1}\|_{0}^{2} &- \|\tilde{e}_{N}^{n}\|_{0}^{2} + \|\tilde{e}_{N}^{n+1} - \tilde{e}_{N}^{n}\|_{0}^{2} + 2\delta t \|\bar{e}_{N}^{n+1}\|_{0}^{2} = 2\delta t (R^{n+1}, \tilde{e}_{N}^{n+1}) \\ &- 2((I - \Pi_{N}^{1})(u(t^{n+1}) - u(t^{n})), \tilde{e}_{N}^{n+1}) + \frac{2\delta t S}{\varepsilon^{2}} (\tilde{e}_{N}^{n+1} - \tilde{e}_{N}^{n}, \bar{e}_{N}^{n+1}) \\ &+ \frac{2\delta t}{\varepsilon^{2}} (f(u(t^{n+1})) - f(u_{N}^{n}), \bar{e}_{N}^{n+1}) - 2\delta t (\check{e}_{N}^{n+1}, \bar{e}_{N}^{n+1}) \\ &- \frac{2S\delta t}{\varepsilon^{2}} (\Pi_{N}^{1}(u(t^{n+1}) - u(t^{n})), \bar{e}_{N}^{n+1}) := \mathbf{I} + \mathbf{II} + \mathbf{III} + \mathbf{IV} + \mathbf{V} + \mathbf{VI}. \end{split}$$
(3.15)

Similarly as in the proof of Theorem 2.1, using the Cauchy-Schwarz inequality and (2.34), we derive

$$\begin{split} \mathbf{I} &\leq \varepsilon^{4} \delta t \|R^{n+1}\|_{0}^{2} + \frac{\delta t}{\varepsilon^{4}} \|\tilde{e}_{N}^{n+1}\|_{0}^{2}; \\ \mathbf{II} &\leq 2\varepsilon^{4} \int_{t^{n}}^{t^{n+1}} \|(I - \Pi_{N}^{1})u_{t}(t)\|_{0}^{2} dt + \frac{\delta t}{2\varepsilon^{4}} \|\tilde{e}_{N}^{n+1}\|_{0}^{2}; \\ \mathbf{III} &\leq \frac{\delta t}{4} \|\bar{e}_{N}^{n+1}\|_{0}^{2} + \frac{4\delta t S^{2}}{\varepsilon^{4}} \|\tilde{e}_{N}^{n+1} - \tilde{e}_{N}^{n}\|^{2}; \\ \mathbf{IV} &\leq \frac{\delta t}{4} \|\bar{e}_{N}^{n+1}\|_{0}^{2} + C_{7} \left( \frac{\delta t L^{2}}{\varepsilon^{4}} \|\tilde{e}_{N}^{n+1} - \tilde{e}_{N}^{n}\|_{0}^{2} + \frac{\delta t^{2} L^{2}}{\varepsilon^{4}} \int_{t^{n}}^{t^{n+1}} \|(I - \Pi_{N}^{1})u_{t}(t)\|_{0}^{2} dt \\ &\quad + \frac{\delta t^{2} L^{2}}{\varepsilon^{4}} \int_{t^{n}}^{t^{n+1}} \|u_{t}(\cdot, t)\|_{0}^{2} dt + \frac{\delta t L^{2}}{\varepsilon^{4}} (\|\tilde{e}_{N}^{n+1}\|_{0}^{2} + \|\tilde{e}_{N}^{n+1}\|_{0}^{2}) \right); \\ \mathbf{V} &\leq \frac{\delta t}{4} \|\bar{e}_{N}^{n+1}\|_{0}^{2} + 4\delta t \|\check{e}_{N}^{n+1}\|_{0}^{2}; \\ \mathbf{VI} &\leq \frac{\delta t}{4} \|\bar{e}_{N}^{n+1}\|_{0}^{2} + \frac{4S^{2} \delta t^{2}}{\varepsilon^{4}} (\int_{t^{n}}^{t^{n+1}} \|(I - \Pi_{N}^{1})u_{t}(t)\|_{0}^{2} dt + \int_{t^{n}}^{t^{n+1}} \|u_{t}(t)\|_{0}^{2} dt). \end{split}$$

