

ENERGY STABLE SECOND ORDER LINEAR SCHEMES FOR THE ALLEN-CAHN PHASE-FIELD EQUATION*

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Abstract. Phase-field model is a powerful mathematical tool to study the dynamics of interface and morphology changes in fluid mechanics and material sciences. However, numerically solving a phase field model for a real problem is a challenging task due to the non-convexity of the bulk energy and the small interface thickness parameter in the equation. In this paper, we propose two stabilized second order semi-implicit linear schemes for the Allen-Cahn phase-field equation based on backward differentiation formula and Crank-Nicolson method, respectively. In both schemes, the nonlinear bulk force is treated explicitly with two second-order stabilization terms, which make the schemes unconditionally energy stable and numerically efficient. By using a known result of the spectrum estimate of the linearized Allen-Cahn operator and some regularity estimates of the exact solution, we obtain an optimal second order convergence in time with a prefactor depending on the inverse of the characteristic interface thickness only in some lower polynomial order. Both 2-dimensional and 3-dimensional numerical results are presented to verify the accuracy and efficiency of proposed schemes.

Keywords. Allen-Cahn equation; energy stable; stabilized semi-implicit scheme; second order scheme; error estimate.

AMS subject classifications. 65M12; 65M15; 65P40.

1. Introduction

In this paper, we consider numerical approximation for the Allen-Cahn equation with Neumann boundary condition

$$\phi_t = \gamma \left(\varepsilon \Delta \phi - \frac{1}{\varepsilon} f(\phi) \right), \quad (x, t) \in \Omega \times (0, T], \quad (1.1)$$

$$\partial_n \phi = 0, \quad (x, t) \in \partial \Omega \times (0, T]. \quad (1.2)$$

Here $\Omega \in R^d, d=2,3$ is a bounded domain with a locally Lipschitz boundary, n is the outward normal, T is a given time, $\phi(x, t)$ is the phase-field variable. $f(\phi)$, the bulk force, is the derivative of a given energy function $F(\phi)$, which is usually non-convex with two or more than two local minima. One commonly used energy function for two-phase problem is the double-well potential $F(\phi) = \frac{1}{4}(\phi^2 - 1)^2$. ε is the thickness of the interface between two phases. γ , called mobility, is related to the characteristic relaxation time of the system. The homogeneous Neumann boundary condition implies that no mass loss occurs across the boundary walls. The Equation (1.1) is introduced by Allen and Cahn [1] to describe the process of phase separation in multi-component alloy systems. It can be regarded as the L^2 gradient flow with respect to the Ginzburg-Landau energy functional

$$E_\varepsilon(\phi) := \int_\Omega \left(\frac{\varepsilon}{2} |\nabla \phi|^2 + \frac{1}{\varepsilon} F(\phi) \right) dx. \quad (1.3)$$

The corresponding energy dissipation is given as

$$\frac{d}{dt} E_\varepsilon(\phi) = -\frac{1}{\gamma} \int_\Omega \|\phi_t\|^2 dx \leq 0. \quad (1.4)$$

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Another popular phase field model is the Cahn-Hilliard equation, which is the H^{-1} gradient flow with respect to the Ginzburg-Landau energy functional. It was originally introduced by Cahn and Hilliard [4] to describe the phase separation and coarsening phenomena in non-uniform systems such as alloys, glasses and polymer mixtures.

The Allen-Cahn equation and the Cahn-Hilliard equation are widely used in modeling many interface problems due to their good mathematical properties (cf. e.g. [7, 14–16, 44, 53]). However, the small parameter ε and the non-convexity of energy function F make the numerical approximation of a phase field equation a challenging task, especially the design of time marching schemes. It is well-known that if a fully explicit or implicit time marching scheme is used, a tiny time step-size is required for the semi-discretized scheme to be stable or uniquely solvable since the nonlinear function F is neither convex nor concave. A very popular approach to obtain unconditionally stable time marching schemes is the so-called convex splitting method which appears to be introduced by Elliott and Stuart [17], and popularized by Eyre [18], in which, the convex part of $F(\phi)$ is treated implicitly and the concave part of $F(\phi)$ is treated explicitly. This method has been applied to various gradient flows (see e.g. [2, 19, 21, 22, 40]). Traditional convex splitting schemes are first order accurate. Recently, several extensions to second order schemes were proposed based on either the Crank-Nicolson scheme (see e.g. [2, 6, 8, 12, 29, 36]), or second order backward differentiation formula (BDF2) [35, 47]. In all convex splitting schemes, no matter first order or second order, one usually obtains a uniquely solvable nonlinear convex problem at each time step.

There are another types of second order unconditionally stable schemes for the phase field equations. In [13], Du and Nicolaides proposed a secant-line method which is energy stable and second order accurate. It is used and extended in several other works, e.g. [2, 3, 9, 20, 25, 26, 54]. Similar to the convex splitting method, the secant-line method leads to nonlinear semi-discretized system, which need special efforts to solve. Recently, an augmented Lagrange multiplier (ALM) method was proposed in [27, 28] to get second order linear energy stable schemes. The idea is generalized as invariant energy quadratization (IEQ) by Yang et al. and successfully applied to handle several very complicated nonlinear phase-field models (see e.g. [30, 49–51]). Based on similar methodology, a new variant called scalar auxiliary variable (SAV) method is developed by Shen et al. [38, 39]. In the ALM and IEQ approach, nonlinear semi-discretized systems are avoided, but one has to solve variable-coefficient systems, while in the SAV scheme, one only needs to solve some linear systems with constant coefficients. Different to other methods, the energy in ALM, IEQ and SAV approaches is a modified one which also depends on the auxiliary variable.

In this study, we focus on numerical methods that are based on semi-implicit discretization and stabilization skill. To improve the numerical stability of solving phase-field equations, semi-implicit schemes were proposed by Chen and Shen [5] and Zhu et al. [55]. Although not unconditionally stable, semi-implicit schemes allow much larger time step-sizes than explicit schemes. To further improve the stability, Xu and Tang proposed stabilized semi-implicit methods for epitaxial growth model in [45]. The proposed schemes have extraordinary numerical stability even though the mathematical proof of the stability is not complete. Similar schemes were developed for phase field equation by He et al. [31] and Shen and Yang [40], where the latter one adopted a mixed form for the Cahn-Hilliard equation, by using a truncated double-well potential such that the assumption $\|f'(\phi)\|_\infty \leq L$ is satisfied, the unconditional energy stability was proved for the first order stabilized scheme. It is worth to mention that with no truncation made to $f(\phi)$, Li et al. [33, 34] proved that the energy stable property can

be obtained as well, but a much larger stability constant needs to be used.

In this paper, we develop two second-order unconditionally energy stable linear schemes for the Allen-Cahn equation based on the schemes proposed in [45] and [40]. The energy dissipation is guaranteed by including two second order stabilization terms, the first one is directly from [45], the other one is inspired by the work [44]. We also carry out an optimal error estimate for the time semi-discretized schemes. For the phase field equations, the error bounds will depend on the factor of $1/\varepsilon$ exponentially if one uses a standard procedure. By using a spectrum estimate result of de Mottoni and Schatzman [10, 11] and Chen [7] for the linearized Allen-Cahn operator, we are able to get an optimal error estimate with a prefactor depending on $1/\varepsilon$ only in some lower polynomial order for small ε . This spectrum estimate argument was first used by Feng and Prohl [23, 24] for an implicit first order scheme for phase field equations. It was also applied by Kessler et al. [32] to derive a posteriori error estimate for adaptive time marching. Similar analysis for a first-order stabilized semi-implicit scheme of the Allen-Cahn equation was given by Yang [48]. Recently, Feng and Li [21], Feng et al. [22] extended this spectrum estimate argument to first order convex splitting scheme coupled with interior penalty discontinuous Galerkin spatial discretization for Allen-Cahn and Cahn-Hilliard equation, respectively. To the best of our knowledge, our analysis is the first such result for second order linear schemes. In summary, the proposed methods have several merits: 1) They are second order accurate; 2) They lead to linear systems with constant coefficients after time discretization; 3) The stability and error analysis is based on weak formulations, so both finite element method and spectral method can be used for spatial discretization to satisfy discretized energy dissipation law. 4) The methods can be easily used in more complicated systems. Note that, similar approach can be extended to the Cahn-Hilliard equation [42, 43], where Lipschitz condition of f is assumed based on physical intuition and the analyses are more tedious.

The remaining part of the paper is organized as follows. In Section 2, we present the two second-order stabilized schemes for the Allen-Cahn equation and prove they are energy stable. The error estimate to derive a convergence rate that does not depend on $1/\varepsilon$ exponentially is then constructed in Section 3. Detailed implementation and numerical experiments for problems in both 2-dimensional and 3-dimensional tensor-product domain are presented in Section 4 to verify our theoretical results. We end the paper with some conclusions in Section 5.

2. The two second order stabilized linear schemes

We first introduce some notations which will be used throughout the paper. We use $\|\cdot\|_{m,p}$ to denote the standard norm of the Sobolev space $W^{m,p}(\Omega)$. In particular, we use $\|\cdot\|_{L^p}$ to denote the norm of $W^{0,p}(\Omega) = L^p(\Omega)$; $\|\cdot\|_m$ to denote the norm of $W^{m,2}(\Omega) = H^m(\Omega)$; and $\|\cdot\|$ to denote the norm of $W^{0,2}(\Omega) = L^2(\Omega)$. Let (\cdot, \cdot) represent the L^2 inner product. For $p \geq 0$, we define $H_0^p(\Omega) := \{u \in H^p(\Omega) | (u, 1) = 0\}$, and denote $L_0^2(\Omega) := H_0^0(\Omega)$.

For any given function $\phi(t)$ of t , we use ϕ^n to denote an approximation of $\phi(n\tau)$, where τ is the step-size. We will frequently use the shorthand notations: $\delta_t \phi^{n+1} := \phi^{n+1} - \phi^n$, $\delta_{tt} \phi^{n+1} := \phi^{n+1} - 2\phi^n + \phi^{n-1}$, $D_\tau \phi^{n+1} := \frac{3\phi^{n+1} - 4\phi^n + \phi^{n-1}}{2\tau} = \frac{1}{\tau} \delta_t \phi^{n+1} + \frac{1}{2\tau} \delta_{tt} \phi^{n+1}$, $\hat{\phi}^{n+\frac{1}{2}} := \frac{3}{2} \phi^n - \frac{1}{2} \phi^{n-1}$ and $\hat{\phi}^{n+1} := 2\phi^n - \phi^{n-1}$. Following identities will be used frequently as well

$$\begin{aligned}
 2(h^{n+1} - h^n, h^{n+1}) &= \|h^{n+1}\|^2 - \|h^n\|^2 + \|h^{n+1} - h^n\|^2, \\
 (D_\tau h^{n+1}, h^{n+1}) &= \frac{1}{4\tau} (\|h^{n+1}\|^2 - \|h^n\|^2)
 \end{aligned}
 \tag{2.1}$$

$$+ \|2h^{n+1} - h^n\|^2 - \|2h^n - h^{n-1}\|^2 + \|\delta_{tt}h^{n+1}\|^2). \tag{2.2}$$

To prove energy stability of the numerical schemes, we assume that the derivative of f in Equation (1.1) is uniformly bounded, i.e.

$$\max_{\phi \in \mathbf{R}} |f'(\phi)| \leq L, \tag{2.3}$$

where L is a non-negative constant.

REMARK 2.1. Note that the commonly used double-well potential does not satisfy the above assumption. But, thanks to the maximum principle that the Allen-Cahn equation has (cf. e.g. [1, 7, 23, 48]), the solution to Equation (1.1) is bounded by value -1 and 1 if the initial condition is bounded by -1 and 1 . So it is safe to modify the double-well energy $F(\phi)$ for $|\phi|$ larger than 1 to be quadratic growth without affecting the exact solution if the initial condition is bounded by -1 and 1 , such that Assumption (2.3) is satisfied. This argument also applies to the Assumption (3.1) in the next section.

2.1. The stabilized linear BDF2 scheme. Suppose $\phi^0 = \phi_0(\cdot)$ and $\phi^1 \approx \phi(\cdot, \tau)$ are given, our stabilized linear BDF2 scheme (SL-BDF2) calculates $\phi^{n+1}, n = 1, 2, \dots, N = T/\tau - 1$ iteratively, using

$$\frac{3\phi^{n+1} - 4\phi^n + \phi^{n-1}}{2\tau\gamma} = \varepsilon\Delta\phi^{n+1} - \frac{1}{\varepsilon}f(2\phi^n - \phi^{n-1}) - A\tau\delta_t\phi^{n+1} - B\delta_{tt}\phi^{n+1}, \tag{2.4}$$

where A and B are two non-negative constants to stabilize the scheme.

THEOREM 2.1. Assume that (2.3) is satisfied. Under the condition

$$A \geq \frac{L}{2\varepsilon\tau} - \frac{1}{\tau^2\gamma}, \quad B \geq \frac{L}{\varepsilon} - \frac{1}{2\tau\gamma}, \tag{2.5}$$

the following energy dissipation law

$$E_B^{n+1} \leq E_B^n - \frac{\varepsilon}{2}\|\nabla\delta_t\phi^{n+1}\|^2 - \left(\frac{1}{\tau\gamma} + A\tau - \frac{L}{2\varepsilon}\right)\|\delta_t\phi^{n+1}\|^2 - \left(\frac{1}{4\tau\gamma} + \frac{B}{2} - \frac{L}{2\varepsilon}\right)\|\delta_{tt}\phi^{n+1}\|^2, \quad \forall n \geq 1, \tag{2.6}$$

holds for the scheme (2.4), where

$$E_B^{n+1} = E_\varepsilon(\phi^{n+1}) + \left(\frac{1}{4\tau\gamma} + \frac{L}{2\varepsilon} + \frac{B}{2}\right)\|\delta_t\phi^{n+1}\|^2. \tag{2.7}$$

Proof. Pairing (2.4) with $\delta_t\phi^{n+1}$, we get

$$\begin{aligned} \left(\frac{1}{\gamma}D_\tau\phi^{n+1}, \delta_t\phi^{n+1}\right) &= \varepsilon(\Delta\phi^{n+1}, \delta_t\phi^{n+1}) - \frac{1}{\varepsilon}(f(\hat{\phi}^{n+1}), \delta_t\phi^{n+1}) \\ &\quad - A\tau\|\delta_t\phi^{n+1}\|^2 - B(\delta_{tt}\phi^{n+1}, \delta_t\phi^{n+1}). \end{aligned} \tag{2.8}$$

