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An improved error analysis for a second-order numerical scheme for the Cahn–Hilliard equation

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ABSTRACT

In this paper we present an error analysis for a second order accurate numerical scheme for the 2-D and 3-D Cahn–Hilliard (CH) equation, with an improved convergence constant. The unique solvability, unconditional energy stability, and a uniform-in-time H^2 stability of this numerical scheme have already been established. However, a standard error estimate gives a convergence constant in an order of $\exp(CT\varepsilon^{-m_0})$, with m_0 a positive integer and the interface width parameter ε being small, which comes from the application of discrete Gronwall inequality. To overcome this well-known difficulty, we apply a spectrum estimate for the linearized Cahn–Hilliard operator (Alikakos and Fusco, 1993; Chen, 1994; Feng and Prohl, 2004), perform a detailed numerical analysis, and get an improved estimate, in which the convergence constant depends on $\frac{1}{\varepsilon}$ only in a polynomial order, instead of the exponential order.

1. Introduction

Suppose that $\Omega = (0, L_x) \times (0, L_y) \times (0, L_z)$. For any $\phi \in H^1_{\rm per}(\Omega)$, we define an energy of the form

$$E(\phi) = \int_\Omega \left\{ \varepsilon^{-1} \left(\frac{1}{4}\phi^4 - \frac{1}{2}\phi^2 \right) + \frac{\varepsilon}{2}|\nabla\phi|^2 \right\} d\mathbf{x}, \tag{1.1}$$

where the interface width parameter $\varepsilon > 0$ is a small constant. See [1] for a detailed derivation of E. The conserved gradient dynamics on Ω is given by

$$\partial_t\phi = \nabla \cdot (\mathcal{M}(\phi)\nabla\mu), \quad \mu := \delta_\phi E = \varepsilon^{-1}\left(\phi^3 - \phi\right) - \varepsilon\Delta\phi, \tag{1.2}$$

where $\mathcal{M}(\phi) > 0$ is a mobility, and μ is the chemical potential. Periodic boundary conditions are imposed for both the phase field, ϕ, and the chemical potential, μ, as well as the higher order derivatives. It is easy to see that Eq. (1.2) is mass conservative, and the energy (1.1) is non-increasing in time along the solution trajectories of (1.2).

There have been a great deal of existing numerical works for the CH equations and related physical models, and many of them have been analyzed at a mathematical level; see the related Refs. [2–13], *et cetera*. In particular, it is observed

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that, in the numerical error analysis for this nonlinear gradient flow, the convergence constant is independent of the time step s and spatial grid size h; while it usually depends on the final time T and on the interface parameter ε in a singular way. A careful calculation reveals its dependence on T and ε in the form of $\exp\left(C\varepsilon^{-m_0}T\right)$, with m_0 an integer, which comes from the application of a discrete Gronwall inequality in the analysis.

Meanwhile, there have been a few recent works on the improved convergence constant for the CH equation (1.2). Specifically, Feng and Prohl [14] proved – for a first-order in time, fully discrete finite element scheme – that the convergence constant is of order $O(e^{C_0T}\varepsilon^{-m_0})$, for some positive integer m_0 and a constant $C_0 > 0$ that is independent of ε. Two more recent work of Feng, Li and Xing [15,16] apply a similar technique to analyze a first-order in time, discontinuous Galerkin (DG) scheme for the Allen–Cahn/Cahn–Hilliard equations. Such an elegant improvement was based on a subtle spectrum analysis for the linearized Cahn–Hilliard operator (with certain given structure assumptions of the solution), provided in earlier PDE analysis literature [17–21], *et cetera*.

On the other hand, all these existing works dealt with a first order temporal discretization. A direct extension of this numerical analysis technique to a second order (in time) scheme poses a serious challenge, due to the complicated form of the nonlinear terms and lack of a uniform-in-time estimate for the higher order H^m norms of the numerical solution.

In this paper we provide such an improved error estimate for a second order scheme to the CH equation, which has been introduced in a recent article [22]. For simplicity of presentation, we focus on the semi-discrete case, without spatial discretization; an extension to the fully discrete scheme could be carried out in an appropriate manner. The energy stability turns out to play an important role in the long time numerical simulation of the gradient flows. Among the numerical approaches to ensure the energy stability, the convex-splitting idea, originated by Eyre's pioneering work [23], has attracted a great deal of attention. See the related works for the phase field crystal (PFC) equation and the modified version [24–30], epitaxial thin film growth models [31–36], ternary system [37], the Cahn–Hilliard–Hele–Shaw (CHHS) and related models [38–46].