Combining the above inequalities into (3.15), we arrive at

$$\begin{split} \|\tilde{e}_{N}^{n+1}\|_{0}^{2} &- \|\tilde{e}_{N}^{n}\|_{0}^{2} + \|\tilde{e}_{N}^{n+1} - \tilde{e}_{N}^{n}\|_{0}^{2} + \delta t \|\tilde{e}_{N}^{n+1}\|_{0}^{2} \\ \leq & \delta t \varepsilon^{4} \|R^{n+1}\|_{0}^{2} + 4 \delta t \|\check{e}_{N}^{n+1}\|_{0}^{2} + \frac{C_{8} \delta t}{\varepsilon^{4}} (\|\tilde{e}_{N}^{n+1}\|_{0}^{2} + \|\tilde{e}_{N}^{n}\|_{0}^{2} + \|\hat{e}_{N}^{n+1}\|_{0}^{2}) \\ &+ 2 \varepsilon^{4} \int_{t^{n}}^{t^{n+1}} \|(I - \Pi_{N}^{1})u_{t}(\cdot, t)\|^{2} dt \\ &+ \frac{C_{9} \delta t^{2}}{\varepsilon^{4}} (\int_{t^{n}}^{t^{n+1}} \|(I - \Pi_{N}^{1})u_{t}(\cdot, t)\|^{2} dt + \int_{t^{n}}^{t^{n+1}} \|u_{t}(\cdot, t)\|^{2} dt). \end{split}$$
(3.16)

Summing up the above inequality for  $n = 0, 1, \dots, k$   $(k \leq \frac{T}{\delta t} - 1)$  and using (2.25) and (2.29), we obtain

$$\begin{split} \|\tilde{e}_{N}^{n+1}\|_{0}^{2} &- \|\tilde{e}_{0}^{n}\|_{0}^{2} + \delta t \sum_{n=0}^{k} \|\bar{e}_{N}^{n+1}\|_{0}^{2} \\ &\leq 4\delta t \sum_{n=0}^{k} \|\check{e}_{N}^{n+1}\|_{0}^{2} + \delta t^{2} (\varepsilon^{4} \|u_{tt}\|_{L^{2}(0,T;L^{2})}^{2} + \frac{C_{9}}{\varepsilon^{4}} \|u_{t}\|_{L^{2}(0,T;L^{2})}^{2}) \\ &+ \frac{C_{8}\delta t}{\varepsilon^{4}} \sum_{n=0}^{k} (\|\tilde{e}_{N}^{n+1}\|^{2} + \|\tilde{e}_{N}^{n}\|_{0}^{2} + \|\hat{e}_{N}^{n+1}\|_{0}^{2}) \\ &+ \varepsilon^{4} N^{-2m} \|u_{t}\|_{L^{2}(0,T;H^{m})}^{2} + \frac{C_{9}\delta t^{2}}{\varepsilon^{4}} N^{-2m} \|u_{t}\|_{L^{2}(0,T;H^{m})}^{2}. \end{split}$$

Applying the discrete Gronwall lemma to the above inequality, we can then conclude by using the triangular inequality, (2.24) and (4.3).

3.2.2. Second-order implicit scheme. The spectral-Galerkin method for the second-order implicit scheme (3.10) reads: Given  $u_N^0 = \prod_N^1 u_0$ , for  $n \ge 0$  find  $u_N^{n+1}, w_N^{n+1} \in Y_N$  such that

$$\frac{1}{\delta t}(u_N^{n+1} - u_N^n, q_N) + (\nabla w_N^{n+1}, \nabla q_N) = 0, \forall q_N \in Y_N 
(\frac{\nabla u_N^{n+1} + \nabla u_N^n}{2}, \nabla \psi_N) + (\tilde{f}(u_N^n, u_N^{n+1}), \psi_N) = (w_N^{n+1}, \psi_N), \forall \psi_N \in Y_N.$$
(3.17)