By integration by parts, following identities hold

$$\left(\frac{1}{\gamma}D_\tau\phi^{n+1}, \delta_t\phi^{n+1}\right) = \frac{1}{\tau\gamma}\|\delta_t\phi^{n+1}\|^2 + \frac{1}{4\tau\gamma}(\|\delta_t\phi^{n+1}\|^2 - \|\delta_t\phi^n\|^2 + \|\delta_{tt}\phi^{n+1}\|^2), \tag{2.9}$$

$$\varepsilon(\Delta\phi^{n+1}, \delta_t\phi^{n+1}) = -\frac{\varepsilon}{2}(\|\nabla\phi^{n+1}\|^2 - \|\nabla\phi^n\|^2 + \|\nabla\delta_t\phi^{n+1}\|^2), \tag{2.10}$$

$$-B(\delta_{tt}\phi^{n+1}, \delta_t\phi^{n+1}) = -\frac{B}{2}\|\delta_t\phi^{n+1}\|^2 + \frac{B}{2}\|\delta_t\phi^n\|^2 - \frac{B}{2}\|\delta_{tt}\phi^{n+1}\|^2. \tag{2.11}$$

To handle the term involving f in (2.8), we expand $F(\phi^{n+1})$ and $F(\phi^n)$ at $\hat{\phi}^{n+1}$ as

$$\begin{aligned} F(\phi^{n+1}) &= F(\hat{\phi}^{n+1}) + f(\hat{\phi}^{n+1})(\phi^{n+1} - \hat{\phi}^{n+1}) + \frac{1}{2}f'(\zeta_1^n)(\phi^{n+1} - \hat{\phi}^{n+1})^2, \\ F(\phi^n) &= F(\hat{\phi}^{n+1}) + f(\hat{\phi}^{n+1})(\phi^n - \hat{\phi}^{n+1}) + \frac{1}{2}f'(\zeta_2^n)(\phi^n - \hat{\phi}^{n+1})^2, \end{aligned}$$

where ζ_1^n is a number between ϕ^{n+1} and $\hat{\phi}^{n+1}$, ζ_2^n is a number between ϕ^n and $\hat{\phi}^{n+1}$. Taking the difference of above two equations, using the fact $\phi^{n+1} - \hat{\phi}^{n+1} = \delta_{tt}\phi^{n+1}$ and $\phi^n - \hat{\phi}^{n+1} = -\delta_t\phi^n$, we obtain

$$\begin{aligned} F(\phi^{n+1}) - F(\phi^n) - f(\hat{\phi}^{n+1})\delta_t\phi^{n+1} &= \frac{1}{2}f'(\zeta_1^n)(\delta_{tt}\phi^{n+1})^2 - \frac{1}{2}f'(\zeta_2^n)(\delta_t\phi^n)^2 \\ &\leq \frac{L}{2}|\delta_{tt}\phi^{n+1}|^2 + \frac{L}{2}|\delta_t\phi^n|^2. \end{aligned} \tag{2.12}$$

Taking inner product of the above equation with constant $1/\varepsilon$, then combining the result with (2.8), (2.9), (2.10) and (2.11), we obtain

$$\begin{aligned} &\frac{1}{\varepsilon}(F(\phi^{n+1}) - F(\phi^n), 1) + \frac{\varepsilon}{2}(\|\nabla\phi^{n+1}\|^2 - \|\nabla\phi^n\|^2) \\ &\quad + \frac{1}{4\tau\gamma}(\|\delta_t\phi^{n+1}\|^2 - \|\delta_t\phi^n\|^2) + \left(\frac{L}{2\varepsilon} + \frac{B}{2}\right)(\|\delta_t\phi^{n+1}\|^2 - \|\delta_t\phi^n\|^2) \\ &\leq -\frac{1}{4\tau\gamma}\|\delta_{tt}\phi^{n+1}\|^2 - \frac{1}{\tau\gamma}\|\delta_t\phi^{n+1}\|^2 - \frac{\varepsilon}{2}\|\nabla\delta_t\phi^{n+1}\|^2 - A\tau\|\delta_t\phi^{n+1}\|^2 \\ &\quad + \frac{L}{2\varepsilon}\|\delta_t\phi^{n+1}\|^2 - \frac{B}{2}\|\delta_{tt}\phi^{n+1}\|^2 + \frac{L}{2\varepsilon}\|\delta_{tt}\phi^{n+1}\|^2. \end{aligned} \tag{2.13}$$

Combining the above equation and the inequality $\frac{1}{\tau\gamma} + A\tau \geq \frac{L}{2\varepsilon}$, $\frac{B}{2} + \frac{1}{4\tau\gamma} \geq \frac{L}{2\varepsilon}$, we get energy dissipation law (2.6). \square

REMARK 2.2. From Equation (2.5), we see that the SL-BDF2 scheme is stable with any non-negative A including $A=0$, if

$$\tau \leq \frac{2\varepsilon}{L\gamma}. \tag{2.14}$$

If one takes time step size even smaller,

$$\tau \leq \frac{\varepsilon}{2L\gamma}, \tag{2.15}$$

then the SL-BDF2 scheme is stable with any non-negative A and B , including the case $A=B=0$.

On the other hand, if we take

$$A = \max_{\tau \geq 0} \left\{ \frac{L}{2\varepsilon\tau} - \frac{1}{\tau^2\gamma} \right\} = \frac{\gamma L^2}{16\varepsilon^2}, \quad B = \frac{L}{\varepsilon}, \tag{2.16}$$

then the SL-BDF2 scheme is unconditionally stable for any τ .

2.2. The stabilized linear Crank-Nicolson scheme. Suppose $\phi^0 = \phi_0(\cdot)$ and $\phi^1 \approx \phi(\cdot, \tau)$ are given, our stabilized linear Crank-Nicolson scheme (SL-CN) calculates $\phi^{n+1}, n = 1, 2, \dots, N = T/\tau - 1$ iteratively, using

$$\frac{\phi^{n+1} - \phi^n}{\tau\gamma} = \varepsilon\Delta\left(\frac{\phi^{n+1} + \phi^n}{2}\right) - \frac{1}{\varepsilon}f\left(\frac{3}{2}\phi^n - \frac{1}{2}\phi^{n-1}\right) - A\tau\delta_t\phi^{n+1} - B\delta_{tt}\phi^{n+1}, \quad (2.17)$$

where A and B are two non-negative constants.

THEOREM 2.2. *Assume that (2.3) is satisfied. Under the condition*

$$A \geq \frac{L}{2\varepsilon\tau} - \frac{1}{\tau^2\gamma}; \quad B \geq \frac{L}{2\varepsilon}, \quad (2.18)$$

the following energy law holds

$$E_C^{n+1} \leq E_C^n - \left(\frac{1}{\tau\gamma} + A\tau - \frac{L}{2\varepsilon}\right)\|\delta_t\phi^{n+1}\|^2 - \left(\frac{B}{2} - \frac{L}{4\varepsilon}\right)\|\delta_{tt}\phi^{n+1}\|^2, \quad \forall n \geq 1, \quad (2.19)$$

for the scheme (2.17), where we define

$$E_C^{n+1} = E(\phi^{n+1}) + \left(\frac{L}{4\varepsilon} + \frac{B}{2}\right)\|\delta_t\phi^{n+1}\|^2. \quad (2.20)$$

Proof. Pairing the Equation (2.17) with $\delta_t\phi^{n+1}$, we get

$$\begin{aligned} \frac{1}{\tau\gamma}\|\delta_t\phi^{n+1}\|^2 &= -\frac{\varepsilon}{2}(\|\nabla\phi^{n+1}\|^2 - \|\nabla\phi^n\|^2) - \frac{1}{\varepsilon}\left(f\left(\frac{3}{2}\phi^n - \frac{1}{2}\phi^{n-1}\right), \phi^{n+1} - \phi^n\right) \\ &\quad - A\tau\|\delta_t\phi^{n+1}\|^2 - \frac{B}{2}(\|\delta_t\phi^{n+1}\|^2 - \|\delta_t\phi^n\|^2 + \|\delta_{tt}\phi^{n+1}\|^2). \end{aligned} \quad (2.21)$$

We use Taylor expansion at $\hat{\phi}^{n+\frac{1}{2}} = \frac{3}{2}\phi^n - \frac{1}{2}\phi^{n-1}$,

$$F(\phi^{n+1}) = F(\hat{\phi}^{n+\frac{1}{2}}) + f(\hat{\phi}^{n+\frac{1}{2}})(\phi^{n+1} - \hat{\phi}^{n+\frac{1}{2}}) + \frac{1}{2}f'(\eta_1^n)(\phi^{n+1} - \hat{\phi}^{n+\frac{1}{2}})^2, \quad (2.22)$$

$$F(\phi^n) = F(\hat{\phi}^{n+\frac{1}{2}}) + f(\hat{\phi}^{n+\frac{1}{2}})(\phi^n - \hat{\phi}^{n+\frac{1}{2}}) + \frac{1}{2}f'(\eta_2^n)(\phi^n - \hat{\phi}^{n+\frac{1}{2}})^2. \quad (2.23)$$

Subtracting (2.23) from (2.22), we obtain

$$\begin{aligned} F(\phi^{n+1}) - F(\phi^n) &= f(\hat{\phi}^{n+\frac{1}{2}})(\phi^{n+1} - \phi^n) + \frac{1}{2}f'(\eta_1^n)(\phi^{n+1} - \hat{\phi}^{n+\frac{1}{2}})^2 \\ &\quad - \frac{1}{2}(f'(\eta_1^n) + f'(\eta_2^n) - f'(\eta_1^n))(\phi^n - \hat{\phi}^{n+\frac{1}{2}})^2 \\ &= f\left(\frac{3}{2}\phi^n - \frac{1}{2}\phi^{n-1}\right)(\phi^{n+1} - \phi^n) + \frac{1}{2}f'(\eta_1^n)\delta_t\phi^{n+1}\delta_{tt}\phi^{n+1} \\ &\quad - \frac{1}{8}(f'(\eta_2^n) - f'(\eta_1^n))(\delta_t\phi^n)^2, \end{aligned} \quad (2.24)$$

which gives us

$$\begin{aligned} &\frac{1}{\varepsilon}\left(f\left(\frac{3}{2}\phi^n - \frac{1}{2}\phi^{n-1}\right), \phi^{n+1} - \phi^n\right) \\ &= \frac{1}{\varepsilon}(F(\phi^{n+1}) - F(\phi^n), 1) - \frac{1}{2\varepsilon}(f'(\eta_1^n), \delta_t\phi^{n+1}\delta_{tt}\phi^{n+1}) + \frac{1}{8\varepsilon}(f'(\eta_2^n) - f'(\eta_1^n), (\delta_t\phi^n)^2). \end{aligned} \quad (2.25)$$

Plugging (2.25) into (2.21), we obtain

$$\begin{aligned} & \frac{\varepsilon}{2}(\|\nabla\phi^{n+1}\|^2 - \|\nabla\phi^n\|^2) + \frac{1}{\varepsilon}(F(\phi^{n+1}) - F(\phi^n), 1) + \frac{B}{2}(\|\delta_t\phi^{n+1}\|^2 - \|\delta_t\phi^n\|^2) \\ & \leq -\frac{1}{\tau\gamma}\|\delta_t\phi^{n+1}\|^2 - A\tau\|\delta_t\phi^{n+1}\|^2 + \frac{L}{4\varepsilon}\|\delta_t\phi^{n+1}\|^2 + \frac{L}{4\varepsilon}\|\delta_t\phi^n\|^2 \\ & \quad + \frac{L}{4\varepsilon}\|\delta_{tt}\phi^{n+1}\|^2 - \frac{B}{2}\|\delta_{tt}\phi^{n+1}\|^2. \end{aligned} \tag{2.26}$$

By the definition of E_C^{n+1} and $A\tau + \frac{1}{\tau\gamma} \geq \frac{L}{2\varepsilon}$, $\frac{B}{2} \geq \frac{L}{4\varepsilon}$, we get the desired results. \square

REMARK 2.3. If we take

$$A = \frac{\gamma L^2}{16\varepsilon^2}, \quad B = \frac{L}{2\varepsilon}, \tag{2.27}$$

then the SL-CN scheme is unconditionally stable for any τ .

On the other hand, by using the inequality $\|\delta_{tt}\phi^{n+1}\|^2 \leq 2\|\delta_t\phi^{n+1}\|^2 + 2\|\delta_t\phi^n\|^2$, it is easy to prove that when $A = B = 0$, the SL-CN scheme (2.17) is stable for

$$\tau \leq \frac{2\varepsilon}{3L\gamma}. \tag{2.28}$$

REMARK 2.4. To make SL-BDF2 and SL-CN scheme unconditionally stable, i.e. stable for any time step size $\tau > 0$, we need to take $A \sim O(\gamma/\varepsilon^2)$. It seems that A needs to be very large in a real simulation since physically ε is very small. But actually, it is not necessary. It is proved that the numerical interface for the Allen-Cahn equation converges with the rate $O(\varepsilon^2|\ln\varepsilon|^2)$ if no singularities appear [21, 23], which suggests that we don't need to take ε as small as the width of a physical interface. Furthermore, A has a linear dependence on the value of γ . It was showed by Magaletti et al. [37] and Xu et al. [46] that the phase-field Cahn-Hilliard–Navier-Stokes model for binary fluids has a fast convergence with respect to ε when the phenomenological mobility $\gamma \sim O(\varepsilon^2)$. When coupled with hydrodynamics, what is a proper choice for the mobility γ in the Allen-Cahn model is an interesting question. We leave this to a future study.

REMARK 2.5. Recently, Li, Qiao and Tang [34], Li and Qiao [33] studied several first order and second order stabilized semi-implicit Fourier schemes, respectively, for the Cahn-Hilliard equation with double-well potential

$$F(\phi) = \frac{1}{4}(\phi^2 - 1)^2. \tag{2.29}$$

Without a Lipschitz condition on $F'(\phi)$, they proved that those schemes are unconditionally stable when a very large stability constant A is used. For example, according to Theorem 1.3 in [33], for a classical second order semi-implicit stabilized scheme proposed by Xu and Tang [45] applied to the Cahn-Hilliard equation, the stabilization constant A needs to be as large as $O(|\ln\varepsilon|^2/\varepsilon^8)$ to make the scheme unconditionally stable (Note that the A in [33] corresponds to εB in this paper). However, the constants A, B in this paper are only of order $O(\gamma/\varepsilon^2), O(1/\varepsilon)$, respectively. The reasons are in two aspects. Firstly, the Cahn-Hilliard equation is much harder to solve than the Allen-Cahn equation. For the Allen-Cahn equation, since its solution satisfies a maximum principle, it is reasonable to modify F defined in (2.29) for $|\phi| > 1$, such that the Lipschitz condition

(2.3) is satisfied. Secondly, we use two stabilization terms instead of only one stabilization term, the extra one helps to maintain the stability for larger time step sizes. The approach presented in this paper can be extended to the Cahn-Hilliard equation with quadratic growth energy as well [42, 43].

3. Convergence analysis

In this section, we shall establish the error estimate of the two proposed schemes for the Allen-Cahn equation in the norm of $l^\infty(0, T; L^2) \cap l^2(0, T; H^1)$. We will show that, if the interface is well developed in the initial condition, the error bounds depend on $1/\varepsilon$ only in some lower polynomial order for small ε . Let $\phi(t^n)$ be the exact solution at time $t = t^n$ to the Allen-Cahn Equation (1.1) and ϕ^n be the solution at time $t = t^n$ to the time discrete numerical scheme (2.4) (or (2.17)); we define error function $e^n := \phi^n - \phi(t^n)$. Obviously $e^0 = 0$.