Among these energy stable works, extensive numerical experiments have shown a great advantage of the second order temporal splitting over the standard first order one in terms of numerical efficiency and accuracy. In addition, the second order energy stable scheme for the CH equation, as reported in [22,42,47,48], enjoys many advantages over the standard second order temporal approximations [8,49–52], in particular in terms of the unconditional energy stability, unconditionally unique solvability, the availability of a uniform-in-time H^2 numerical stability, et cetera.

On other hand, a careful calculation reveals that, for the error estimate reported in [22,42,47,48], the convergence constant depends on $\frac{1}{\varepsilon}$ in an exponential growth form, which comes from the application of discrete Gronwall inequality in the analysis. To overcome this difficulty, we have to derive a uniform-in-time (discrete) H^{m_0} (for $m_0 \geq 3$) bound for the numerical solution. In more detail, these bounds are dependent upon the initial H^{m_0} data, $\frac{1}{\varepsilon}$ (in a polynomial form), and independent of T. Since this bound is available for any $m_0 \geq 3$, a subtle observation implies that $\|\phi^{m+1} - \phi^m\|_{H^\ell}$ (with ϕ the numerical solution, ℓ an integer) is of order $O(s)$, with the constant independent of T, using certain discrete Hölder and Sobolev estimates. In other words, we are able to derive a uniform-in-time $O(s)$ estimate for $\|\phi^{m+1} - \phi^m\|_{H^\ell}$, independent of the convergence analysis. Moreover, we observe that, a difference analysis between $\phi^{m+1} - \phi^m$ and $\phi^m - \phi^{m-1}$ leads to a uniform-in-time $O(s^2)$ estimate for $\|\phi^{m+1} - 2\phi^m + \phi^{m-1}\|_{H^\ell}$, and the constant is dependent upon $\frac{1}{\varepsilon}$ in a polynomial form, independent of T.

Such a refined estimate is crucial to the improved error analysis in an H^{-1} norm. Both the error function for the chemical potential and the numerical error function are evaluated at the time instant $t^{m+1/2}$, and their differences with the exact numerical forms are analyzed with the help of $\|\phi^{m+1} - 2\phi^m + \phi^{m-1}\|_{H^\ell}$ estimate (for certain integer ℓ), which has been proved to be of order $O(s^2)$. Consequently, with all these preliminary estimates at hand, we could apply the spectrum analysis for the linearized Cahn–Hilliard operator [17–19], and arrive at an H^{-1} error estimate of order $O(s^2)$, with the convergence constant in the form of $O(e^{C_0T}\varepsilon^{-m_0})$, with C_0 independent of ε.

To simplify the presentation greatly, we employ no spatial discretization and work on a periodic domain. We deal only with the temporal discretization herein. In Section 2 we review the numerical scheme and its mathematical properties, such as the unique solvability, unconditional energy stability, and a uniform-in-time (discrete) H^2 stability. The higher order H^{m_0} (for $m_0 \geq 3$) numerical stability analysis is presented in Section 3. Subsequently, a uniform-in-time estimate for both $\|\phi^{m+1} - \phi^m\|_{H^\ell}$ and $\|\phi^{m+1} - 2\phi^m + \phi^{m-1}\|_{H^\ell}$ is provided in that section. In Section 4 we present the primary result of the paper, namely, an H^{-1} error estimate of order $O(s^2)$, with the convergence constant dependent on $\frac{1}{\varepsilon}$ in a polynomial form. Finally, some concluding remarks are made in Section 5.

2. Review of the numerical scheme and a few stability results

For simplicity, we assume that $\Omega = (0, 1)^3$. Let $M \in \mathbb{Z}^+$, and set $s := T/M$, where T is the final time. For simplicity of presentation, we take $\mathcal{M} \equiv 1$. The second order accurate, semi-discrete numerical scheme can be expressed in weak form as follows [22]: for $1 \leq m \leq M-1$, given $\phi^m, \phi^{m-1} \in H^1_{\rm per}(\Omega)$, find $\phi^{m+1}, \mu^{m+1/2} \in H^1_{\rm per}(\Omega)$, such that

$$\left(\phi^{m+1} - \phi^m, \nu\right) + s\left(\nabla\mu^{m+1/2}, \nabla\nu\right) = 0, \qquad \forall\ \nu \in H^1_{\rm per}(\Omega), \tag{2.1}$$

$$\varepsilon^{-1}\left(\chi\left(\phi^{m+1}, \phi^m\right) - \breve{\phi}^{m+1/2}, \psi\right) + \varepsilon\left(\nabla\hat{\phi}^{m+1/2}, \nabla\psi\right) - \left(\mu^{m+1/2}, \psi\right) = 0, \qquad \forall\ \psi \in H^1_{\rm per}(\Omega), \tag{2.2}$$