**Theorem 3.2.** Given T > 0, we assume that, for some  $m \ge 1$ ,  $u, w \in C(0, T; H^m(\Omega))$ ,  $u_t \in L^2(0, T; H^m(\Omega)) \cap L^2(0, T; L^4(\Omega))$ ,  $u_{tt} \in L^2(0, T; H^2(\Omega))$  and  $u_{ttt} \in L^2(0, T; L^2(\Omega))$ . Then the solution of (3.17) satisfies

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$$E(u_N^{n+1}) \le E(u_N^n),$$

and the following error estimate holds

$$\|u(t^{k}) - u_{N}^{k}\|_{0} + \left(\delta t \sum_{n=0}^{k} \|w(t^{n+\frac{1}{2}}) - \frac{1}{2}(w_{N}^{n+1} + w_{N}^{n})\|_{0}^{2}\right)^{\frac{1}{2}} \le C(\varepsilon, T)(K_{7}(u, \varepsilon)\delta t^{2} + K_{8}(u, \varepsilon)N^{-m}), \quad \forall 0 \le k \le \frac{T}{\delta t},$$

where

$$C(\varepsilon, T) \sim \exp(T/\varepsilon^{4});$$
  

$$K_{7}(u, \varepsilon)$$
  

$$= \varepsilon^{2} \|u_{ttt}\|_{L^{2}(0,T;L^{2})} + \|u_{tt}\|_{L^{2}(0,T;H^{2})} + \frac{1}{\varepsilon^{2}} (\|u_{tt}\|_{L^{2}(0,T;L^{2})} + \|u_{t}\|_{L^{2}(0,T;L^{4})});$$
  

$$K_{8}(u, \varepsilon) = \|u_{0}\|_{m} + \varepsilon^{2} \|u_{t}\|_{L^{2}(0,T;H^{m})} + \frac{1}{\varepsilon^{2}} \|u\|_{C(0,T;H^{m})} + \|w\|_{C(0,T;H^{m})}.$$

*Proof.* The proof of Lemma 3.3 is obviously valid for the full discrete case. For the error estimates, we denote, in addition to (3.13),

$$\bar{e}_N^{n+1/2} = \Pi_N^1 w(t^{n+1/2}) - w_N^{n+1}, \quad \check{e}_N^{n+1/2} = \Pi_N^1 w(t^{n+1/2}) - \Pi_N^1 w(t^{n+1/2}).$$

Subtracting (3.17) from (3.1) at  $t^{n+1/2}$ , we find

$$\left(\frac{\tilde{e}_{N}^{n+1} - \tilde{e}_{N}^{n}}{\delta t}, q_{N}\right) + \left(\nabla \bar{e}_{N}^{n+1/2}, \nabla q_{N}\right) \\
= \frac{1}{\delta t} \left(\left(\Pi_{N}^{1} - I\right)\left(u(t^{n+1}) - u(t^{n}), q_{N}\right) + \left(R_{1}^{n+1/2}, q_{N}\right), \quad \forall q_{N} \in Y_{N}; \\
\left(\nabla \tilde{e}_{N}^{n+1/2}, \nabla \psi_{N}\right) + \frac{1}{\varepsilon^{2}} \left(f(u(t^{n+1/2})) - \tilde{f}(u_{N}^{n}, u_{N}^{n+1}), \psi_{N}\right) \\
= \left(\check{e}_{N}^{n+1/2} + \bar{e}_{N}^{n+1/2}, \psi_{N}\right) + \left(R_{2}^{n+1/2}, \psi_{N}\right), \quad \forall \psi_{N} \in Y_{N}.$$
(3.18)