Before presenting the detailed error analysis, we first make some assumptions. For simplicity, we take $\gamma = 1$ in this section, and assume $0 < \varepsilon < 1$. We use notation \lesssim in the way that $f \lesssim g$ means that $f \leq Cg$ with positive constant C independent of τ, ε .

ASSUMPTION 3.1. We make following assumptions on $f: f = F'$, for $F \in C^4(\mathbf{R})$, such that f' and f'' are uniformly bounded, i.e. f satisfies (2.3) and

$$\max_{\phi \in \mathbf{R}} |f''(\phi)| \leq L_2, \tag{3.1}$$

where L_2 is a non-negative constant.

Since the solution of Allen-Cahn equation satisfies maximum principle (see Remark 2.1), one can always modify $f(\phi)$ for large $|\phi|$ such that Assumption 3.1 holds without affecting the exact solution.

ASSUMPTION 3.2.

(i) We assume that there exist non-negative constants σ_1 such that

$$E_\varepsilon(\phi^0) := \frac{\varepsilon}{2} \|\nabla \phi^0\|^2 + \frac{1}{\varepsilon} \|F(\phi^0)\|_{L^1} \lesssim \varepsilon^{-2\sigma_1}, \tag{3.2}$$

$$\|\phi_t^0\|^2 \lesssim \varepsilon^{-2\sigma_1-1}, \tag{3.3}$$

$$\|\nabla \phi_t^0\|^2 \lesssim \varepsilon^{-2\sigma_1-3}, \tag{3.4}$$

$$\|\nabla \phi_{tt}^0\|^2 \lesssim \varepsilon^{-2\sigma_1-7}. \tag{3.5}$$

(ii) Assume that an appropriate scheme is used to calculate the numerical solution at first step, such that

$$E_\varepsilon(\phi^1) \leq E_\varepsilon(\phi^0) \lesssim \varepsilon^{-2\sigma_1}, \tag{3.6}$$

$$\frac{1}{\tau} \|\delta_t \phi^1\|^2 \lesssim \varepsilon^{-2\sigma_1}. \tag{3.7}$$

Then it is easy to get

$$E_C^1 \lesssim \varepsilon^{-2\sigma_1}, \tag{3.8}$$

$$E_B^1 \lesssim \varepsilon^{-2\sigma_1}. \tag{3.9}$$

(iii) There exists a constant $\sigma_0 > 0$,

$$\|e^1\|^2 + \varepsilon \|\nabla e^1\|^2 \lesssim \varepsilon^{-\sigma_0} \tau^4. \tag{3.10}$$

Given Assumptions 3.1 and 3.2 (i), we have following estimates for the exact solution to the Allen-Cahn equation.

LEMMA 3.1. *Let ϕ be the exact solution of (1.1), under the condition of Assumption 3.1 and 3.2 (i), the following regularities hold:*

- (i) $\int_0^\infty \|\phi_t\|^2 dt + E_\varepsilon(\phi) \lesssim \varepsilon^{-2\sigma_1}$;
- (ii) $2\varepsilon \int_0^\infty \|\nabla \phi_t\|^2 dt + \text{ess sup}_{[0,\infty]} \|\phi_t\|^2 \lesssim \varepsilon^{-2\sigma_1-1}$;
- (iii) $\int_0^\infty \|\phi_{tt}\|^2 dt + \text{ess sup}_{[0,\infty]} \varepsilon \|\nabla \phi_t\|^2 \lesssim \varepsilon^{-2\sigma_1-2}$;
- (iv) $\varepsilon \int_0^\infty \|\Delta \phi_{tt}\|^2 dt + \text{ess sup}_{[0,\infty]} \|\nabla \phi_{tt}\|^2 \lesssim \varepsilon^{-4\sigma_1-8}$;
- (v) $\int_0^\infty \|\phi_{ttt}\|^2 dt + \text{ess sup}_{[0,\infty]} \varepsilon \|\nabla \phi_{tt}\|^2 \lesssim \varepsilon^{-4\sigma_1-7}$.

Proof. Taking $\gamma = 1$ in Equation (1.1), we have

$$\phi_t - \varepsilon \Delta \phi = -\frac{1}{\varepsilon} f(\phi). \tag{3.11}$$

- (i) Pairing (3.11) with ϕ_t and taking integration by parts on the second term, we get

$$\|\phi_t\|^2 + \frac{\varepsilon}{2} \frac{d}{dt} \|\nabla \phi\|^2 = -\frac{1}{\varepsilon} (f(\phi), \phi_t) = -\frac{1}{\varepsilon} \frac{d}{dt} \int_\Omega |F(\phi)| dx. \tag{3.12}$$

After integration over $[0, \infty]$ and using the inequality (3.2), we obtain (i).

- (ii) We differentiate (3.11) in time to obtain

$$\phi_{tt} - \varepsilon \Delta \phi_t = -\frac{1}{\varepsilon} f(\phi)_t. \tag{3.13}$$

Pairing (3.13) with ϕ_t yields

$$\frac{1}{2} \frac{d}{dt} \|\phi_t\|^2 + \varepsilon \|\nabla \phi_t\|^2 = -\frac{1}{\varepsilon} (f'(\phi) \phi_t, \phi_t) \leq \frac{1}{\varepsilon} \|f'(\phi)\|_{L^\infty} \|\phi_t\|^2. \tag{3.14}$$

Integrating (3.14) over $[0, \infty)$, yields

$$\text{ess sup}_{[0,\infty]} \|\phi_t\|^2 + 2\varepsilon \int_0^\infty \|\nabla \phi_t\|^2 \lesssim \frac{2}{\varepsilon} \|f'(\phi)\|_{L^\infty} \int_0^\infty \|\phi_t\|^2 dt + \|\phi_t^0\|^2. \tag{3.15}$$

The assertion then follows from (i) and the inequality (3.3).

- (iii) Testing (3.13) with ϕ_{tt} , we get

$$\begin{aligned} \|\phi_{tt}\|^2 + \frac{\varepsilon}{2} \frac{d}{dt} \|\nabla \phi_t\|^2 &= -\frac{1}{\varepsilon} (f'(\phi) \phi_t, \phi_{tt}) \\ &\leq \frac{1}{2\varepsilon^2} \|f'(\phi)\|_{L^\infty}^2 \|\phi_t\|^2 + \frac{1}{2} \|\phi_{tt}\|^2. \end{aligned} \tag{3.16}$$

Integrating (3.16) over $[0, \infty)$, we get

$$\int_0^\infty \|\phi_{tt}\|^2 dt + \text{ess sup}_{[0,\infty]} \varepsilon \|\nabla \phi_t\|^2 \lesssim \frac{1}{\varepsilon^2} \|f'(\phi)\|_{L^\infty}^2 \int_0^\infty \|\phi_t\|^2 dt + \varepsilon \|\nabla \phi_t^0\|^2. \tag{3.17}$$

By using (i) and the inequality (3.4) of Assumption 3.2, we obtain (iii).

(iv) We differentiate (3.13) in time to derive

$$\phi_{ttt} - \varepsilon \Delta \phi_{tt} = -\frac{1}{\varepsilon} f(\phi)_{tt}. \tag{3.18}$$

Testing (3.18) with $-\Delta \phi_{tt}$ and using $H^1(\Omega) \hookrightarrow L^4(\Omega)$ for $d \leq 4$, we have

$$\begin{aligned} & \frac{1}{2} \frac{d}{dt} \|\nabla \phi_{tt}\|^2 + \varepsilon \|\Delta \phi_{tt}\|^2 = \frac{1}{\varepsilon} (f(\phi)_{tt}, \Delta \phi_{tt}) = \frac{1}{\varepsilon} (f''(\phi) \phi_t^2 + f'(\phi) \phi_{tt}, \Delta \phi_{tt}) \\ & \leq \frac{1}{\varepsilon^3} (\|f''(\phi)\|_{L^\infty}^2 \|\phi_t\|_{L^4}^4 + \|f'(\phi)\|_{L^\infty}^2 \|\phi_{tt}\|^2) + \frac{\varepsilon}{2} \|\Delta \phi_{tt}\|^2 \\ & \leq \frac{1}{\varepsilon^3} (C_s \|f''(\phi)\|_{L^\infty}^2 (\|\nabla \phi_t\|^4 + \|\phi_t\|^4) + \|f'(\phi)\|_{L^\infty}^2 \|\phi_{tt}\|^2) + \frac{\varepsilon}{2} \|\Delta \phi_{tt}\|^2. \end{aligned} \tag{3.19}$$

Integrating (3.19) over $[0, \infty)$, we obtain

$$\begin{aligned} & \operatorname{ess\,sup}_{[0, \infty]} \|\nabla \phi_{tt}\|^2 + \varepsilon \int_0^\infty \|\Delta \phi_{tt}\|^2 \\ & \lesssim \frac{2}{\varepsilon^3} \left(C_s \|f''(\phi)\|_{L^\infty}^2 \int_0^\infty (\|\nabla \phi_t\|^4 + \|\phi_t\|^4) dt + \|f'(\phi)\|_{L^\infty}^2 \int_0^\infty \|\phi_{tt}\|^2 dt \right) \\ & \quad + \|\nabla \phi_{tt}^0\|^2 \\ & \leq \frac{2}{\varepsilon^3} C_s \|f''(\phi)\|_{L^\infty}^2 \left(\operatorname{ess\,sup}_{[0, \infty]} \|\nabla \phi_t\|^2 \int_0^\infty \|\nabla \phi_t\|^2 dt + \operatorname{ess\,sup}_{[0, \infty]} \|\phi_t\|^2 \int_0^\infty \|\phi_t\|^2 dt \right) \\ & \quad + \frac{2}{\varepsilon^3} \|f'(\phi)\|_{L^\infty}^2 \int_0^\infty \|\phi_{tt}\|^2 dt + \|\nabla \phi_{tt}^0\|^2. \end{aligned} \tag{3.20}$$

The assertion then follows from (i), (ii), (iii) and the inequality (3.5).

(v) Testing (3.18) with ϕ_{ttt} , we have

$$\begin{aligned} & \|\phi_{ttt}\|^2 + \frac{\varepsilon}{2} \frac{d}{dt} \|\nabla \phi_{tt}\|^2 = -\frac{1}{\varepsilon} (f(\phi)_{tt}, \phi_{ttt}) \\ & \leq \frac{1}{\varepsilon^2} (\|f''(\phi)\|_{L^\infty}^2 \|\phi_t\|_{L^4}^4 + \|f'(\phi)\|_{L^\infty}^2 \|\phi_{tt}\|^2) + \frac{1}{2} \|\phi_{ttt}\|^2. \end{aligned} \tag{3.21}$$

Integrating in time yields

$$\begin{aligned} & \int_0^\infty \|\phi_{ttt}\|^2 + \operatorname{ess\,sup}_{[0, \infty]} \varepsilon \|\nabla \phi_{tt}\|^2 \\ & \lesssim \frac{2}{\varepsilon^2} C_s \|f''(\phi)\|_{L^\infty}^2 \left(\operatorname{ess\,sup}_{[0, \infty]} \|\nabla \phi_t\|^2 \int_0^\infty \|\nabla \phi_t\|^2 dt + \operatorname{ess\,sup}_{[0, \infty]} \|\phi_t\|^2 \int_0^\infty \|\phi_t\|^2 dt \right) \\ & \quad + \frac{2}{\varepsilon^2} \|f'(\phi)\|_{L^\infty}^2 \int_0^\infty \|\phi_{tt}\|^2 dt + \varepsilon \|\nabla \phi_{tt}^0\|^2. \end{aligned} \tag{3.22}$$

The assertion then follows from (i), (ii), (iii) and the inequality (3.5). □

3.1. Convergence analysis of the SL-BDF2 scheme. Now, we present our first error estimate result, which is a coarse estimate obtained by a standard approach.

PROPOSITION 3.1 (Coarse error estimate). *Given Assumptions 3.1, 3.2, $\forall \tau \leq \frac{1}{12}$, following error estimates hold for the SL-BDF2 scheme (2.4).*

$$\frac{1}{2} \|e^{n+1}\|^2 + \|2e^{n+1} - e^n\|^2 + 2A\tau^2 \|e^{n+1}\|^2 + 4\varepsilon\tau \|\nabla e^{n+1}\|^2$$

$$\begin{aligned}
 & + 2A\tau^2 \|\delta_t e^{n+1}\|^2 + \|\delta_{tt} e^{n+1}\|^2 + 4B\tau \|e^{n+1}\|^2 \\
 \lesssim & \|e^n\|^2 + \|2e^n - e^{n-1}\|^2 + 2A\tau^2 \|e^n\|^2 \\
 & + \varepsilon^{-(4\sigma_1+7)} \tau^4 + 4\left(B^2 + \frac{L^2}{\varepsilon^2}\right) \tau \|2e^n - e^{n-1}\|^2, \quad n \geq 1,
 \end{aligned} \tag{3.23}$$

and

$$\begin{aligned}
 & \max_{1 \leq n \leq N} (\|e^{n+1}\|^2 + 2\|2e^{n+1} - e^n\|^2 + 4A\tau^2 \|e^{n+1}\|^2) + 8\varepsilon\tau \sum_{n=1}^N \|\nabla e^{n+1}\|^2 \\
 & + 4A\tau^2 \sum_{n=1}^N \|\delta_t e^{n+1}\|^2 + 2 \sum_{n=1}^N \|\delta_{tt} e^{n+1}\|^2 + 8B\tau \sum_{n=1}^N \|e^{n+1}\|^2 \\
 \lesssim & \exp\left(80\left(B^2 + \frac{L^2}{\varepsilon^2}\right)T + 12T\right) \varepsilon^{-\max\{4\sigma_1+7, \sigma_0\}} \tau^4.
 \end{aligned} \tag{3.24}$$

Proof. By taking the difference of Equation (1.1) and (2.4), we obtain the following error equation

$$\begin{aligned}
 D_\tau e^{n+1} = & \tilde{R}_1^{n+1} + \varepsilon \Delta e^{n+1} - \frac{1}{\varepsilon} [f(2\phi^n - \phi^{n-1}) - f(\phi(t^{n+1}))] \\
 & - A\tau \delta_t e^{n+1} - B\delta_{tt} e^{n+1} - A\tilde{R}_2^{n+1} - B\tilde{R}_3^{n+1},
 \end{aligned} \tag{3.25}$$

where

$$\begin{aligned}
 D_\tau e^{n+1} & := \frac{3e^{n+1} - 4e^n + e^{n-1}}{2\tau}, \\
 \tilde{R}_1^{n+1} & := \phi_t(t^{n+1}) - D_\tau \phi(t^{n+1}), \\
 \tilde{R}_2^{n+1} & := \tau \delta_t \phi(t^{n+1}) = \tau(\phi(t^{n+1}) - \phi(t^n)), \\
 \tilde{R}_3^{n+1} & := \delta_{tt} \phi(t^{n+1}) = \phi(t^{n+1}) - 2\phi(t^n) + \phi(t^{n-1}).
 \end{aligned}$$