where

$$\chi\left(\phi^{m+1},\phi^{m}\right) := \frac{1}{4}\left(\phi^{m+1}+\phi^{m}\right)\left(\left(\phi^{m+1}\right)^{2}+\left(\phi^{m}\right)^{2}\right), \tag{2.3}$$

$$\breve{\phi}^{m+1/2} := \frac{3}{2}\phi^{m}-\frac{1}{2}\phi^{m-1}, \tag{2.4}$$

$$\hat{\phi}^{m+1/2} := \frac{3}{4}\phi^{m+1}+\frac{1}{4}\phi^{m-1}. \tag{2.5}$$

Meanwhile, ours is a two-step method, requiring either a special starting strategy or two starting values. For simplicity of presentation, we will assume that both $\phi^0, \phi^1 \in H^1_{\rm per}(\Omega)$ are given and correspond to the true PDE solution, Φ. In other words,

$$\phi^0 := \Phi(\,\cdot\,,0) \quad \text{and} \quad \phi^1 := \Phi(\,\cdot\,,s), \tag{2.6}$$

so that, among other properties,

$$E(\phi^1)+\int_0^s \|\nabla\mu(t)\|^2\,dt = E(\phi^0) \quad \text{and} \quad (\phi^1-\phi^0,1)=0,$$

where μ is the exact (true) chemical potential of the PDE. The local truncation error of the proposed scheme is second-order with respect to time.

Meanwhile, as demonstrated in [22,42], the original energy functional E is not guaranteed to be non-increasing in time; however, we can guarantee the dissipation of another modified energy. To be precise, for all $\psi, \phi \in H^1_{\rm per}(\Omega)$, define an alternate numerical energy via

$$\widetilde{E}(\phi,\psi) := E(\phi)+\frac{1}{4\varepsilon}\|\phi-\psi\|^2+\frac{\varepsilon}{8}\|\nabla_h(\phi-\psi)\|^2. \tag{2.7}$$

Note that this energy is consistent with the energy (1.1). For example, suppose that $u : \Omega\times[0,T]\to\mathbb{R}$ is a sufficiently regular, Ω-periodic function and set $u_s := u(\,\cdot\,,t_0+s)$. Then, clearly, $\widetilde{E}(u_0,u_s)\to E(u(\,\cdot\,,t_0))$, as $s\to 0$.

The unique solvability and unconditional energy stability for the second order scheme (2.1) have been established for the fully discrete case [22]; the analysis for the semi-discrete scheme is even simpler, and we recall it in the next theorem.

Theorem 2.1. *The second-order scheme (2.1) is uniquely solvable for any time step-size $s>0$, and it is mass conserving,* i.e., $\left(\phi^{m+1}-\phi^m,1\right)=0$, *for all $0\le m\le M-1$. In addition, suppose that $\phi^{m+1},\ \phi^m,\ \phi^{m-1}\in H^1_{\rm per}(\Omega)$ are solutions to (2.1). The second-order scheme (2.1) is unconditionally energy stable with respect to (2.7), meaning that for any time step-size $s>0$ and any $1\le m\le M-1$, $\widetilde{E}(\phi^{m+1},\phi^m)\le\widetilde{E}(\phi^m,\phi^{m-1})$. More precisely,*

$$\widetilde{E}(\phi^{m+1},\phi^m)+s\left\|\nabla\mu^{m+1/2}\right\|^2+R\left(\widetilde{\Delta}_s\phi^m\right)=\widetilde{E}(\phi^m,\phi^{m-1}), \tag{2.8}$$

where

$$R\left(\widetilde{\Delta}_s\phi^m\right) := \frac{\varepsilon}{8}\left\|\nabla\left(\widetilde{\Delta}_s\phi^m\right)\right\|^2+\frac{1}{4\varepsilon}\left\|\widetilde{\Delta}_s\phi^m\right\|^2, \tag{2.9}$$

and

$$\widetilde{\Delta}_s\phi^m := \phi^{m+1}-2\phi^m+\phi^{m-1}.$$

If $\phi^0,\phi^1\in H^1_{\rm per}(\Omega)$ are given as in (2.6), where the exact PDE solution, Φ is sufficiently regular, then we have the following stabilities

$$\|\nabla\phi\|^2_{L^\infty(0,T;L^2)} := \max_{0\le m\le M}\left\|\nabla\phi^m\right\|^2\le C_{1,\varepsilon}=:C_1\varepsilon^{-k_1}, \tag{2.10}$$

$$\|\phi\|^2_{L^\infty(0,T;L^4)} := \max_{0\le m\le M}\left\|\phi^m\right\|^2_{L^4}\le C_{1,\varepsilon}=:C_1\varepsilon^{-k_1}, \tag{2.11}$$

$$\|\phi\|^2_{L^\infty(0,T;H^1)} := \max_{0\le m\le M}\left\|\phi^m\right\|^2_{H^1}\le C_{1,\varepsilon}=:C_1\varepsilon^{-k_1}, \tag{2.12}$$

where k_1 is a positive integer and $C_1>0$ is a constant that is independent of s, T, and ε.