Taking  $q_N = 2\delta t \tilde{e}_N^{n+1/2}$  and  $\psi_N = -2\delta t \bar{e}_N^{n+1/2}$  and summing up the two identities, we derive

$$\begin{split} \|\tilde{e}_{N}^{n+1}\|_{0}^{2} &- \|\tilde{e}_{N}^{n}\|_{0}^{2} + 2\delta t \|\bar{e}_{N}^{n+1/2}\|_{0}^{2} \\ &= 2((\Pi_{N}^{1} - I)(u(t^{n+1}) - u(t^{n})), \tilde{e}_{N}^{n+1/2}) \\ &+ 2\delta t(R_{1}^{n+1/2}, \tilde{e}_{N}^{n+1/2}) \\ &+ \frac{2\delta t}{\varepsilon^{2}}(f(u(t^{n+1/2})) - \tilde{f}(u_{N}^{n}, u_{N}^{n+1}), \bar{e}_{N}^{n+1/2}) \\ &- 2\delta t(\check{e}_{N}^{n+1/2}, \bar{e}_{N}^{n+1/2}) \\ &- 2\delta t(R_{2}^{n+1/2}, \bar{e}_{N}^{n+1/2}) := \mathbf{I} + \mathbf{II} + \mathbf{III} + \mathbf{IV} + \mathbf{V}. \end{split}$$
(3.19)

Similarly as in the proof of Theorem 2.2, by using the Cauchy-Schwarz inequality, (2.42), (2.43) and (2.46), we derive

$$\mathbf{I} \leq \frac{\delta t}{\varepsilon^{4}} \| \tilde{e}_{N}^{n+1/2} \|_{0}^{2} + \varepsilon^{4} \int_{t^{n}}^{t^{n+1}} \| (\Pi_{N}^{1} - I) u_{t}(t) \|_{0}^{2} dt;$$

$$\mathbf{II} \leq \frac{\delta t}{\varepsilon^{4}} \| \tilde{e}_{N}^{n+1/2} \|_{0}^{2} + \delta t^{4} \varepsilon^{4} \int_{t^{n}}^{t^{n+1}} \| u_{ttt}(t) \|_{0}^{2} dt;$$

$$\mathbf{III} \leq \frac{\delta t}{4} \| \tilde{e}_{N}^{n+1/2} \|_{0}^{2} + \frac{4\delta t}{\varepsilon^{4}} \| f(u(t^{n+1/2})) - \tilde{f}(u_{N}^{n}, u_{N}^{n+1}) \|_{0}^{2}$$

$$\leq \frac{\delta t}{4} \| \tilde{e}_{N}^{n+1/2} \|_{0}^{2} + \frac{C_{10} \delta t}{\varepsilon^{4}} (\| \tilde{e}_{N}^{n+1} \|_{0}^{2} + \| \tilde{e}_{N}^{n} \|_{0}^{2} + \| \hat{e}_{N}^{n+1} \|_{0}^{2} + \| \hat{e}_{N}^{n} \|_{0}^{2}) \qquad (3.20)$$

$$+ \frac{C_{11} \delta t^{4}}{\varepsilon^{4}} \int_{t^{n}}^{t^{n+1}} (\| u_{tt}(t) \|_{0}^{2} + \| u_{t}^{2}(t) \|_{0}^{2}) dt;$$

$$\mathbf{IV} \leq \frac{\delta t}{4} \| \tilde{e}_{N}^{n+1/2} \|_{0}^{2} + 4\delta t \| \check{e}_{N}^{n+1/2} \|_{0}^{2};$$

$$\mathbf{V} \leq \frac{\delta t}{4} \| \tilde{e}_{N}^{n+1/2} \|_{0}^{2} + 4\delta t^{4} \int_{t^{n}}^{t^{n+1}} \| u_{tt}(t) \|_{2}^{2} dt.$$