Pairing (3.25) with e^{n+1} , we obtain

$$\begin{aligned}
 & (D_\tau e^{n+1}, e^{n+1}) + \varepsilon \|\nabla e^{n+1}\|^2 + A\tau (\delta_t e^{n+1}, e^{n+1}) \\
 = & (\tilde{R}_1^{n+1}, e^{n+1}) - A(\tilde{R}_2^{n+1}, e^{n+1}) - B(\tilde{R}_3^{n+1}, e^{n+1}) \\
 & - B(\delta_{tt} e^{n+1}, e^{n+1}) - \frac{1}{\varepsilon} (f(2\phi^n - \phi^{n-1}) - f(\phi(t^{n+1})), e^{n+1}) \\
 = & : J_1 + J_2 + J_3 + J_4 + J_5.
 \end{aligned} \tag{3.26}$$

First, for the terms on the left-hand side of (3.26), using identity (2.2), we have

$$\begin{aligned}
 (D_t e^{n+1}, e^{n+1}) & = \frac{1}{4\tau} (\|e^{n+1}\|^2 + \|2e^{n+1} - e^n\|^2) \\
 & - \frac{1}{4\tau} (\|e^n\|^2 + \|2e^n - e^{n-1}\|^2) + \frac{1}{4\tau} \|\delta_{tt} e^{n+1}\|^2,
 \end{aligned} \tag{3.27}$$

and using identity (2.1), we get

$$A\tau (\delta_t e^{n+1}, e^{n+1}) = \frac{1}{2} A\tau (\|e^{n+1}\|^2 - \|e^n\|^2 + \|\delta_t e^{n+1}\|^2). \tag{3.28}$$

Then we estimate the terms on the right-hand side of (3.26).

$$J_1 = (\tilde{R}_1^{n+1}, e^{n+1}) \leq \|\tilde{R}_1^{n+1}\|^2 + \frac{1}{4}\|e^{n+1}\|^2, \tag{3.29}$$

$$J_2 = -A(\tilde{R}_2^{n+1}, e^{n+1}) \leq A^2\|\tilde{R}_2^{n+1}\|^2 + \frac{1}{4}\|e^{n+1}\|^2, \tag{3.30}$$

$$J_3 = -B(\tilde{R}_3^{n+1}, e^{n+1}) \leq B^2\|\tilde{R}_3^{n+1}\|^2 + \frac{1}{4}\|e^{n+1}\|^2 \tag{3.31}$$

$$\begin{aligned} J_4 &= -B(\delta_{tt}e^{n+1}, e^{n+1}) = -B(e^{n+1} - (2e^n - e^{n-1}), e^{n+1}) \\ &\leq -B\|e^{n+1}\|^2 + B^2\|2e^n - e^{n-1}\|^2 + \frac{1}{4}\|e^{n+1}\|^2. \end{aligned} \tag{3.32}$$

$$\begin{aligned} J_5 &= -\frac{1}{\varepsilon}(f(2\phi^n - \phi^{n-1}) - f(\phi(t^{n+1})), e^{n+1}) \\ &\leq \frac{L}{\varepsilon}(|2\phi^n - \phi^{n-1} - \phi(t^{n+1})|, |e^{n+1}|) \\ &= \frac{L}{\varepsilon}(|2e^n - e^{n-1} - \delta_{tt}\phi(t^{n+1})|, |e^{n+1}|) \\ &\leq \frac{L^2}{\varepsilon^2}\|2e^n - e^{n-1}\|^2 + \frac{L^2}{\varepsilon^2}\|\tilde{R}_3^{n+1}\|^2 + \frac{1}{2}\|e^{n+1}\|^2. \end{aligned} \tag{3.33}$$

Combining (3.26)-(3.33) together, yields

$$\begin{aligned} &\frac{1}{4\tau}(\|e^{n+1}\|^2 + \|2e^{n+1} - e^n\|^2) + \frac{1}{2}A\tau\|e^{n+1}\|^2 \\ &\quad + \frac{1}{2}A\tau\|\delta_{tt}e^{n+1}\|^2 + \varepsilon\|\nabla e^{n+1}\|^2 + \frac{1}{4\tau}\|\delta_{tt}e^{n+1}\|^2 + B\|e^{n+1}\|^2 \\ &\leq \frac{1}{4\tau}(\|e^n\|^2 + \|2e^n - e^{n-1}\|^2) + \frac{1}{2}A\tau\|e^n\|^2 \\ &\quad + \|\tilde{R}_1^{n+1}\|^2 + A^2\|\tilde{R}_2^{n+1}\|^2 + \left(B^2 + \frac{L^2}{\varepsilon^2}\right)\|\tilde{R}_3^{n+1}\|^2 \\ &\quad + \left(B^2 + \frac{L^2}{\varepsilon^2}\right)\|2e^n - e^{n-1}\|^2 + \frac{3}{2}\|e^{n+1}\|^2. \end{aligned} \tag{3.34}$$

By using Taylor expansions in integral form, one can get estimates for the residuals

$$\|\tilde{R}_1^{n+1}\|^2 \leq 8\tau^3 \int_{t_{n-1}}^{t_{n+1}} \|\phi_{ttt}(t)\|^2 dt \lesssim \tau^3 \varepsilon^{-4\sigma_1 - 7}, \tag{3.35}$$

$$\|\tilde{R}_2^{n+1}\|^2 \leq \tau^3 \int_{t_n}^{t_{n+1}} \|\phi_t(t)\|^2 dt \lesssim \tau^3 \varepsilon^{-2\sigma_1}, \tag{3.36}$$

$$\|\tilde{R}_3^{n+1}\|^2 \leq 6\tau^3 \int_{t_{n-1}}^{t_{n+1}} \|\phi_{tt}(t)\|^2 dt \lesssim \tau^3 \varepsilon^{-2\sigma_1 - 2}. \tag{3.37}$$

Taking $\tau \leq \frac{1}{12}$, combining (3.35)-(3.37) and the assumptions about the first step error, by using a discrete Grönwall’s inequality, we obtain (3.24). (3.23) is obtained without using Grönwall’s inequality. □

Proposition 3.1 is the usual error estimate, in which the error growth depends on $1/\varepsilon$ exponentially. To obtain a finer estimate on the error, we will need to use a spectral estimate of the linearized Allen-Cahn operator by Chen [7] for the case when the interface is well developed in the Allen-Cahn system.

LEMMA 3.2. *Let ϕ be the exact solution of the Allen-Cahn Equation (1.1) with interfaces being well developed in the initial condition (i.e. conditions (1.9)-(1.15) in [7] are satisfied). Then there exist $0 < \varepsilon_0 \ll 1$ and positive constant C_0 such that the principal eigenvalue of the linearized Allen-Cahn operator $\mathcal{L}_{AC} := -(\varepsilon\Delta - \frac{1}{\varepsilon}f'(\phi)I)/\varepsilon$ satisfies for all $t \in [0, T]$*

$$\lambda_{CH} = \inf_{0 \neq v \in H^1(\Omega)} \frac{\varepsilon \|\nabla v\|^2 + \frac{1}{\varepsilon} (f'(\phi(\cdot, t))v, v)}{\varepsilon \|v\|^2} \geq -C_0, \tag{3.38}$$

for $\varepsilon \in (0, \varepsilon_0)$.

THEOREM 3.1. *Suppose all of the Assumptions 3.1, 3.2 hold. Let time step τ satisfy the following constraint*

$$\tau \lesssim \min \left\{ \varepsilon^2, \varepsilon^{\frac{1}{3} \max\{4\sigma_1+7, \sigma_0\} + \frac{5}{3} - \frac{2}{d}}, \varepsilon^{\frac{1}{4} \max\{4\sigma_1+7, \sigma_0\} + \frac{9}{2(6-d)}} \right\}, \tag{3.39}$$

then the solution of (2.4) satisfies the following error estimate

$$\begin{aligned} & \max_{1 \leq n \leq N} \{ \|e^{n+1}\|^2 + 2\|2e^{n+1} - e^n\|^2 + 4A\tau^2 \|e^{n+1}\|^2 \} \\ & + 4A\tau^2 \sum_{n=1}^N \|\delta_t e^{n+1}\|^2 + \varepsilon^2 \sum_{n=1}^N \|\nabla e^{n+1}\|^2 \\ & \leq \exp(8T(C_0\varepsilon + L + 2)) \varepsilon^{-\max\{4\sigma_1+7, \sigma_0\}} \tau^4. \end{aligned} \tag{3.40}$$

Proof. We refine the result of Proposition 3.1 by re-estimating J_4 in Equation (3.26) as

$$J_4 = -B(\delta_{tt}e^{n+1}, e^{n+1}) \leq B^2 \|\delta_{tt}e^{n+1}\|^2 + \frac{1}{4} \|e^{n+1}\|^2, \tag{3.41}$$

and rewriting J_5 as

$$J_5 = J_6 + J_7, \tag{3.42}$$

$$\begin{aligned} J_6 &= -\frac{1}{\varepsilon} (f(2\phi^n - \phi^{n-1}) - f(\phi^{n+1}), e^{n+1}) \\ &\leq \frac{L}{\varepsilon} (|\delta_{tt}e^{n+1}| + |\tilde{R}_3^{n+1}|, |e^{n+1}|) \\ &\leq \frac{L^2}{\varepsilon^2} \left(\|\delta_{tt}e^{n+1}\|^2 + \|\tilde{R}_3^{n+1}\|^2 \right) + \frac{1}{2} \|e^{n+1}\|^2, \end{aligned} \tag{3.43}$$

$$\begin{aligned} J_7 &= -\frac{1}{\varepsilon} (f(\phi^{n+1}) - f(\phi(t^{n+1})), e^{n+1}) \\ &\leq -\frac{1}{\varepsilon} (f'(\phi(t^{n+1}))e^{n+1}, e^{n+1}) + \frac{L_2}{\varepsilon} \|e^{n+1}\|_{L^3}^3. \end{aligned} \tag{3.44}$$

The spectrum estimate (3.38) give us

$$\varepsilon \|\nabla e^{n+1}\|^2 + \frac{1}{\varepsilon} (f'(\phi(t^{n+1}))e^{n+1}, e^{n+1}) \geq -\varepsilon C_0 \|e^{n+1}\|^2. \tag{3.45}$$

Applying (3.45) with a scaling factor $-(1-\varepsilon)$, we get

$$-(1-\varepsilon) \frac{1}{\varepsilon} (f'(\phi(t^{n+1}))e^{n+1}, e^{n+1}) \leq C_0\varepsilon(1-\varepsilon) \|e^{n+1}\|^2 + (1-\varepsilon)\varepsilon \|\nabla e^{n+1}\|^2. \tag{3.46}$$

On the other hand,

$$-(f'(\phi(t^{n+1}))e^{n+1}, e^{n+1}) \leq L\|e^{n+1}\|^2. \tag{3.47}$$

Now, we estimate the L^3 term in (3.44) by interpolating L^3 between L^2 and H^1

$$\|e^{n+1}\|_{L^3}^3 \leq K(\|\nabla e^{n+1}\|^{\frac{d}{2}}\|e^{n+1}\|^{\frac{6-d}{2}} + \|e^{n+1}\|^3),$$

where K is a constant independent of ε and τ . We continue the estimate by using Young's inequality

$$\frac{L_2}{\varepsilon}\|e^{n+1}\|_{L^3}^3 \leq \frac{d}{6}\varepsilon^{\frac{3}{d}}\|\nabla e^{n+1}\|^3 + \frac{6-d}{6}\left(\frac{L_2K}{\varepsilon^{\frac{3}{d}}}\right)^{\frac{6}{6-d}}\|e^{n+1}\|^3 + \frac{L_2K}{\varepsilon}\|e^{n+1}\|^3. \tag{3.48}$$

Substituting (3.46), (3.47) and (3.48) into (3.44), we get

$$\begin{aligned} J_7 \leq & (C_0\varepsilon(1-\varepsilon) + L)\|e^{n+1}\|^2 + (1-\varepsilon)\varepsilon\|\nabla e^{n+1}\|^2 + \frac{d}{6}\varepsilon^{\frac{3}{d}}\|\nabla e^{n+1}\|^3 \\ & + \left(\frac{6-d}{6}\left(\frac{L_2K}{\varepsilon^{\frac{3}{d}}}\right)^{\frac{6}{6-d}} + \frac{L_2K}{\varepsilon}\right)\|e^{n+1}\|^3. \end{aligned} \tag{3.49}$$

Substituting the estimate of (3.27)-(3.31), (3.41)-(3.43) and (3.49) into (3.26), we get

$$\begin{aligned} & \frac{1}{4\tau}((\|e^{n+1}\|^2 + \|2e^{n+1} - e^n\|^2) - (\|e^n\|^2 + \|2e^n - e^{n-1}\|^2)) \\ & + \frac{1}{2}A\tau(\|e^{n+1}\|^2 - \|e^n\|^2) + \frac{1}{2}A\tau\|\delta_t e^{n+1}\|^2 + \frac{1}{4\tau}\|\delta_{tt} e^{n+1}\|^2 + \varepsilon^2\|\nabla e^{n+1}\|^2 \\ \leq & \|\tilde{R}_1^{n+1}\|^2 + A^2\|\tilde{R}_2^{n+1}\|^2 + \left(B^2 + \frac{L^2}{\varepsilon^2}\right)\|\tilde{R}_3^{n+1}\|^2 \\ & + \left(C_0\varepsilon(1-\varepsilon) + L + \frac{3}{2} + G^{n+1}\right)\|e^{n+1}\|^2 + \left(B^2 + \frac{L^2}{\varepsilon^2}\right)\|\delta_{tt} e^{n+1}\|^2 \\ & + Q^{n+1}\|\nabla e^{n+1}\|^2, \end{aligned} \tag{3.50}$$

where $Q^{n+1} = \frac{d}{6}\varepsilon^{\frac{3}{d}}\|\nabla e^{n+1}\|$, $G^{n+1} = \left(\frac{6-d}{6}\left(\frac{L_2K}{\varepsilon^{\frac{3}{d}}}\right)^{\frac{6}{6-d}} + \frac{L_2K}{\varepsilon}\right)\|e^{n+1}\|$.

If Q^{n+1} is uniformly bounded by constant $\frac{\varepsilon^2}{2}$, G^{n+1} is uniformly bounded by constant $\frac{1}{2}$, then choose $\tau \leq \max\{\frac{\varepsilon^2}{4(B^2\varepsilon^2 + L^2)}, \frac{1}{8(C_0\varepsilon(1-\varepsilon) + L + 2)}\}$; by Grönwall's inequality and the first step error estimate (3.10) in Assumption 3.2, we will get the finer error estimate (3.40).