A uniform-in-time $L^\infty(0,T;H^2)$ bound of the numerical solution has also been established in [22] at the fully discrete level. Using similar techniques, the estimate can be established at the semi-discrete level:

Theorem 2.2. *Assume that the hypotheses of Theorem 2.1 hold. Then, if $s\le C\varepsilon^{-1}$, where $C>0$ is a certain constant that is independent of ε, we have*

$$\|\phi\|^2_{L^\infty(0,T;H^2)} := \max_{0\le m\le M}\left\|\phi^m\right\|^2_{H^2}\le C_{2,\varepsilon}=:C_2\varepsilon^{-k_2}, \tag{2.13}$$

where k_2 is a positive integer and $C_2>0$ is a constant that is independent of s, T, and ε.

Remark 2.3. We shall assume, from this point forward, that $\phi^0, \phi^1 \in H^1_{\text{per}}(\Omega)$ have sufficient additional spatial regularity to guarantee that $\phi^k \in H^{m_0}_{\text{per}}(\Omega)$, for all $k = 2, \ldots, M$, for $m_0 \in \mathbb{N}$ as large as desired.

3. Some estimates of the numerical scheme

3.1. $L^\infty(0, T; H^{m_0})$ ($m_0 \geq 3$) bound of the scheme

The uniform-in-time H^1 and H^2 bound of the numerical solution have been demonstrated in [22]. Meanwhile, these two bounds are not sufficient to assure an error estimate with the desired improved convergence constant. In this section, we establish the uniform-in-time H^{m_0} bound, for any $m_0 \geq 3$, of the numerical solution. We will see that such a bound depends on ε^{-1} to some integer power.

Theorem 3.1. *Assume that the hypotheses of Theorem 2.1 hold. Then, if $s \leq {}^{176C_R^2}/_{45\varepsilon}$, where $C_R > 0$ is a constant of elliptic regularity, used below, we have*

$$\|\phi\|_{L^\infty(0,T;H^3)} := \max_{0\leq m\leq M} \left\|\phi^m\right\|_{H^3} \leq C_{3,\varepsilon} =: C_3\varepsilon^{-k_3}, \tag{3.1}$$

where k_3 is a positive integer and $C_3 > 0$ is a constant that is independent of s, T, and ε.

Proof. Taking $\nu = \Delta^3\phi^{m+1}$ in (2.1) gives

$$\begin{aligned} &-\left(\phi^{m+1} - \phi^m, \Delta^3\phi^{m+1}\right) - \varepsilon^{-1}s\left(\Delta^3\phi^{m+1}, \Delta\breve{\phi}^{m+1/2}\right) \\ &\quad + \varepsilon^{-1}s\left(\Delta^3\phi^{m+1}, \Delta\chi(\phi^{m+1}, \phi^m)\right) - \varepsilon s\left(\Delta^3\phi^{m+1}, \Delta^2\hat{\phi}^{m+1/2}\right) = 0. \end{aligned} \tag{3.2}$$

An application of integration-by-parts using periodic boundary conditions yields

$$\begin{aligned} -\left(\phi^{m+1} - \phi^m, \Delta^3\phi^{m+1}\right) &= \left(\nabla\Delta(\phi^{m+1} - \phi^m), \nabla\Delta\phi^{m+1}\right) \\ &= \frac{1}{2}\left(\left\|\nabla\Delta\phi^{m+1}\right\|^2 - \left\|\nabla\Delta\phi^m\right\|_2^2\right) \\ &\quad + \frac{1}{2}\left\|\nabla\Delta(\phi^{m+1} - \phi^m)\right\|^2. \end{aligned} \tag{3.3}$$

For the concave diffusion term, we have

$$\begin{aligned} \left(\Delta^3\phi^{m+1}, \Delta\breve{\phi}^{m+1/2}\right) &= -\left(\nabla\Delta^2\phi^{m+1}, \nabla\Delta\breve{\phi}^{m+1/2}\right) \\ &\leq \alpha\left\|\nabla\Delta^2\phi^{m+1}\right\|^2 + \frac{1}{4\alpha}\left\|\nabla\Delta\breve{\phi}^{m+1/2}\right\|^2 \\ &\leq \alpha\left\|\nabla\Delta^2\phi^{m+1}\right\|^2 + \frac{9}{8\alpha}\left\|\nabla\Delta\phi^m\right\|^2 + \frac{1}{8\alpha}\left\|\nabla\Delta\phi^{m-1}\right\|^2, \end{aligned} \tag{3.4}$$