Combing the above inequalities into (3.19), we derive

$$\begin{split} \|\tilde{e}_{N}^{n+1}\|_{0}^{2} - \|\tilde{e}_{N}^{n}\|_{0}^{2} + \delta t \|\tilde{e}_{N}^{n+1/2}\|_{0}^{2} &\leq 4\delta t \|\check{e}_{N}^{n+1/2}\|_{0}^{2} + \delta t^{4}\varepsilon^{4} \int_{t^{n}}^{t^{n+1}} \|u_{ttt}(t)\|_{0}^{2} \\ &+ \frac{C_{12}\delta t}{\varepsilon^{4}} (\|\tilde{e}_{N}^{n+1}\|_{0}^{2} + \|\tilde{e}_{N}^{n}\|_{0}^{2} + \|\hat{e}_{N}^{n+1}\|_{0}^{2} + \|\hat{e}_{N}^{n}\|_{0}^{2}) \\ &+ \varepsilon^{4} \int_{t^{n}}^{t^{n+1}} \|(\Pi_{N}^{1} - I)u_{t}(t)\|_{0}^{2} dt \\ &+ \frac{C_{11}\delta t^{4}}{\varepsilon^{4}} \int_{t^{n}}^{t^{n+1}} (\|u_{tt}(t)\|_{0}^{2} + \|u_{t}^{2}(t)\|_{0}^{2}) dt \\ &+ 4\delta t^{4} \int_{t^{n}}^{t^{n+1}} \|u_{tt}(t)\|_{2}^{2} dt. \end{split}$$
(3.21)

Summing up the above inequality for  $n = 0, 1, \dots, k$   $(k \leq \frac{T}{\delta t} - 1)$ , and using (4.3), we arrive at

$$\begin{split} \|\tilde{e}_{N}^{n+1}\|_{0}^{2} &- \|\tilde{e}_{N}^{0}\|_{0}^{2} + \delta t \sum_{n=0}^{k} \|\bar{e}_{N}^{n+1/2}\|_{0}^{2} \leq \frac{C_{12}\delta t}{\varepsilon^{4}} \sum_{n=0}^{k} (\|\tilde{e}_{N}^{n+1}\|_{0}^{2} + \|\tilde{e}_{N}^{n}\|_{0}^{2}) \\ &+ \frac{\delta t^{4}}{\varepsilon^{4}} (\|u_{tt}\|_{L^{2}(0,T;L^{2})}^{2} + \|u_{t}\|_{L^{2}(0,T;L^{4})}^{2}) + \delta t^{4} \|u_{tt}\|_{L^{2}(0,T;H^{2})}^{2} + \delta t^{4} \varepsilon^{4} \|u_{ttt}\|_{L^{2}(0,T;L^{2})}^{2} \\ &+ N^{-2m} (\|w\|_{C(0,T;H^{m})}^{2} + \frac{1}{\varepsilon^{4}} \|u\|_{C(0,T;H^{m})}^{2} + \varepsilon^{4} \|u_{t}\|_{L^{2}(0,T;H^{m})}^{2}). \end{split}$$

We can then conclude by applying the discrete Gronwall lemma to the above inequality, and by using the triangular inequality and (2.25).

#### 4. Miscellaneous remarks.

4.1. **Generalizations.** The stability results in Sections 2 and 3 are obtained for (semi-discretized) time discretization schemes. Since all the stability results are proved from a weak formulation, it is obvious that these results are also valid for any spatial discretization whose weak formulation is simply the restriction of the continuous-in-space weak formulation onto a finite dimensional subspace, including in particular Galerkin finite-element methods and spectral-Galerkin methods.

Similarly, while we only considered error estimates with a spectral-Galerkin approximation, it is clear that these error estimates can also be directly extended to Galerkin finite-element methods, except that the spatial convergence order m in the error estimates will be fixed to be the order of the finite element approximation.

Often times, it is computationally more efficient to use, instead of  $Y_N$ , the space (cf. [20])

$$Y_N^0 = \{ u \in Y_N : \frac{\partial u}{\partial n} |_{\partial \Omega} = 0 \}.$$
(4.1)

With this approximation space, we can construct special basis functions in  $Y_N^0$  such that the stiffness and mass matrices are very sparse and can be efficiently solved by using a matrix diagonalization method, we refer to [20] for more detail on this matter.