We prove this by induction. Assuming that the finer estimate holds for all first $n \leq N$ time steps:

$$\begin{aligned} & \max_{1 \leq n \leq N} \{\|e^n\|^2 + 2\|2e^n - e^{n-1}\|^2 + 4A\tau^2\|e^n\|^2\} \\ & + 4A\tau^2 \sum_{n=1}^N \|\delta_t e^n\|^2 + 4\tau\varepsilon^2 \sum_{n=1}^N \|\nabla e^n\|^2 \\ \leq & \exp(8T(C_0\varepsilon + L + 2))\varepsilon^{-\max\{4\sigma_1 + 7, \sigma_0\}}\tau^4. \end{aligned} \tag{3.51}$$

Combining (3.51) with the coarse estimate (3.23) leads to

$$\|e^{N+1}\|^2 + 2\|2e^{N+1} - e^N\|^2 + 4A\tau^2\|e^{N+1}\|^2$$

$$\begin{aligned}
 &+4A\tau^2\|\delta_t e^{N+1}\|^2+8\varepsilon\tau\|\nabla e^{N+1}\|^2+2\|\delta_{tt}e^{N+1}\|^2+8B\tau\|e^{N+1}\|^2 \\
 &\lesssim\varepsilon^{-\max\{4\sigma_1+7,\sigma_0\}}\tau^4, \quad N\geq 1.
 \end{aligned}
 \tag{3.52}$$

Then by taking $\tau \lesssim \varepsilon^{\frac{1}{3}\max\{4\sigma_1+7,\sigma_0\}+\frac{5}{3}-\frac{2}{d}}$, we have

$$Q^{N+1} \lesssim \varepsilon^{\frac{3}{d}} \varepsilon^{-\frac{1}{2}\max\{4\sigma_1+7,\sigma_0\}-\frac{1}{2}} \tau^{\frac{3}{2}} \lesssim \frac{\varepsilon^2}{2},
 \tag{3.53}$$

By taking $\tau \lesssim \varepsilon^{\frac{1}{4}\max\{4\sigma_1+7,\sigma_0\}+\frac{9}{2(6-d)}}$, we have

$$G^{N+1} \lesssim \varepsilon^{-\frac{9}{6-d}} \varepsilon^{-\frac{1}{2}\max\{4\sigma_1+7,\sigma_0\}} \tau^2 \lesssim \frac{1}{2}.
 \tag{3.54}$$

So, by taking step-sizes as defined in (3.39), the finer error estimate for $N+1$ step can be obtained, and the proof is completed by mathematical induction. \square

3.2. Convergence analysis of the SL-CN scheme. Similar as the error estimate of SL-BDF2 scheme, we first present the coarse error estimate for SL-CN scheme.

PROPOSITION 3.2 (Coarse error estimate). *Given Assumptions 3.1, 3.2, $\forall \tau \lesssim \varepsilon$, following error estimate holds for the SL-CN scheme (2.17).*

$$\begin{aligned}
 &\frac{1}{2}\|e^{n+1}\|^2+2\tau\varepsilon\|\nabla\frac{e^{n+1}+e^n}{2}\|^2+A\tau^2\|e^{n+1}\|^2+B\tau\|e^{n+1}\|^2 \\
 &\lesssim\varepsilon^{-\max\{4\sigma_1+7,\sigma_0\}}\tau^4+2B\tau\|e^n-e^{n-1}\|^2+\frac{2L}{\varepsilon}\tau\|\frac{3}{2}e^n-\frac{1}{2}e^{n-1}\|^2 \\
 &\quad +\left(\frac{5}{2}+\frac{B}{2}+\frac{L}{2\varepsilon}\right)\tau\|e^n\|^2+2A\tau^2\|e^n\|^2+2B\tau\|e^n\|^2, \quad \forall n\geq 1.
 \end{aligned}
 \tag{3.55}$$

and

$$\begin{aligned}
 &\max_{1\leq n\leq N}\left(\|e^{n+1}\|^2+2A\tau^2\|e^{n+1}\|^2+2B\tau\|e^{N+1}\|^2\right)+4\varepsilon\tau\sum_{n=1}^N\|\nabla\frac{e^{n+1}+e^n}{2}\|^2 \\
 &\lesssim\exp\left(17B+5+\frac{11L}{\varepsilon}\right)T\varepsilon^{-\max\{4\sigma_1+7,\sigma_0\}}\tau^4.
 \end{aligned}
 \tag{3.56}$$

Proof. The following equation for the error functions holds:

$$\begin{aligned}
 \frac{e^{n+1}-e^n}{\tau} &=R_1^{n+1}+\varepsilon\Delta\frac{e^{n+1}+e^n}{2}-\frac{1}{\varepsilon}\left(f\left(\frac{3}{2}\phi^n-\frac{1}{2}\phi^{n-1}\right)-f\left(\phi\left(t^{n+\frac{1}{2}}\right)\right)\right) \\
 &\quad -A\tau\delta_t e^{n+1}-AR_2^{n+1}-B\delta_{tt}e^{n+1}-BR_3^{n+1}+\varepsilon\Delta R_4^{n+1}.
 \end{aligned}
 \tag{3.57}$$

where

$$R_1^{n+1}=\phi_t^{n+\frac{1}{2}}-\frac{\phi(t^{n+1})-\phi(t^n)}{\tau},
 \tag{3.58}$$

$$R_2^{n+1}=\tau(\phi(t^{n+1})-\phi(t^n)),
 \tag{3.59}$$

$$R_3^{n+1}=\phi(t^{n+1})-2\phi(t^n)+\phi(t^{n-1}),
 \tag{3.60}$$

$$R_4^{n+1}=\frac{\phi(t^{n+1})+\phi(t^n)}{2}-\phi\left(t^{n+\frac{1}{2}}\right).
 \tag{3.61}$$

Pairing (3.57) with $\frac{e^{n+1}+e^n}{2}$, we get

$$\begin{aligned} & \frac{1}{2\tau}(\|e^{n+1}\|^2 - \|e^n\|^2) + \varepsilon \|\nabla \frac{e^{n+1}+e^n}{2}\|^2 + \frac{A\tau}{2}(\|e^{n+1}\|^2 - \|e^n\|^2) \\ &= \left(R_1^{n+1}, \frac{e^{n+1}+e^n}{2}\right) - A\left(R_2^{n+1}, \frac{e^{n+1}+e^n}{2}\right) - B\left(R_3^{n+1}, \frac{e^{n+1}+e^n}{2}\right) \\ & \quad + \varepsilon\left(\Delta R_4^{n+1}, \frac{e^{n+1}+e^n}{2}\right) - B\left(\delta_{tt}e^{n+1}, \frac{e^{n+1}+e^n}{2}\right) \\ & \quad - \frac{1}{\varepsilon}\left(f\left(\frac{3}{2}\phi^n - \frac{1}{2}\phi^{n-1}\right) - f\left(\phi(t^{n+\frac{1}{2}})\right), \frac{e^{n+1}+e^n}{2}\right) \\ & =: J_1 + J_2 + J_3 + J_4 + J_5 + J_6 =: J, \end{aligned} \tag{3.62}$$

For the right-hand side of (3.62), by using the Cauchy-Schwarz inequality, we obtain the following estimate:

$$J_1 = \left(R_1^{n+1}, \frac{e^{n+1}+e^n}{2}\right) \leq \|R_1^{n+1}\|^2 + \frac{1}{4}\left\|\frac{e^{n+1}+e^n}{2}\right\|^2, \tag{3.63}$$

$$J_2 = A\left(R_2^{n+1}, \frac{e^{n+1}+e^n}{2}\right) \leq A^2\|R_2^{n+1}\|^2 + \frac{1}{4}\left\|\frac{e^{n+1}+e^n}{2}\right\|^2, \tag{3.64}$$

$$J_3 = -B\left(R_3^{n+1}, \frac{e^{n+1}+e^n}{2}\right) \leq B^2\|R_3^{n+1}\|^2 + \frac{1}{4}\left\|\frac{e^{n+1}+e^n}{2}\right\|^2, \tag{3.65}$$

$$J_4 = \varepsilon\left(\Delta R_4^{n+1}, \frac{e^{n+1}+e^n}{2}\right) \leq \varepsilon^2\|\Delta R_4^{n+1}\|^2 + \frac{1}{4}\left\|\frac{e^{n+1}+e^n}{2}\right\|^2, \tag{3.66}$$

For J_5 on the right-hand side of (3.62), by using the equation $\delta_{tt}e^{n+1} = \delta_t e^{n+1} - \delta_t e^n$, we have

$$\begin{aligned} J_5 &= -B\left(\delta_{tt}e^{n+1}, \frac{e^{n+1}+e^n}{2}\right) \\ &= -\frac{B}{2}(\|e^{n+1}\|^2 - \|e^n\|^2) + \frac{B}{2}(\delta_t e^n, e^{n+1}+e^n) \\ &\leq -\frac{B}{2}(\|e^{n+1}\|^2 - \|e^n\|^2) + B\|e^n - e^{n-1}\|^2 + \frac{B}{4}\left\|\frac{e^{n+1}+e^n}{2}\right\|^2. \end{aligned} \tag{3.67}$$

$$\begin{aligned} J_6 &= -\frac{1}{\varepsilon}\left(f\left(\frac{3}{2}\phi^n - \frac{1}{2}\phi^{n-1}\right) - f\left(\phi(t^{n+\frac{1}{2}})\right), \frac{e^{n+1}+e^n}{2}\right) \\ &\leq \frac{L}{\varepsilon}\left(|R_5^{n+1}|, \left|\frac{e^{n+1}+e^n}{2}\right|\right) + \frac{L}{\varepsilon}\left(\left|\frac{3}{2}e^n - \frac{1}{2}e^{n-1}\right|, \left|\frac{e^{n+1}+e^n}{2}\right|\right) \\ &\leq \frac{L^2}{\varepsilon^2}\|R_5^{n+1}\|^2 + \frac{1}{4}\left\|\frac{e^{n+1}+e^n}{2}\right\|^2 + \frac{L}{\varepsilon}\left\|\frac{3}{2}e^n - \frac{1}{2}e^{n-1}\right\|^2 + \frac{L}{4\varepsilon}\left\|\frac{e^{n+1}+e^n}{2}\right\|^2, \end{aligned} \tag{3.68}$$

where

$$R_5^{n+1} = \frac{3}{2}\phi(t^n) - \frac{1}{2}\phi(t^{n-1}) - \phi(t^{n+\frac{1}{2}}). \tag{3.69}$$

Substituting J_1, \dots, J_6 into (3.62), we have

$$\begin{aligned} & \frac{1}{2\tau}(\|e^{n+1}\|^2 - \|e^n\|^2) + \varepsilon \|\nabla \frac{e^{n+1}+e^n}{2}\|^2 + \frac{A\tau}{2}(\|e^{n+1}\|^2 - \|e^n\|^2) + \frac{B}{2}(\|e^{n+1}\|^2 - \|e^n\|^2) \\ & \leq \|R_1^{n+1}\|^2 + A^2\|R_2^{n+1}\|^2 + B^2\|R_3^{n+1}\|^2 + \varepsilon^2\|\Delta R_4^{n+1}\|^2 + \frac{L^2}{\varepsilon^2}\|R_5^{n+1}\|^2 \\ & \quad + B\|e^n - e^{n-1}\|^2 + \frac{L}{\varepsilon}\left\|\frac{3}{2}e^n - \frac{1}{2}e^{n-1}\right\|^2 + \left(\frac{5}{4} + \frac{B}{4} + \frac{L}{4\varepsilon}\right)\left\|\frac{e^{n+1}+e^n}{2}\right\|^2, \end{aligned} \tag{3.70}$$

By using Taylor expansions in integral form, one can get estimates for the residuals

$$\|R_1^{n+1}\|^2 \leq \tau^3 \int_{t^n}^{t^{n+1}} \|\phi_{tt}(t)\|^2 dt \lesssim \varepsilon^{-2\sigma_1-2} \tau^3, \tag{3.71}$$

$$\|R_2^{n+1}\|^2 \leq \tau^3 \int_{t^n}^{t^{n+1}} \|\phi_t(t)\|^2 dt \lesssim \varepsilon^{-2\sigma_1} \tau^3, \tag{3.72}$$

$$\|R_3^{n+1}\|^2 \leq 6\tau^3 \int_{t^{n-1}}^{t^{n+1}} \|\phi_{tt}(t)\|^2 dt \lesssim \varepsilon^{-2\sigma_1-2} \tau^3, \tag{3.73}$$

$$\|\Delta R_4^{n+1}\|^2 \leq \tau^3 \int_{t^n}^{t^{n+1}} \|\Delta \phi_{tt}(t)\|^2 dt \lesssim \varepsilon^{-4\sigma_1-9} \tau^3, \tag{3.74}$$

$$\|R_5^{n+1}\|^2 \leq \tau^3 \int_{t^{n-1}}^{t^{n+1}} \|\phi_{tt}(t)\|^2 dt \lesssim \varepsilon^{-2\sigma_1-2} \tau^3. \tag{3.75}$$

Taking $\tau < 1/(\frac{5}{2} + \frac{B}{2} + \frac{L}{2\varepsilon}) \lesssim \varepsilon$, combining (3.71)-(3.75) and the error assumption of the first step, by using a discrete Grönwall's inequality, one gets (3.56). (3.55) is obtained without using Grönwall's inequality. \square

Proposition 3.2 is the usual error estimate, in which the error growth depends on $1/\varepsilon$ exponentially. Next, we give a finer error estimate by using Lemma 3.2.