for any $\alpha > 0$. Meanwhile, the quantities $\|\nabla\Delta\phi^m\|^2$, $\left\|\nabla\Delta\phi^{m-1}\right\|^2$ can be controlled by

$$\left\|\nabla\Delta\phi^\ell\right\|^2 \leq \frac{1}{4\alpha^2}\left\|\nabla\phi^\ell\right\|^2 + \alpha^2\left\|\nabla\Delta^2\phi^\ell\right\|^2 \leq \frac{C_{1,\varepsilon}}{4\alpha^2} + \alpha^2\left\|\nabla\Delta^2\phi^\ell\right\|^2, \tag{3.5}$$

for any $\alpha > 0$, for $\ell = m, m-1$. A combination of (3.4) and (3.5) shows that

$$\begin{aligned} \left(\Delta^3\phi^{m+1}, \Delta\breve{\phi}^{m+1/2}\right) &\leq \alpha\left\|\nabla\Delta^2\phi^{m+1}\right\|^2 + \frac{9\alpha}{8}\left\|\nabla\Delta^2\phi^m\right\|^2 \\ &\quad + \frac{\alpha}{8}\left\|\nabla\Delta^2\phi^{m-1}\right\|^2 + \frac{5C_{1,\varepsilon}}{16\alpha^3}, \end{aligned} \tag{3.6}$$

for any $\alpha > 0$.

The bi-harmonic diffusion term can be analyzed as follows:

$$\begin{aligned} -\left(\Delta^3\phi^{m+1}, \Delta^2\hat{\phi}^{m+1/2}\right) &= \frac{3}{4}\left\|\nabla\Delta^2\phi^{m+1}\right\|^2 + \frac{1}{4}\left(\nabla\Delta^2\phi^{m+1}, \nabla\Delta^2\phi^{m-1}\right) \\ &\geq \frac{3}{4}\left\|\nabla\Delta^2\phi^{m+1}\right\|^2 - \frac{1}{8}\left(\left\|\nabla\Delta^2\phi^{m+1}\right\|^2 + \left\|\nabla\Delta^2\phi^{m-1}\right\|^2\right) \\ &\geq \frac{5}{8}\left\|\nabla\Delta^2\phi^{m+1}\right\|^2 - \frac{1}{8}\left\|\nabla\Delta^2\phi^{m-1}\right\|^2. \end{aligned} \tag{3.7}$$

As one might expect, all of the difficult work is in dealing with the nonlinear term. Regarding this, we begin with the following inequality:

$$\begin{aligned} -\left(\Delta^3\phi^{m+1}, \Delta\chi(\phi^{m+1}, \phi^m)\right) &= \left(\nabla\Delta^2\phi^{m+1}, \nabla\Delta\chi(\phi^{m+1}, \phi^m)\right) \\ &\leq \left\|\nabla\Delta^2\phi^{m+1}\right\| \cdot \left\|\nabla\Delta\chi(\phi^{m+1}, \phi^m)\right\|. \end{aligned} \tag{3.8}$$

The rest work is focused on obtaining a useful estimate for $\left\|\nabla\Delta\chi(\phi^{m+1},\phi^m)\right\|$. To this end, a detailed expansion and repeated application of Hölder's inequality implies that

$$\begin{aligned}\left\|\nabla\Delta\chi(\phi^{m+1},\phi^m)\right\| \le C\Big\{&\left(\left\|\phi^{m+1}\right\|_{L^\infty}^2+\left\|\phi^m\right\|_{L^\infty}^2\right)\cdot\left(\left\|\phi^{m+1}\right\|_{H^3}+\left\|\phi^m\right\|_{H^3}\right)\\ &+\left(\left\|\phi^{m+1}\right\|_{W^{1,\infty}}^2+\left\|\phi^m\right\|_{W^{1,\infty}}^2\right)\cdot\left(\left\|\phi^{m+1}\right\|_{H^2}+\left\|\phi^m\right\|_{H^2}\right)\\ &+\left(\left\|\nabla\phi^{m+1}\right\|_{L^6}^3+\left\|\nabla\phi^m\right\|_{L^6}^3\right)\Big\}. \end{aligned} \tag{3.9}$$