Introducing the corresponding projection operator  $\hat{\Pi}_N^1 : Y^2(\Omega) := \{ u \in H^2(\Omega) : \frac{\partial u}{\partial n} |_{\partial \Omega} = 0 \} \to Y_N^0$  defined by

$$(\nabla(\widehat{\Pi}_N^1 v - v), \nabla\psi) = 0, \forall \psi \in Y_N^0, \tag{4.2}$$

it is an easy matter to show that

$$\begin{aligned} \|u - \hat{\Pi}_N^1 u\|_k &\lesssim N^{k-m} \|u\|_m, \quad k = 0, 1, 2; \\ \forall u \in Y^m(\Omega) := \{ v \in H^m(\Omega) : \frac{\partial v}{\partial n}|_{\partial\Omega} = 0 \}, \quad m \ge 2. \end{aligned}$$

Then, if we replace the approximation space  $Y_N$  by  $Y_N^0$  in Sections 2 and 3, all the error estimates are still valid for  $m \ge 2$ .

4.2. Effect of spatial accuracy. It has been observed that for interface problems governed by Allen-Cahn or Cahn-Hilliard type equation, spectral methods usually provide much more accurate results using fewer points than lower order methods like finite elements or finite differences. We now give a heuristic argument based on our error estimates.

To fix the idea, let us consider the Allen-Cahn equation (1.1) and its error estimate in (2.31). It is well-known that the solution of the Allen-Cahn equation will develop an interface with thickness of order  $\varepsilon$ . Therefore, it is reasonable to assume that  $\partial_x^m u \sim \varepsilon^{-m}, \forall m \ge 0$ . Hence, the error estimate (2.31) indicates that

$$|u(t^n) - u_N^n||_0 \lesssim C(\varepsilon, T)(K_1(u, \varepsilon)\delta t + N^{-m}\varepsilon^{-1-m}).$$

Since the solution is usually smooth around the interfacial area, it can be expected that the above estimate is valid for all m. Let us ignore for the moment  $C(\varepsilon, T)$ (see Remark 2.3). Then, as soon as  $N > O(\varepsilon^{-1})$ , it can be expected that the error due to the spatial discretization will decay very fast, in fact faster than any algebraic order, as N increases. In practice, it has been found that having 5 - 8points inside the trasitional region is sufficient to represent the interface accurately. On the other hand, for a lower order method, the corresponding error estimate is similar to (2.31) with N replaced by  $h^{-1}$ , but only with a fixed m, e.g., m = 2 for piece-wise linear finite elements or second-order finite differences. Hence, for m = 2, one needs to have  $h \ll \varepsilon^{3/2}$  for the scheme to be convergent, and  $h \sim \varepsilon^3$  for the spatial error to be of order O(h). Therefore, an adaptive procedure is almost necessary for low-order methods to have a desirable accuracy with reasonable cost.

It is clear that similar arguments can be applied to other schemes for the Allen-Cahn and Cahn-Hilliard equations. In fact, the situation is even worse for Cahn-Hilliard equation.

4.3. Numerical tests. In this section, we compare the accuracy of various schemes for a classical benchmark problem (cf. [7]) we describe below.

At the initial state, there is a circular interface boundary with a radius of  $R_0 = 100$  in the rectangular domain of  $(0, 256) \times (0, 256)$ . Such a circular interface is unstable and the driving force will shrink and eventually disappear. It is shown, as the ratio between the radius of the circle and the interfacial thickness goes to infinity, the velocity of the moving interface V approaches to

$$V = \frac{dR}{dt} - \frac{1}{R},\tag{4.4}$$

where R is the radius of the circle at a given time t. After taking the integration, we obtain

$$R = \sqrt{R_0^2 - 2t}.$$
 (4.5)

After mapping the domain to  $(-1, 1) \times (-1, 1)$ , we obtain the following Allen-Cahn equation

$$\phi_t = \gamma(\Delta \phi - \frac{f(\phi)}{\varepsilon^2}), \tag{4.6}$$

with  $\gamma = 6.10351 \times 10^{-5}$  and  $\varepsilon = 0.0078$ . We solved this equation using the secondorder semi-implicit scheme (2.11) with S = 1 and the implicit scheme (2.20). The spectral approximation space  $Y_N^0$  is used. For the scheme (2.11), we only have to solve a Poisson-type equation at each time step so it is computationally very efficient since the Poisson-type equation can be solved efficiently (cf. [20]). For the scheme (2.20), a Newton iteration is required to deal with the nonlinear system at each time step. At each Newton iteration, we need to solve a non-constant coefficient elliptic equation which we solve by a preconditioner CG iteration with a constant-coefficient Poisson-type equation as a preconditioner. In the computations presented below, only 2-4 Newton's iterations are needed and each Newton's iteration requires a few PCG iterations. So the cost of one step for the scheme (2.20) is usually more than 10 times of the cost for one step of (2.11).