THEOREM 3.2. *Suppose all of the Assumptions 3.1, 3.2 hold. Let τ satisfy the following constraint*

$$\tau \lesssim \min \left\{ \varepsilon^2, \varepsilon^{\frac{1}{3} \max\{4\sigma_1+11, \sigma_0\} + \frac{5}{3} - \frac{2}{d}}, \varepsilon^{\frac{1}{4} \max\{4\sigma_1+11, \sigma_0\} + \frac{9}{2(6-d)}} \right\}, \tag{3.76}$$

then the solution of (2.17) satisfies the following error estimate

$$\begin{aligned} & \max_{1 \leq n \leq N} \left\{ \|e^{n+1}\|^2 + 2\varepsilon\tau \|\nabla e^{n+1}\|^2 + \left(2B + 8B^2 + \frac{2L}{\varepsilon} + \frac{2L^2}{\varepsilon^2} \right) \tau \|\delta_t e^{n+1}\|^2 \right\} \\ & + 2\varepsilon^2\tau \sum_{n=1}^N \left\| \nabla \frac{e^{n+1} + e^n}{2} \right\|^2 \\ & \lesssim \exp((12 + 4C_0\varepsilon + 4L)T) \varepsilon^{-\max\{4\sigma_1+11, \sigma_0\}} \tau^4. \end{aligned} \tag{3.77}$$

Proof. To get better convergence results, we re-estimate J_5 in (3.67) as

$$J_5 = -B \left(\delta_{tt} e^{n+1}, \frac{e^{n+1} + e^n}{2} \right) \leq B^2 \|\delta_{tt} e^{n+1}\|^2 + \frac{1}{4} \left\| \frac{e^{n+1} + e^n}{2} \right\|^2. \tag{3.78}$$

For J_6 , we have

$$\begin{aligned} J_6 &= -\frac{1}{\varepsilon} \left(f\left(\frac{3}{2}\phi^n - \frac{1}{2}\phi^{n-1}\right) - f\left(\phi\left(t^{n+\frac{1}{2}}\right)\right), \frac{e^{n+1} + e^n}{2} \right) \\ &= -\frac{1}{\varepsilon} \left(f\left(\frac{3}{2}\phi^n - \frac{1}{2}\phi^{n-1}\right) - f\left(\frac{\phi^{n+1} + \phi^n}{2}\right), \frac{e^{n+1} + e^n}{2} \right) \\ &\quad - \frac{1}{\varepsilon} \left(f\left(\frac{\phi^{n+1} + \phi^n}{2}\right) - f\left(\phi\left(t^{n+\frac{1}{2}}\right)\right), \frac{e^{n+1} + e^n}{2} \right) \\ &:= J_7 + J_8. \end{aligned} \tag{3.79}$$

$$\begin{aligned}
J_7 &= -\frac{1}{\varepsilon} \left(f\left(\frac{3}{2}\phi^n - \frac{1}{2}\phi^{n-1}\right) - f\left(\frac{\phi^{n+1} + \phi^n}{2}\right), \frac{e^{n+1} + e^n}{2} \right) \\
&\leq \frac{L}{2\varepsilon} \left(|\delta_{tt}\phi^{n+1}|, \left|\frac{e^{n+1} + e^n}{2}\right| \right) \\
&= \frac{L}{2\varepsilon} \left(|\delta_{tt}e^{n+1} + R_3^{n+1}|, \left|\frac{e^{n+1} + e^n}{2}\right| \right) \\
&\leq \frac{L^2}{4\varepsilon^2} \|\delta_{tt}e^{n+1}\|^2 + \frac{L^2}{4\varepsilon^2} \|R_3^{n+1}\|^2 + \frac{1}{2} \left\| \frac{e^{n+1} + e^n}{2} \right\|^2. \tag{3.80}
\end{aligned}$$

By Taylor expansion, there exists $\vartheta^{n+1} \in \left(\frac{\phi^{n+1} + \phi^n}{2}, \phi(t^{n+\frac{1}{2}})\right)$ such that

$$\begin{aligned}
J_8 &= -\frac{1}{\varepsilon} \left(f\left(\frac{\phi^{n+1} + \phi^n}{2}\right) - f\left(\phi(t^{n+\frac{1}{2}})\right), \frac{e^{n+1} + e^n}{2} \right) \\
&= -\frac{1}{\varepsilon} \left(f'\left(\phi(t^{n+\frac{1}{2}})\right) \left(\frac{e^{n+1} + e^n}{2} + R_4^{n+1}\right), \frac{e^{n+1} + e^n}{2} \right) \\
&\quad - \frac{1}{2\varepsilon} \left(f''\left(\vartheta^{n+1}\right) \left(\frac{e^{n+1} + e^n}{2} + R_4^{n+1}\right)^2, \frac{e^{n+1} + e^n}{2} \right) \\
&\leq -\frac{1}{\varepsilon} \left(f'\left(\phi(t^{n+\frac{1}{2}})\right) \frac{e^{n+1} + e^n}{2}, \frac{e^{n+1} + e^n}{2} \right) + \frac{L_2}{\varepsilon} \left\| \frac{e^{n+1} + e^n}{2} \right\|_{L^3}^3 \\
&\quad + \frac{1}{\varepsilon^2} C_2 \|R_4^{n+1}\|^2 + \frac{1}{2} \left\| \frac{e^{n+1} + e^n}{2} \right\|^2, \tag{3.81}
\end{aligned}$$

where $L^2 + 4L_2^2 \|\phi(t)\|_\infty^2 \leq L^2 + 4L_2^2 C^2 =: C_2$. For the first term on the right-hand side of (3.81), we use the spectrum estimate (3.38) to get

$$\varepsilon \left\| \nabla \frac{e^{n+1} + e^n}{2} \right\|_{L^2}^2 + \frac{1}{\varepsilon} \left(f'\left(\phi(t^{n+\frac{1}{2}})\right) \frac{e^{n+1} + e^n}{2}, \frac{e^{n+1} + e^n}{2} \right) \geq -C_0 \varepsilon \left\| \frac{e^{n+1} + e^n}{2} \right\|^2. \tag{3.82}$$

Applying (3.82) with a scaling factor $(1 - \varepsilon)$, we get

$$\begin{aligned}
&-(1 - \varepsilon) \frac{1}{\varepsilon} \left(f'\left(\phi(t^{n+1})\right) \frac{e^{n+1} + e^n}{2}, \frac{e^{n+1} + e^n}{2} \right) \\
&\leq C_0 \varepsilon (1 - \varepsilon) \left\| \frac{e^{n+1} + e^n}{2} \right\|^2 + (1 - \varepsilon) \varepsilon \left\| \nabla \frac{e^{n+1} + e^n}{2} \right\|^2. \tag{3.83}
\end{aligned}$$

On the other hand,

$$-\left(f'\left(\phi(t^{n+1})\right) \frac{e^{n+1} + e^n}{2}, \frac{e^{n+1} + e^n}{2} \right) \leq L \left\| \frac{e^{n+1} + e^n}{2} \right\|^2. \tag{3.84}$$

Now, we estimate the L^3 term. By interpolating L^3 between L^2 and H^1 , we get

$$\left\| \frac{e^{n+1} + e^n}{2} \right\|_{L^3}^3 \leq K \left(\left\| \nabla \frac{e^{n+1} + e^n}{2} \right\|^{\frac{d}{2}} \left\| \frac{e^{n+1} + e^n}{2} \right\|^{\frac{6-d}{2}} + \left\| \frac{e^{n+1} + e^n}{2} \right\|^3 \right),$$

where K is a constant independent of ε and τ . We continue the estimate by using Young's inequality

$$\begin{aligned}
&\frac{L_2}{\varepsilon} K \left(\left\| \nabla \frac{e^{n+1} + e^n}{2} \right\|^{\frac{d}{2}} \left\| \frac{e^{n+1} + e^n}{2} \right\|^{\frac{6-d}{2}} \right) \\
&\leq \frac{d}{6} \varepsilon^{\frac{3}{d}} \left\| \nabla \frac{e^{n+1} + e^n}{2} \right\|^3 + \frac{6-d}{6} \left(\frac{L_2 K}{\varepsilon^{\frac{3}{2}}} \right)^{\frac{6}{6-d}} \left\| \frac{e^{n+1} + e^n}{2} \right\|^3. \tag{3.85}
\end{aligned}$$

Substituting (3.83), (3.84) and (3.85) into (3.81), we get

$$\begin{aligned}
 J_8 \leq & (C_0\varepsilon(1-\varepsilon) + L) \left\| \frac{e^{n+1} + e^n}{2} \right\|^2 + (1-\varepsilon)\varepsilon \left\| \nabla \frac{e^{n+1} + e^n}{2} \right\|^2 \\
 & + \frac{d}{6} \varepsilon^{\frac{3}{2}} \left\| \nabla \frac{e^{n+1} + e^n}{2} \right\|^3 + \left(\frac{6-d}{6} \left(\frac{L_2 K}{\varepsilon^{\frac{3}{2}}} \right)^{\frac{6-d}{6}} + \frac{L_2}{\varepsilon} K \right) \left\| \frac{e^{n+1} + e^n}{2} \right\|^3 \\
 & + \frac{1}{\varepsilon^2} C_2 \|R_4^{n+1}\|^2 + \frac{1}{2} \left\| \frac{e^{n+1} + e^n}{2} \right\|^2.
 \end{aligned} \tag{3.86}$$

Substituting J_1, \dots, J_8 into (3.62), we have

$$\begin{aligned}
 & \frac{1}{2\tau} (\|e^{n+1}\|^2 - \|e^n\|^2) + \frac{A\tau}{2} (\|e^{n+1}\|^2 - \|e^n\|^2) + \varepsilon^2 \left\| \nabla \frac{e^{n+1} + e^n}{2} \right\|^2 \\
 \leq & \|R_1^{n+1}\|^2 + A^2 \|R_2^{n+1}\|^2 + B^2 \|R_3^{n+1}\|^2 + \varepsilon^2 \|\Delta R_4^{n+1}\|^2 + \frac{L^2}{4\varepsilon^2} \|R_3^{n+1}\|^2 + \frac{C_2}{\varepsilon^2} \|R_4^{n+1}\|^2 \\
 & + \frac{9}{4} \left\| \frac{e^{n+1} + e^n}{2} \right\|^2 + \left(B^2 + \frac{L^2}{4\varepsilon^2} \right) \|\delta_{tt} e^{n+1}\|^2 + (C_0\varepsilon(1-\varepsilon) + L) \left\| \frac{e^{n+1} + e^n}{2} \right\|^2 \\
 & + \frac{d}{6} \varepsilon^{\frac{3}{2}} \left\| \nabla \frac{e^{n+1} + e^n}{2} \right\|^3 + \left(\frac{6-d}{6} \left(\frac{L_2 K}{\varepsilon^{\frac{3}{2}}} \right)^{\frac{6-d}{6}} + \frac{L_2 K}{\varepsilon} \right) \left\| \frac{e^{n+1} + e^n}{2} \right\|^3.
 \end{aligned} \tag{3.87}$$

To control the 8th term on the right-hand side, we pair (3.57) with $\delta_t e^{n+1}$ to get

$$\begin{aligned}
 & \frac{1}{\tau} \|\delta_t e^{n+1}\|^2 + \frac{\varepsilon}{2} (\|\nabla e^{n+1}\|^2 - \|\nabla e^n\|^2) + A\tau \|\delta_t e^{n+1}\|^2 \\
 & + \frac{B}{2} (\|\delta_t e^{n+1}\|^2 - \|\delta_t e^n\|^2 + \|\delta_{tt} e^{n+1}\|^2) \\
 = & (R_1^{n+1}, \delta_t e^{n+1}) - A(R_2^{n+1}, \delta_t e^{n+1}) - B(R_3^{n+1}, \delta_t e^{n+1}) \\
 & + \varepsilon(\Delta R_4^{n+1}, \delta_t e^{n+1}) - \frac{1}{\varepsilon} \left(f\left(\frac{3}{2}\phi^n - \frac{1}{2}\phi^{n-1}\right) - f\left(\phi(t^{n+\frac{1}{2}})\right), \delta_t e^{n+1} \right) \\
 =: & \tilde{J}_1 + \tilde{J}_2 + \tilde{J}_3 + \tilde{J}_4 + \tilde{J}_5 =: \tilde{J}, \quad n \geq 1.
 \end{aligned} \tag{3.88}$$

Analogously, applying the method for J_1, \dots, J_4 to $\tilde{J}_1, \dots, \tilde{J}_4$, yields

$$\tilde{J}_1 = (R_1^{n+1}, \delta_t e^{n+1}) \leq \varepsilon \|R_1^{n+1}\|^2 + \frac{1}{4\varepsilon} \|\delta_t e^{n+1}\|^2, \tag{3.89}$$

$$\tilde{J}_2 = -A(R_2^{n+1}, \delta_t e^{n+1}) \leq A^2 \varepsilon \|R_2^{n+1}\|^2 + \frac{1}{4\varepsilon} \|\delta_t e^{n+1}\|^2, \tag{3.90}$$

$$\tilde{J}_3 = B(R_3^{n+1}, \delta_t e^{n+1}) \leq B^2 \varepsilon \|R_3^{n+1}\|^2 + \frac{1}{4\varepsilon} \|\delta_t e^{n+1}\|^2, \tag{3.91}$$

$$\tilde{J}_4 = \varepsilon(\Delta R_4^{n+1}, \delta_t e^{n+1}) \leq \varepsilon^3 \|\Delta R_4^{n+1}\|^2 + \frac{1}{4\varepsilon} \|\delta_t e^{n+1}\|^2. \tag{3.92}$$

For \tilde{J}_5 of (3.88), we have

$$\begin{aligned}
 \tilde{J}_5 & = -\frac{1}{\varepsilon} \left(f\left(\frac{3}{2}\phi^n - \frac{1}{2}\phi^{n-1}\right) - f\left(\phi(t^{n+\frac{1}{2}})\right), \delta_t e^{n+1} \right) \\
 & \leq -\frac{1}{\varepsilon} \left(f'(\xi^{n+1}) \left(-\frac{1}{2} \delta_{tt} e^{n+1} - \frac{1}{2} R_3^{n+1} + \frac{e^{n+1} + e^n}{2} + R_4^{n+1} \right), \delta_t e^{n+1} \right) \\
 & \leq \frac{L}{2\varepsilon} \left(\frac{3}{2} \|\delta_t e^{n+1}\|^2 + \|\delta_t e^n\|^2 \right) + \frac{L^2}{4\varepsilon} \|R_3^{n+1}\|^2 + \frac{L^2}{\varepsilon} \|R_4^{n+1}\|^2 + \frac{1}{2\varepsilon} \|\delta_t e^{n+1}\|^2
 \end{aligned}$$

$$+ \frac{1}{4} \left\| \frac{e^{n+1} + e^n}{2} \right\|^2 + \frac{L^2}{\varepsilon^2} \|\delta_t e^{n+1}\|^2. \quad (3.93)$$

Substituting $\tilde{J}_1, \dots, \tilde{J}_5$ into (3.88), we have

$$\begin{aligned} & \frac{1}{\tau} \|\delta_t e^{n+1}\|^2 + \frac{\varepsilon}{2} (\|\nabla e^{n+1}\|^2 - \|\nabla e^n\|^2) + \frac{L}{2\varepsilon} (\|\delta_t e^{n+1}\|^2 - \|\delta_t e^n\|^2) \\ & + A\tau \|\delta_t e^{n+1}\|^2 + \frac{B}{2} (\|\delta_t e^{n+1}\|^2 - \|\delta_t e^n\|^2 + \|\delta_{tt} e^{n+1}\|^2) \\ & \leq \varepsilon \|R_1^{n+1}\|^2 + A^2 \varepsilon \|R_2^{n+1}\|^2 + B^2 \varepsilon \|R_3^{n+1}\|^2 + \varepsilon^3 \|\Delta R_4^{n+1}\|^2 + \frac{L^2}{4\varepsilon} \|R_3^{n+1}\|^2 \\ & + \frac{L^2}{\varepsilon} \|R_4^{n+1}\|^2 + \left(\frac{5L}{4\varepsilon} + \frac{3}{2\varepsilon} + \frac{L^2}{\varepsilon^2} \right) \|\delta_t e^{n+1}\|^2 + \frac{1}{4} \left\| \frac{e^{n+1} + e^n}{2} \right\|^2. \end{aligned} \quad (3.94)$$