Meanwhile, based on the uniform-in-time H^2 bound (2.13) for the numerical solution, the following Sobolev inequalities are available:

$$\left\|\phi^\ell\right\|_{H^2}\le C_{2,\varepsilon}, \tag{3.10}$$

$$\left\|\phi^\ell\right\|_{L^\infty}+\left\|\nabla\phi^\ell\right\|_{L^6}\le C\left\|\phi^\ell\right\|_{H^2}\le CC_{2,\varepsilon}, \tag{3.11}$$

$$\begin{aligned}\left\|\phi^\ell\right\|_{W^{1,\infty}}&\le C\|\phi^\ell\|_{H^2}^{\frac34}\cdot\left\|\phi^\ell\right\|_{H^4}^{\frac14}\\ &\le C\left(\|\phi^\ell\|_{H^2}^{\frac34}\cdot\left\|\Delta^2\phi^\ell\right\|^{\frac14}+\left\|\phi^\ell\right\|_{H^2}\right)\\ &\le C\left(\left\|\phi^\ell\right\|_{H^2}^{\frac56}\cdot\left\|\nabla\Delta^2\phi^\ell\right\|^{\frac16}+\left\|\phi^\ell\right\|_{H^2}\right)\\ &\le C\left(C_{2,\varepsilon}^{\frac56}\cdot\left\|\nabla\Delta^2\phi^\ell\right\|^{\frac16}+C_{2,\varepsilon}\right),\end{aligned} \tag{3.12}$$

$$\begin{aligned}\left\|\phi^\ell\right\|_{H^3}&\le C\left\|\phi^\ell\right\|_{H^2}^{\frac23}\cdot\left\|\phi^\ell\right\|_{H^5}^{\frac13}\\ &\le C\left(\left\|\phi^\ell\right\|_{H^2}^{\frac23}\cdot\left\|\nabla\Delta^2\phi^\ell\right\|^{\frac13}+\left\|\phi^\ell\right\|_{H^2}\right)\\ &\le C\left(C_{2,\varepsilon}^{\frac23}\cdot\left\|\nabla\Delta^2\phi^\ell\right\|^{\frac13}+C_{2,\varepsilon}\right),\end{aligned} \tag{3.13}$$

for $\ell=m,m+1$, where the Gagliado–Nirenberg inequality [53] has been extensively used. In more details, the first step of (3.12) stands for an application of Gagliado–Nirenberg inequality, while the second step is based on the following elliptic regularity

$$\|\phi^\ell\|_{H^4}\le C(\|\phi^\ell\|_{H^2}+\|\Delta^2\phi^\ell\|),$$

which is always valid for ϕ^ℓ satisfying periodic boundary condition, i.e, both ϕ^ℓ, $\Delta\phi^\ell$ and $\Delta^2\phi^\ell$ are periodic. The third step of (3.12) is based on the following inequalities

$$\begin{aligned}&\left\|\Delta^2\phi^\ell\right\|^2=(\Delta^2\phi^\ell,\Delta^2\phi^\ell)=-(\nabla\Delta\phi^\ell,\nabla\Delta^2\phi^\ell)\le\|\nabla\Delta\phi^\ell\|\cdot\|\nabla\Delta^2\phi^\ell\|,\\ &\left\|\nabla\Delta\phi^\ell\right\|^2=(\nabla\Delta\phi^\ell,\nabla\Delta\phi^\ell)=-(\Delta\phi^\ell,\Delta^2\phi^\ell)\le\|\Delta\phi^\ell\|\cdot\|\Delta^2\phi^\ell\|,\\ \text{so that }\ &\left\|\Delta^2\phi^\ell\right\|\le\|\Delta\phi^\ell\|^{\frac13}\cdot\|\nabla\Delta^2\phi^\ell\|^{\frac23}\le\|\phi^\ell\|_{H^2}^{\frac13}\cdot\|\nabla\Delta^2\phi^\ell\|^{\frac23},\end{aligned}$$

in which the integration by parts and periodic boundary conditions have been extensively used. Inequality (3.13) could be derived in a similar manner. The first step stands for an application of weighed interpolation inequality, while the second step is based on the following elliptic regularity

$$\|\phi^\ell\|_{H^5}\le C(\|\phi^\ell\|_{H^2}+\|\nabla\Delta^2\phi^\ell\|),$$

which is always valid for ϕ^ℓ satisfying periodic boundary condition, i.e, both ϕ^ℓ, $\Delta\phi^\ell$ and $\Delta^2\phi^\ell$, $\nabla\Delta^2\phi^\ell$ are periodic. In turn, a substitution of (3.11)–(3.13) into (3.9) yields

$$\left\|\nabla\Delta\chi(\phi^{m+1},\phi^m)\right\|\le C\left(C_{2,\varepsilon}^{\frac83}\left(\left\|\nabla\Delta^2\phi^{m+1}\right\|^{\frac13}+\left\|\nabla\Delta^2\phi^m\right\|^{\frac13}\right)+C_{2,\varepsilon}^3\right). \tag{3.14}$$