In all computations, we used  $513 \times 513$  points to ensure that the error is dominated by time discretization errors. In Figure 4.1, we plot the evolution of the radius obtained by the second-order implicit scheme (I2), stabilized first-order and secondorder semi-implicit schemes (SSI1 and SSI2) with the stabilization constant S = 1. Four different time step sizes  $\delta t = 0.1, 0.01, 0.005, 0.001$  are used. We observe that all three schemes perform quite well for this problem. The scheme SSI1 has the largest error while the schemes SSI2 and I2 have similar accuracy. Note that the scheme I2 is an order of magnitude more expensive than the scheme SSI2.

4.4. **Concluding remarks.** We presented in this paper stability analyses and error estimates for a number of commonly used numerical schemes for the Allen-Cahn and Cahn-Hilliard equations.



FIGURE 4.1. Comparison between the second-order implicit scheme (I2), stabilized second-order semi-implicit scheme (SSI2) and stabilized first-order semi-implicit scheme (SSI1).

We showed that the semi-implicit schemes without stabilization are energy stable under reasonable conditions; we also shown that, at least in the first-order case, the stabilized version is unconditionally energy stable. Since the stabilized schemes only requires solving a constant-coefficient second-order (resp. fourth-order) equation for the Allen-Cahn (resp. Cahn-Hilliard) problem, they are computationally very efficient. On the other hand, the implicit schemes are obviously unconditionally stable but requires solving a nonlinear system at each time step.

We also carried out an error analysis for selected schemes with a spectral-Galerkin approximation, as an example. The error estimates reveal that high-order methods, such as spectral methods, are preferable for interface problems governed by Allen-Cahn and Cahn-Hilliard equations, and that an adaptive procedure is probably necessary for low order methods to achieve desired accuracy with reasonable cost.

The stability results and error estimates derived in this paper are based on a weak formulation so they can be applied to other spatial discretizations, such as Galerkin finite element methods, which are based on a weak formulation.

#### REFERENCES

- S. M. Allen and J. W. Cahn, A microscopic theory for antiphase boundary motion and its application to antiphase domain coarsening, Acta Metall. Mater., 27 (1979), 1085–1095.
- [2] D. M. Anderson, G. B. McFadden and A. A. Wheeler, *Diffuse-interface methods in fluid mechanics*, Annual Review Of Fluid Mechanics, **30**, 139–165, Annu. Rev. Fluid Mech., 30, Annual Reviews, Palo Alto, CA, (1998).