By combining (3.87) and (3.94), we get

$$\begin{aligned} & \frac{1}{2\tau} (\|e^{n+1}\|^2 - \|e^n\|^2) + \frac{\varepsilon}{2} (\|\nabla e^{n+1}\|^2 - \|\nabla e^n\|^2) + \frac{A\tau}{2} (\|e^{n+1}\|^2 - \|e^n\|^2) \\ & + \left(\frac{B}{2} + 2B^2 + \frac{L}{2\varepsilon} + \frac{L^2}{2\varepsilon^2} \right) (\|\delta_t e^{n+1}\|^2 - \|\delta_t e^n\|^2) \\ & + A\tau \|\delta_t e^{n+1}\|^2 + \frac{B}{2} \|\delta_{tt} e^{n+1}\|^2 + \frac{1}{\tau} \|\delta_t e^{n+1}\|^2 + \varepsilon^2 \left\| \nabla \frac{e^{n+1} + e^n}{2} \right\|^2 \\ & \leq (1 + \varepsilon) \left(\|R_1^{n+1}\|^2 + A^2 \|R_2^{n+1}\|^2 + B^2 \|R_3^{n+1}\|^2 + \varepsilon^2 \|\Delta R_4^{n+1}\|^2 + \frac{L^2}{4\varepsilon^2} \|R_3^{n+1}\|^2 \right) \\ & + \left(\frac{C_2}{\varepsilon^2} + \frac{L^2}{\varepsilon} \right) \|R_4^{n+1}\|^2 + \left(4B^2 + 2\frac{L^2}{\varepsilon^2} + \frac{5L}{4\varepsilon} + \frac{3}{2\varepsilon} \right) \|\delta_t e^{n+1}\|^2 \\ & + \left(\frac{5}{2} + C_0 \varepsilon (1 - \varepsilon) + L \right) \left\| \frac{e^{n+1} + e^n}{2} \right\|^2 + G^{n+1} \left\| \frac{e^{n+1} + e^n}{2} \right\|^2 \\ & + Q^{n+1} \left\| \nabla \frac{e^{n+1} + e^n}{2} \right\|^2, \end{aligned} \quad (3.95)$$

where $Q^{n+1} = \frac{d}{6} \varepsilon^{\frac{3}{d}} \left\| \nabla \frac{e^{n+1} + e^n}{2} \right\|$, $G^{n+1} = \left(\frac{6-d}{6} \left(\frac{L_2 K}{\varepsilon^{\frac{3}{2}}} \right)^{\frac{6}{6-d}} + \frac{L_2 K}{\varepsilon} \right) \left\| \frac{e^{n+1} + e^n}{2} \right\|$. Taking $\tau \leq 1 / \left(4B^2 + 2\frac{L^2}{\varepsilon^2} + \frac{5L}{4\varepsilon} + \frac{3}{2\varepsilon} \right)$, if Q^{n+1} is uniformly bounded by constant $\frac{\varepsilon^2}{2}$, G^{n+1} is uniformly bounded by constant $\frac{1}{2}$, then by Grönwall's inequality, we get the finer error estimate (3.77).

We prove this by induction. Assuming that the finer estimate (3.77) holds for all first N time steps, the coarse estimate (3.55) leads to

$$\begin{aligned} & \|e^{N+1}\|^2 + 2\tau\varepsilon \left\| \nabla \frac{e^{N+1} + e^N}{2} \right\|^2 + A\tau^2 \|e^{N+1}\|^2 + B\tau \|e^{N+1}\|^2 \\ & \lesssim \varepsilon^{-\max\{4\sigma_1+11, \sigma_0\}} \tau^4. \end{aligned} \quad (3.96)$$

Then, if $\tau \lesssim \varepsilon^{\frac{1}{3} \max\{4\sigma_1+11, \sigma_0\} + \frac{5}{3} - \frac{2}{d}}$, we have

$$Q^{N+1} \lesssim \varepsilon^{\frac{3}{d}} \varepsilon^{-\frac{1}{2} \max\{4\sigma_1+11, \sigma_0\} - \frac{1}{2}} \tau^{\frac{3}{2}} \lesssim \frac{\varepsilon^2}{2}. \quad (3.97)$$

If $\tau \lesssim \varepsilon^{\frac{1}{4} \max\{4\sigma_1+11, \sigma_0\} + \frac{9}{2(6-d)}}$, we have

$$G^{N+1} \lesssim \varepsilon^{-\frac{9}{6-d}} \varepsilon^{-\frac{1}{2} \max\{4\sigma_1+11, \sigma_0\}} \tau^2 \lesssim \frac{1}{2}. \quad (3.98)$$

By taking τ that satisfies inequality (3.76), we get the finer error estimate for $N + 1$ step, and the proof is completed by mathematical induction. \square

REMARK 3.1. Theorems 3.2 and 3.1 are valid for the special cases i) $A = 0$, ii) $B = 0$, iii) both $A = 0$ and $B = 0$, since the conditions (2.5) and (2.18) are not used in the proof. On the other hand, in Theorems 3.2 and 3.1, the step size needs to be smaller than ε^2 to guarantee the convergence, which is much stronger than the requirement for the unstabilized schemes (i.e. the case $A = B = 0$) to be stable.

REMARK 3.2. The proofs of Theorem 3.1 and Theorem 3.2 are inspired by the works [21, 24, 32] and [22] for first order convex splitting schemes. The main difference is that we use a mathematical induction to handle high order terms coming from the L^3 term, while a generalized Grönwall’s lemma is used in [21, 22], and a continuation argument is used in [32].

REMARK 3.3. For the case that $\gamma = O(1/\varepsilon)$, we can get similar second order convergence results where the constant does not depend on $1/\varepsilon$ exponentially for both SL-BDF2 and SL-CN schemes. Take the SL-BDF2 scheme as an example. By using a Cauchy inequality with ε , one can put an ε in front of the $\|e^{n+1}\|^2$ terms in (3.29), (3.30), (3.31), (3.41) and (3.43). Then, by replacing the factor $(1 - \varepsilon)$ in (3.46) with $1 - \varepsilon^2$, and multiplying (3.47) by ε , we can get an estimate similar to (3.40) for time steps small enough, but the exponential factor now scales like $\exp(O(\varepsilon)T)$.

4. Implementation and numerical results

In this section, we numerically verify that our schemes are second order accurate in time and energy stable.

We use the commonly used double-well potential $F(\phi) = \frac{1}{4}(\phi^2 - 1)^2$. Since the exact solution satisfies the maximum principle $|\phi| \leq 1$, it is a common practice to modify $F(\phi)$ to have a quadratic growth for $|\phi| > 1$, such that a global Lipschitz condition is satisfied (cf. e.g. [9, 40]). To get a C^4 smooth double-well potential with quadratic growth, we introduce $\hat{F}(\phi) \in C^\infty(\mathbf{R})$ as a smooth mollification of

$$\hat{F}(\phi) = \begin{cases} \frac{11}{2}(\phi - 2)^2 + 6(\phi - 2) + \frac{9}{4}, & \phi > 2, \\ \frac{1}{4}(\phi^2 - 1)^2, & \phi \in [-2, 2], \\ \frac{11}{2}(\phi + 2)^2 - 6(\phi + 2) + \frac{9}{4}, & \phi < -2. \end{cases} \tag{4.1}$$

with a mollification parameter much smaller than 1, to replace $F(\phi)$. Note that the truncation points -2 and 2 used here are for convenience only. Other values outside of region $[-1, 1]$ can be used as well. For simplicity, we still denote the modified function \hat{F} by F .

4.1. Space discretization and implementation. To test the numerical scheme, we solve (1.1) in a 2-dimensional domain $\Omega = [-1, 1]^2$ and a 3-dimensional domain $\Omega = [-1, 1]^3$. We use a Legendre Galerkin method similar as in [41, 52] for spatial discretization. For example, we define

$$V_M = \text{span}\{\varphi_k(x)\varphi_j(y)\varphi_i(z), k, j, i = 0, \dots, M - 1\} \in H^1(\Omega),$$

as Galerkin approximation space for ϕ^{n+1} in 3-dimensional case. Here $\varphi_0(x) = L_0(x); \varphi_1(x) = L_1(x); \varphi_k(x) = L_k(x) - L_{k+2}(x), k = 2, \dots, M - 1$. $L_k(x)$ denotes the Legendre polynomial of degree k . Then the full discretized form for the SL-BDF2 scheme reads:

Find $(\phi^{n+1}, \mu^{n+1}) \in (V_M)^2$ such that

$$\frac{1}{2\tau\gamma}(3\phi^{n+1} - 4\phi^n + \phi^{n-1}, \omega) = -\varepsilon(\nabla\phi^{n+1}, \nabla\varphi) - \frac{1}{\varepsilon}(f(2\phi^n - \phi^{n-1}), \varphi) - A\tau(\delta_t\phi^{n+1}, \varphi) - B(\delta_{tt}\phi^{n+1}, \varphi), \quad \forall \varphi \in V_M. \quad (4.2)$$

This is a linear system with constant coefficients for ϕ^{n+1} , which can be efficiently solved. We use a spectral transform with double quadrature points to eliminate the aliasing error and efficiently evaluate the integration $(f(2\phi^n - \phi^{n-1}), \varphi)$ in Equation (4.2).

Given ϕ^0 , to start the second order schemes, we use following first order stabilized scheme with smaller time steps to generate ϕ^1 ,

$$\frac{\varphi^{n+1} - \varphi^n}{\tau\gamma} = \varepsilon\Delta\varphi^{n+1} - \frac{1}{\varepsilon}f(\varphi^n) - A\delta_t\varphi^{n+1}, \quad n=0, \dots, m-1, \quad (4.3)$$

where $\varphi^0 = \phi^0$, $\varphi^1 = \phi^m$.

We take $\varepsilon = 0.075$ and $M = 63$ and use random initial values ϕ_0 to test the stability and accuracy of the proposed schemes. For the 3-dimensional case, the initial value is given as $\{\phi_0(x_i, y_j, z_k)\} \in \mathbf{R}^{2M \times 2M \times 2M}$ with x_i, y_j, z_k are tensor product Legendre-Gauss quadrature points and $\phi_0(x_i, y_j, z_k)$ is a uniformly distributed random number between -1 and 1 (shown in the first picture of Figure 4.1);

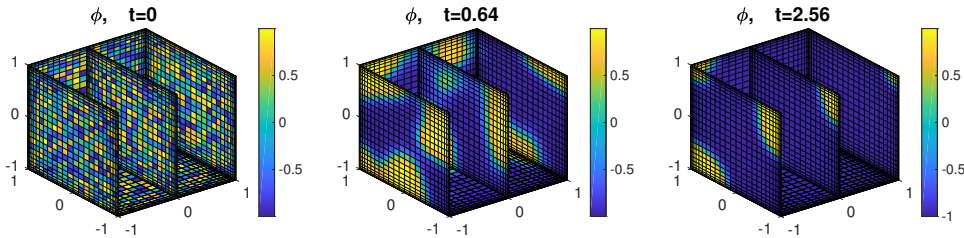


FIG. 4.1. The view of five different slices of the initial value ϕ_0 and the corresponding solution. (First) the random initial values ϕ_0 ; (Second) ϕ_1 , the solution at $t=0.64$ of the Allen-Cahn equation with initial value ϕ_0 ; (Third) the solution at $t=2.56$ of the Allen-Cahn equation with initial value ϕ_0 . Equation parameters $\gamma = 1$, $\varepsilon = 0.075$.

τ	SL-BDF2			SL-CN		
	$B=0$	$B=5$	$B=10$	$B=0$	$B=5$	$B=10$
10	3	2	1	3	2	1
1	30	20	10	30	20	10
0.1	100	0	0	200	100	0
0.01	0	0	0	0	0	0

TABLE 4.1. The minimum values of A (only values $\{0, 1, \dots, 5\} \cup \{10, 15, \dots, 50\} \cup \{100, 150, \dots, 500\}$ are tested for A) to make SL-BDF2 and SL-CN scheme stable when B and τ taking different values. The results are from 3-dimensional simulations with $\gamma = 1$, $\varepsilon = 0.075$.

4.2. Stability results. We present the required minimum values of A (resp. B) with different B (resp. A) and τ values for stably solving the Allen-Cahn Equation (1.1)

τ	SL-BDF2			SL-CN		
	$A=0$	$A=10$	$A=20$	$A=0$	$A=10$	$A=20$
10	20	0	0	30	0	0
1	20	10	5	30	10	3
0.1	10	10	10	10	10	10
0.01	0	0	0	0	0	0

TABLE 4.2. The minimum values of B (only values $\{0,1,\dots,5\} \cup \{10,15,\dots,50\}$ are tested for B) to make scheme SL-BDF2 and SL-CN stable when A and τ taking different values. The results are from 3-dimensional simulations with $\gamma=1, \varepsilon=0.075$.

τ	SL-BDF2			SL-CN		
	$B=0$	$B=5$	$B=10$	$B=0$	$B=5$	$B=10$
10	3	2	1	4	2	1
1	35	20	20	30	20	10
0.1	100	10	0	200	100	0
0.01	0	0	0	0	0	0

TABLE 4.3. The minimum values of A (only values $\{0,1,\dots,5\} \cup \{10,15,\dots,50\} \cup \{100,150,\dots,500\}$ are tested for A) to make SL-BDF2 and SL-CN scheme stable when B and τ taking different values. The results are from 2-dimensional simulations with $\gamma=1, \varepsilon=0.075$.

τ	SL-BDF2			SL-CN		
	$A=0$	$A=10$	$A=20$	$A=0$	$A=10$	$A=20$
10	20	0	0	20	0	0
1	20	15	0	20	10	3
0.1	10	5	2	10	10	10
0.01	0	0	0	0	0	0

TABLE 4.4. The minimum values of B (only values $\{0,1,\dots,5\} \cup \{10,15,\dots,50\}$ are tested for B) to make scheme SL-BDF2 and SL-CN stable when A and τ taking different values. The results are from 2-dimensional simulations with $\gamma=1, \varepsilon=0.075$.

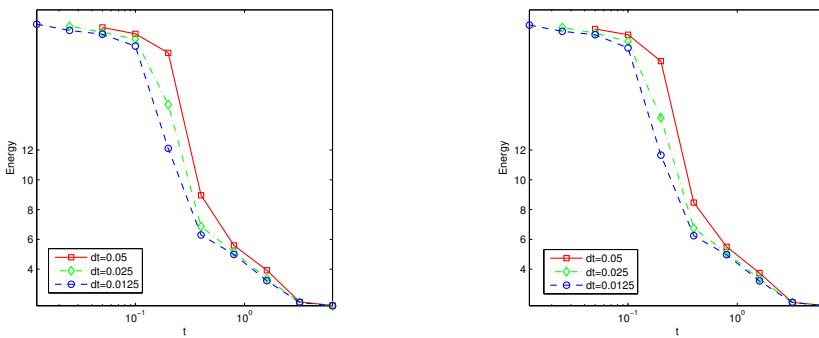


FIG. 4.2. The discrete energy dissipation of the two schemes solving the Allen-Cahn equation with initial value ϕ_1 , and parameters $\gamma=1, \varepsilon=0.075$. (Left) result of SL-BDF2 scheme; (Right) result of SL-CN scheme.

in 3-dimensional case in Table 4.1 (resp. 4.2). Here by “stably solving”, we mean that the energy keeps dissipating in first 1024 time steps. The corresponding 2-dimensional

τ	L^2 Error	Order	H^1 Error	Order
0.032	3.21 E-01		3.41	
0.016	1.19E-01	1.425	1.49	1.189
8E-3	2.90E-02	2.043	3.68E-01	2.021
4E-3	7.15E-03	2.019	8.91E-02	2.047
2E-3	1.82E-03	1.976	2.26E-02	1.980
1E-3	4.50E-04	2.016	5.58E-03	2.016

TABLE 4.5. *The convergence of the SL-BDF2 scheme with $B=5$, $A=10$ for the Allen-Cahn equation with initial value ϕ_1 , parameters $\gamma=0.5, \varepsilon=0.05$. The errors are calculated at $T=1.28$.*

τ	L^2 Error	Order	H^1 Error	Order
0.032	2.84E-01		3.11	
0.016	9.71E-02	1.548	1.25	1.320
8E-3	2.19E-02	2.152	2.76E-01	2.178
4E-3	5.33E-03	2.035	6.63E-02	2.055
2E-3	1.34E-03	1.997	1.66E-02	2.000
1E-3	3.27E-04	2.031	4.06E-03	2.032

TABLE 4.6. *The convergence of the SL-CN scheme with $B=5$, $A=10$ for the Allen-Cahn equation with initial value ϕ_1 , parameters $\gamma=0.5, \varepsilon=0.05$. The errors are calculated at $T=1.28$.*

results are given in Table 4.3 and 4.4. Those results are obtained by using initial value ϕ_0 , the results for the cases taking initial value ϕ_1 are similar. From those tables, we see that the maximum required A values are of order $O(\varepsilon^2)$ and the maximum required B values are of order $O(\varepsilon)$. For τ small enough, both schemes are stable with $A=0$ and $B=0$. This is consistent with our analysis result. On the other hand, by using a nonzero B , e.g. $B=10$, the requirement for a large A will be dramatically reduced.