Going back to (3.8), we arrive at

$$\begin{aligned}-\left(\Delta^3\phi^{m+1},\Delta\chi(\phi^{m+1},\phi^m)\right)&\le CC_{2,\varepsilon}^{\frac83}\left(\left\|\nabla\Delta^2\phi^{m+1}\right\|^{\frac43}+\left\|\nabla\Delta^2\phi^{m+1}\right\|\cdot\left\|\nabla\Delta\phi^m\right\|^{\frac13}\right)\\ &\quad+CC_{2,\varepsilon}^3\left\|\nabla\Delta^2\phi^{m+1}\right\|\\ &\le\frac{\varepsilon^2}{16}\left(\left\|\nabla\Delta^2\phi^{m+1}\right\|^2+\left\|\nabla\Delta^2\phi^m\right\|^2\right)\\ &\quad+C\varepsilon^{-4}C_{2,\varepsilon}^8+C\varepsilon^{-2}C_{2,\varepsilon}^6,\end{aligned} \tag{3.15}$$

in which the Young's inequality was repeatedly applied in the last step.

A combination of (3.2), (3.3), (3.6), (3.7) and (3.15) results in

$$\begin{aligned}&\left\|\nabla\Delta\phi^{m+1}\right\|^2-\left\|\nabla\Delta\phi^{m}\right\|^2+\Big(\frac{9\varepsilon}{8}-\frac{2\alpha}{\varepsilon}\Big)s\left\|\nabla\Delta^2\phi^{m+1}\right\|^2\\&\qquad\le\Big(\frac{9\alpha}{4\varepsilon}+\frac{\varepsilon}{8}\Big)s\left\|\nabla\Delta^2\phi^{m}\right\|^2+\Big(\frac{\varepsilon}{4}+\frac{\alpha}{4\varepsilon}\Big)s\left\|\nabla\Delta^2\phi^{m-1}\right\|^2+s\hat{C}_{3,\varepsilon},\end{aligned}\tag{3.16}$$

with

$$\hat{C}_{3,\varepsilon}:=C(\varepsilon^{-5}C_{2,\varepsilon}^8+\varepsilon^{-3}C_{2,\varepsilon}^6)+\frac{5C_{1,\varepsilon}}{8\alpha^3\varepsilon}.$$

Choosing $\alpha=\frac{1}{16}\varepsilon^2$ fixes $\hat{C}_{3,\varepsilon}$ and yields

$$\begin{aligned}&\left\|\nabla\Delta\phi^{m+1}\right\|^2-\left\|\nabla\Delta\phi^{m}\right\|^2+\varepsilon s\left\|\nabla\Delta^2\phi^{m+1}\right\|^2\\&\qquad\le\frac{17\varepsilon}{64}s\Big(\left\|\nabla\Delta^2\phi^{m}\right\|^2+\left\|\nabla\Delta^2\phi^{m-1}\right\|^2\Big)+s\hat{C}_{3,\varepsilon}.\end{aligned}\tag{3.17}$$

Now, adding $\frac{7\varepsilon}{16}\left\|\nabla\Delta^2\phi^{m}\right\|^2$ to both sides of the last inequality gives

$$\begin{aligned}&\left\|\nabla\Delta\phi^{m+1}\right\|^2+\varepsilon s\left\|\nabla\Delta^2\phi^{m+1}\right\|^2+\frac{7\varepsilon s}{16}\left\|\nabla\Delta^2\phi^{m}\right\|^2\\&\qquad\le\left\|\nabla\Delta\phi^{m}\right\|^2+\frac{45\varepsilon s}{64}\left\|\nabla\Delta^2\phi^{m}\right\|^2+\frac{17\varepsilon s}{64}\left\|\nabla\Delta^2\phi^{m-1}\right\|^2+s\hat{C}_{3,\varepsilon}.\end{aligned}\tag{3.18}$$

We define a modified "energy"

$$G^m:=\left\|\nabla\Delta\phi^{m}\right\|^2+\frac{45\varepsilon s}{64}\left\|\nabla\Delta^2\phi^{m}\right\|^2+\frac{17\varepsilon s}{64}\left\|\nabla\Delta^2\phi^{m-1}\right\|^2.\tag{3.19}$$

Then, it follows that

$$G^{m+1}+\frac{19\varepsilon s}{64}\left\|\nabla\Delta^2\phi^{m+1}\right\|_2^2+\frac{11\varepsilon s}{64}\left\|\nabla\Delta^2\phi^{m}\right\|_2^2\le G^m+s\hat{C}_{3,\varepsilon}.\tag{3.20}$$