- [3] Luis A. Caffarelli and Nora E. Muler, An L<sup>∞</sup> bound for solutions of the Cahn-Hilliard equation, Arch. Rational Mech. Anal., 133 (1995), 129–144.
- [4] J. W. Cahn and J. E. Hilliard, Free energy of a nonuniform system. I. Interfacial free energy, J. Chem. Phys., 28 (1958), 258–267.
- [5] C. Canuto, M. Y. Hussaini, A. Quarteroni and T. A. Zang, "Spectral Methods," Fundamentals in single domains. Scientific Computation, Springer-Verlag, Berlin, 2006.
- [6] L. Q. Chen, *Phase-field models for microstructure evolution*, Annual Review of Material Research, **32** (2002), 113.
- [7] L. Q. Chen and J. Shen, Applications of semi-implicit Fourier-spectral method to phase-field equations, Comput. Phys. Comm., 108 (1998), 147–158.
- [8] N. Condette, C. Melcher and E. Süli, Spectral approximation of pattern-forming nonlinear evolution equations with double-well potentials of quadratic growth, to appear in Math. Comp..
- [9] Q. Du, C. Liu and X. Wang, Simulating the deformation of vesicle membranes under elastic bending energy in three dimensions, J. Comput. Phys., 212 (2006), 757–777.
- [10] Qiang Du and R. A. Nicolaides, Numerical analysis of a continuum model of phase transition, SIAM J. Numer. Anal., 28 (1991), 1310–1322.
- [11] David J. Eyre, Unconditionally gradient stable time marching the Cahn-Hilliard equation, In "Computational and Mathematical Models of Microstructural Evolution" (San Francisco, CA, 1998), 39–46, Mater. Res. Soc. Sympos. Proc., 529, MRS, Warrendale, PA, 1998.
- [12] Xiaobing Feng and Andreas Prohl, Numerical analysis of the Allen-Cahn equation and approximation for mean curvature flows, Numer. Math., 94 (2003), 33–65.
- [13] Xiaobing Feng and Andreas Prohl, Error analysis of a mixed finite element method for the Cahn-Hilliard equation, Numer. Math., 99 (2004), 47–84.
- [14] Z. Hu, S. M. Wise, C. Wang and J. S. Lowengrub, Stable and efficient finite-difference nonlinear-multigrid schemes for the phase field crystal equation, J. Comput. Phys., 228 (2009), 5323–5339.
- [15] Daniel Kessler, Ricardo H. Nochetto and Alfred Schmidt, A posteriori error control for the Allen-Cahn problem: circumventing Gronwall's inequality, M2AN Math. Model. Numer. Anal., 38 (2004), 129–142.
- [16] D. Khismatullin, Y. Renardy and M. Renardy, Development and implementation of vof-prost for 3d viscoelastic liquid-liquid simulations, J. Non-Newt. Fluid Mech., 140 (1992), 120–131.
- [17] C. Liu and J. Shen, A phase field model for the mixture of two incompressible fluids and its approximation by a Fourier-spectral method, Physica D, **179** (2003), 211–228.
- [18] C. Liu, J. Shen and X. Yang, Dynamics of defect motion in nematic liquid crystal flow: Modeling and numerical simulation, Comm. Comput. Phys. 2 (2007), 1184–1198.
- [19] J. Lowengrub and L. Truskinovsky, Quasi-incompressible cahn-hilliard fluids and topological transitions, R. Soc. Lond. Proc. Ser. A Math. Phys. Eng. Sci., 454 (1998), 2617–2654.
- [20] J. Shen, Efficient spectral-Galerkin method I. direct solvers for second- and fourth-order equations by using Legendre polynomials, SIAM J. Sci. Comput., 15 (1994), 1489–1505.
- [21] Jie Shen, On error estimates of the projection methods for the Navier-Stokes equations: First-order schemes, SIAM J. Numer. Anal., 29 (1992), 57–77.
- [22] S. M. Wise, C. Wang and J. S. Lowengrub, An energy-stable and convergent finite-difference scheme for the phase field crystal equation, SIAM J. Numer. Anal., 47 (2009), 2269–2288.
- [23] Chuanju Xu and Tao Tang, Stability analysis of large time-stepping methods for epitaxial growth models, SIAM J. Numer. Anal., 44 (2006), 1759–1779.
- [24] X. Yang, Error analysis of stabilized semi-implicit method of Allen-Cahn equation, Disc. Conti. Dyn. Sys.-B, 11 (2009), 1057–1070.
- [25] X. Yang, J. J. Feng, C. Liu and J. Shen, Numerical simulations of jet pinching-off and drop formation using an energetic variational phase-field method, J. Comput. Phys., 218 (2006), 417–428.
- [26] Xingde Ye, The Legendre collocation method for the Cahn-Hilliard equation, J. Comput. Appl. Math., 150 (2003), 87–108.
- [27] P. Yue, J. J. Feng, C. Liu and J. Shen, A diffuse-interface method for simulating two-phase flows of complex fluids, J. Fluid Mech., **515** (2004), 293–317.
- [28] J. Zhang and Q. Du, Numerical studies of discrete approximations to the Allen-Cahn equation in the sharp interface limit, to appear in SIAM J. Scient. Comput..

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