To check the energy dissipation property, we present in Figure 4.2 the log-log plot of the energy versus time for the two schemes using different time step-sizes. We see that the energy decaying property is maintained.

4.3. Accuracy results. We take initial value ϕ_1 (see the second plot in Figure 4.1) for (1.1) to test the accuracy of the two schemes in a 2-dimensional domain $\Omega = [-1, 1] \times [-1, 1]$. The Allen-Cahn equation with the time relaxation parameter $\gamma=0.5$ is solved from $t=0$ to $T=1.28$. To calculate the numerical error, we use the numerical result generated using $\tau=10^{-4}$ as a reference to the exact solution. The results are given in Table 4.5 and Table 4.6. We see that the schemes are second order accurate in both L^2 and H^1 norm.

5. Conclusions

We proposed two second order stabilized linear schemes, namely the SL-BDF2 and the SL-CN scheme, for the phase-field Allen-Cahn equation. In both schemes, the nonlinear bulk forces are treated explicitly with two additional linear stabilization terms to guarantee unconditionally energy stable schemes. The schemes lead to linear systems with constant coefficients and thus can be efficiently solved. An optimal error estimate is given by using a spectrum argument to remove the exponential dependence on $1/\varepsilon$. The error analysis also holds for the special cases when one of the stabilization constants or both of them take zero values. Numerical results verified the stability and accuracy of the proposed schemes.

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REFERENCES

- [1] 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**:1085–1095, 1979. [1](#), [2.1](#)
- [2] A. Baskaran, P. Zhou, Z. Hu, C. Wang, S. M. Wise, and J. S. Lowengrub, *Energy stable and efficient finite-difference nonlinear multigrid schemes for the modified phase field crystal equation*, J. Comput. Phys., **250**:270–292, 2013. [1](#)
- [3] B. Benesová, C. Melcher, and E. Süli, *An implicit midpoint spectral approximation of nonlocal Cahn–Hilliard equations*, SIAM J. Numer. Anal., **52**:1466–1496, 2014. [1](#)
- [4] J. W. Cahn and J. E. Hilliard, *Free energy of a nonuniform system. I. interfacial free energy*, J. Chem. Phys., **28**:258–267, 1958. [1](#)
- [5] L. Chen and J. Shen, *Applications of semi-implicit Fourier-spectral method to phase field equations*, Comput. Phys. Commun., **108**:147–158, 1998. [1](#)
- [6] W. Chen, C. Wang, X. Wang, and S. M. Wise, *A linear iteration algorithm for a second-order energy stable scheme for a thin film model without slope selection*, J. Sci. Comput., **59**:574–601, 2014. [1](#)
- [7] X. Chen, *Spectrum for the Allen-Cahn, Cahn-Hilliard, and phase-field equations for generic interfaces*, Commun. Part. Diff. Eqs., **19**:1371–1395, 1994. [1](#), [2.1](#), [3.1](#), [3.2](#)
- [8] K. Cheng, C. Wang, S. M. Wise, and X. Yue, *A second-order, weakly energy-stable pseudo-spectral scheme for the Cahn-Hilliard equation and its solution by the homogeneous linear iteration method*, J. Sci. Comput., **69**:1083–1114, 2016. [1](#)
- [9] N. Condatte, C. Melcher, and E. Süli, *Spectral approximation of pattern-forming nonlinear evolution equations with double-well potentials of quadratic growth*, Math. Comput., **80**:205–223, 2011. [1](#), [4](#)
- [10] P. de Mottoni and M. Schatzman, *Évolution géométrique d’interfaces. (Geometrical evolution of interfaces)*, C. R. Acad. Sci. Sbr. I, **309**:453–458, 1989. [1](#)
- [11] P. de Mottoni and M. Schatzman, *Geometrical evolution of developed interfaces*, T. Am. Math. Soc., **347**:1533–1589, 1995. [1](#)
- [12] A. E. Diegel, C. Wang, and S. M. Wise, *Stability and convergence of a second order mixed finite element method for the Cahn-Hilliard equation*, IMA J. Numer. Anal., **36**:1867–1897, 2016. [1](#)
- [13] Q. Du and R. A. Nicolaides, *Numerical analysis of a continuum model of phase transition*, SIAM J. Numer. Anal., **28**:1310–1322, 1991. [1](#)
- [14] K. R. Elder and M. Grant, *Modeling elastic and plastic deformations in nonequilibrium processing using phase field crystals*, Phys. Rev. E, **70**:051605, 2004. [1](#)
- [15] C. Elliott and H. Garcke, *On the Cahn-Hilliard equation with degenerate mobility*, SIAM J. Math. Anal., **27**:404–423, 1996. [1](#)
- [16] C. M. Elliott, *The Cahn-Hilliard model for the kinetics of phase separation*, in Mathematical Models for Phase Change Problems, International Series of Numerical Mathematics, Springer, **88**:35–73, 1989. [1](#)
- [17] C. M. Elliott and A. M. Stuart, *The global dynamics of discrete semilinear parabolic equations*, SIAM J. Numer. Anal., **30**:1622–1663, 1993. [1](#)
- [18] D. J. Eyre, *Unconditionally gradient stable time marching the Cahn-Hilliard equation*, Comput. Math. Mode. Microstructural Evolution, **529**:39–46, 1998. [1](#)
- [19] W. Feng, Z. Guan, J. Lowengrub, C. Wang, S. M. Wise, and Y. Chen, *A uniquely solvable, energy stable numerical scheme for the functionalized Cahn-Hilliard equation and its convergence analysis*, J. Sci. Comput., **76**(3):1938–1967, 2018. [1](#)
- [20] X. Feng, *Fully discrete finite element approximations of the Navier–Stokes–Cahn-Hilliard diffuse interface model for two-phase fluid flows*, SIAM J. Numer. Anal., **44**:1049–1072, 2006. [1](#)
- [21] X. Feng and Y. Li, *Analysis of symmetric interior penalty discontinuous Galerkin methods for the Allen-Cahn equation and the mean curvature flow*, IMA J. Numer. Anal., **35**:1622–1651, 2015. [1](#), [2.4](#), [3.2](#)
- [22] X. Feng, Y. Li, and Y. Xing, *Analysis of mixed interior penalty discontinuous Galerkin methods for the Cahn-Hilliard equation and the Hele-Shaw flow*, SIAM J. Numer. Anal., **54**:825–847, 2016. [1](#), [3.2](#)

- [23] X. Feng and A. Prohl, *Numerical analysis of the Allen-Cahn equation and approximation for mean curvature flows*, Numer. Math., **94**:33–65, 2003. [1](#), [2.1](#), [2.4](#)
- [24] X. Feng and A. Prohl, *Error analysis of a mixed finite element method for the Cahn-Hilliard equation*, Numer. Math., **99**:47–84, 2004. [1](#), [3.2](#)
- [25] D. Furihata, *A stable and conservative finite difference scheme for the Cahn-Hilliard equation*, Numer. Math., **87**:675–699, 2001. [1](#)
- [26] H. Gomez and T. J. R. Hughes, *Provably unconditionally stable, second-order time-accurate, mixed variational methods for phase-field models*, J. Comput. Phys., **230**:5310–5327, 2011. [1](#)
- [27] F. Guilln-Gonzlez and G. Tierra, *On linear schemes for a Cahn-Hilliard diffuse interface model*, J. Comput. Phys., **234**:140–171, 2013. [1](#)
- [28] F. Guilln-Gonzlez and G. Tierra, *Second order schemes and time-step adaptivity for Allen-Cahn and Cahn-Hilliard models*, Comput. Math. Appl., **68**:821–846, 2014. [1](#)
- [29] J. Guo, C. Wang, S. M. Wise, and X. Yue, *An H^2 convergence of a second-order convex-splitting, finite difference scheme for the three-dimensional Cahn-Hilliard equation*, Commun. Math. Sci., **14**:489–515, 2016. [1](#)
- [30] D. Han, A. Brylev, X. Yang, and Z. Tan, *Numerical analysis of second order, fully discrete energy stable schemes for phase field models of two phase incompressible flows*, J. Sci. Comput., **70**:965–989, 2017. [1](#)
- [31] Y. He, Y. Liu, and T. Tang, *On large time-stepping methods for the Cahn-Hilliard equation*, Appl. Numer. Math., **57**:616–628, 2007. [1](#)
- [32] D. Kessler, R. H. Nochetto, and A. Schmidt, *A posteriori error control for the Allen-Cahn problem: circumventing Grönwall’s inequality*, ESAIM: Math. Model. Numer. Anal., **38**:129–142, 2004. [1](#), [3.2](#)
- [33] D. Li and Z. Qiao, *On second order semi-implicit Fourier spectral methods for 2D Cahn-Hilliard equations*, J. Sci. Comput., **70**:301–341, 2017. [1](#), [2.5](#), [2.5](#)
- [34] D. Li, Z. Qiao, and T. Tang, *Characterizing the stabilization size for semi-implicit Fourier-spectral method to phase field equations*, SIAM J. Numer. Anal., **54**:1653–1681, 2016. [1](#), [2.5](#)
- [35] W. Li, W. Chen, C. Wang, Y. Yan, and R. He, *A second order energy stable linear scheme for a thin film model without slope selection*, J. Sci. Comput., **76**(3):1905–1937, 2018. [1](#)
- [36] X. Li, Z. Qiao, and H. Zhang, *A second-order convex splitting scheme for a Cahn-Hilliard equation with variable interfacial parameters*, J. Comput. Math., **35**:693–710, 2017. [1](#)
- [37] F. Magaletti, F. Picano, M. Chinappi, L. Marino, and C. M. Casciola, *The sharp-interface limit of the Cahn-Hilliard Navier-Stokes model for binary fluids*, J Fluid. Mech., **714**:95–126, 2013. [2.4](#)
- [38] J. Shen, J. Xu, and J. Yang, *A new class of efficient and robust energy stable schemes for gradient flows*, [arXiv:1710.01331](#), 2017. [1](#)
- [39] J. Shen, J. Xu, and J. Yang, *The scalar auxiliary variable (SAV) approach for gradient flows*, J. Comput. Phys., **353**:407–416, 2017. [1](#)
- [40] J. Shen and X. Yang, *Numerical approximations of Allen-Cahn and Cahn-Hilliard equations*, Discrete Contin. Dyn. A., **28**:1669–1691, 2010. [1](#), [4](#)
- [41] J. Shen, X. Yang, and H. Yu, *Efficient energy stable numerical schemes for a phase field moving contact line model*, J. Comput. Phys., **284**:617–630, 2015. [4.1](#)
- [42] L. Wang and H. Yu, *Convergence analysis of an unconditionally energy stable linear Crank-Nicolson scheme for the Cahn-Hilliard equation*, J. Math. Study, **51**:89–114, 2017. [1](#), [2.5](#)
- [43] L. Wang and H. Yu, *On efficient second order stabilized semi-implicit schemes for the Cahn-Hilliard phase-field equation*, J. Sci. Comput., **77**(2):1185–1209, 2018. [1](#), [2.5](#)
- [44] X. Wu, G. J. van Zwieten, and K. G. van der Zee, *Stabilized second-order convex splitting schemes for Cahn-Hilliard models with application to diffuse-interface tumor-growth models*, Int. J. Numer. Meth. Biomed. Engng., **30**:180–203, 2014. [1](#)
- [45] C. Xu and T. Tang, *Stability analysis of large time-stepping methods for epitaxial growth models*, SIAM J. Num. Anal., **44**:1759–1779, 2006. [1](#), [2.5](#)
- [46] X. Xu, Y. Di, and H. Yu, *Sharp-interface limits of a phase-field model with a generalized Navier slip boundary condition for moving contact lines*, J. Fluid Mech., **849**:805–833, 2018. [2.4](#)
- [47] Y. Yan, W. Chen, C. Wang, and S. Wise, *A second-order energy stable BDF numerical scheme for the Cahn-Hilliard equation*, Commun. Comput. Phys., **23**:572–602, 2018. [1](#)
- [48] X. Yang, *Error analysis of stabilized semi-implicit method of Allen-Cahn equation*, Discrete. Cont. Dyn. B., **11**:1057–1070, 2009. [1](#), [2.1](#)
- [49] X. Yang, *Linear, first and second-order, unconditionally energy stable numerical schemes for the phase field model of homopolymer blends*, J. Comput. Phys., **327**:294–316, 2016. [1](#)
- [50] X. Yang and L. Ju, *Efficient linear schemes with unconditional energy stability for the phase field elastic bending energy model*, Comput. Method. Appl. Mech. Eng., **315**:691–712, 2017. [1](#)
- [51] X. Yang and H. Yu, *Efficient second order unconditionally stable schemes for a phase field moving*

- contact line model using an invariant energy quadratization approach*, SIAM J. Sci. Comput., **40(3):B889–B914**, 2018. [1](#)
- [52] H. Yu and X. Yang, *Numerical approximations for a phase-field moving contact line model with variable densities and viscosities*, J. Comput. Phys., **334:665–686**, 2017. [4.1](#)
- [53] 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., **515:293–317**, 2004. [1](#)
- [54] Z. Zhang, Y. Ma, and Z. Qiao, *An adaptive time-stepping strategy for solving the phase field crystal model*, J. Comput. Phys., **249:204–215**, 2013. [1](#)
- [55] J. Zhu, L.-Q. Chen, J. Shen, and V. Tikare, *Coarsening kinetics from a variable-mobility Cahn-Hilliard equation: Application of a semi-implicit Fourier spectral method*, Phys. Rev. E, **60:3564–3572**, 1999. [1](#)