Meanwhile, with the help of the elliptic regularity estimate $\|\nabla\Delta f\|\le C_R\|\nabla\Delta^2 f\|$, the following inequality could be derived:

$$\frac{19\varepsilon}{64}s\left\|\nabla\Delta^2\phi^{m+1}\right\|^2+\frac{11\varepsilon s}{64}\left\|\nabla\Delta^2\phi^{m}\right\|^2\ge\frac{\varepsilon s}{16}\left\|\nabla\Delta^2\phi^{m+1}\right\|^2+\frac{\varepsilon^2 s}{16C_R^2}G^{m+1},\tag{3.21}$$

provided that

$$s\le\frac{176C_R^2}{45\varepsilon}.\tag{3.22}$$

The details are left for interested readers. Note that the condition in (3.22) is very easily satisfied, as the bound on the right-hand-side will typically be greater than 1. As a result, we arrive at

$$\left(1+\frac{\varepsilon s}{16C_R^2}\right)G^{m+1}+\frac{\varepsilon s}{16}\left\|\nabla\Delta^2\phi^{m+1}\right\|^2\le G^m+s\hat{C}_{3,\varepsilon}.\tag{3.23}$$

Applying an induction argument with the last estimate, we get

$$G^{m+1}\le\left(1+\frac{\varepsilon s}{16C_R^2}\right)^{-(m+1)}G^0+\frac{16C_R^2\hat{C}_{3,\varepsilon}}{\varepsilon}\le G^0+\frac{16C_R^2\hat{C}_{3,\varepsilon}}{\varepsilon}.\tag{3.24}$$

Finally, (3.1) is a direct consequence of (3.24) and the elliptic regularity:

$$\begin{aligned}\left\|\phi^{m+1}\right\|_{H^3}&\le C\left(\left\|\phi^{m+1}\right\|+\left\|\nabla\Delta\phi^{m+1}\right\|\right)\\&\le C\left(C_{2,\varepsilon}+\left\|\nabla\Delta\phi^{m+1}\right\|\right)\\&\le C\left(C_{2,\varepsilon}+(G^{m+1})^{1/2}\right)\\&\le C\left(C_{2,\varepsilon}+(G^0)^{1/2}+\frac{4C_R\hat{C}_{3,\varepsilon}^{1/2}}{\varepsilon^{1/2}}\right):=C_{3,\varepsilon}.\end{aligned}\tag{3.25}$$

Note that $C_{3,\varepsilon}$ depends on ε^{-1} in a polynomial form, since $\hat{C}_{3,\varepsilon}$ does. The proof of Theorem 3.1 is complete. □

Using similar tools, a uniform-in-time H^ℓ bound for the numerical solution could be established, for any $\ell\ge3$, by setting $\nu=\Delta^\ell\phi^{m+1}$ in (2.1). The details are left for interested readers.

Theorem 3.2. *Assume that the hypotheses of Theorem 2.1 hold. Then, if $s \le C\varepsilon^{-1}$, where $C > 0$ is a certain constant, we have*

$$\|\phi\|_{L^\infty(0,T;H^\ell)} := \max_{0\le m\le M} \left\|\phi^m\right\|_{H^\ell} \le C_{\ell,\varepsilon} := C_\ell \varepsilon^{-k_\ell}, \tag{3.26}$$

where k_ℓ is a positive integer, which increases as ℓ increases, and $C_\ell > 0$ is a constant independent of s, T, and ε.

Remark 3.3. The global-in-time H^3 bound for the numerical solution, $C_{3,\varepsilon}$ in (3.25), depends singularly on ε. In more details, we have

$$C_{1,\varepsilon} = O(\varepsilon^{-1}), \tag{3.27}$$

$$C_{2,\varepsilon} = O(\varepsilon^{-13}), \quad \text{(for the 3-D case, as derived in [22])}, \tag{3.28}$$

$$\hat{C}_{3,\varepsilon} = O(\varepsilon^{-109}), \tag{3.29}$$

$$C_{3,\varepsilon} = O(\varepsilon^{-55}), \tag{3.30}$$

so that $k_3 = 55$.

In comparison, for the 2-D case, the corresponding index increases at a much lower rate; a careful analysis reveals that $C_{1,\varepsilon} = O(\varepsilon^{-1})$, $C_{2,\varepsilon} = O(\varepsilon^{-(7+\delta)})$, $C_{3,\varepsilon} = O(\varepsilon^{-(9+\delta')})$, (with $\delta > 0$, $\delta' > 0$), so that $k_3 = 10$. This in turn shows that, the higher order H^ℓ norm grows at a much faster rate for the 3-D CH flow than the 2-D version, which comes from different Sobolev inequalities.

3.2. Estimates for $\left\|\phi^{m+1} - \phi^m\right\|_{H^\ell}$ and $\left\|\phi^{m+1} - 2\phi^m + \phi^{m-1}\right\|_{H^\ell}$

The following estimate is needed in later analysis.

Theorem 3.4. *Assume that the hypotheses of Theorem 3.2 hold. Then we have*

$$\max_{0\le m\le M-1} \left\|\phi^{m+1} - \phi^m\right\|_{H^\ell} \le sD_{\ell,\varepsilon} := D_\ell \varepsilon^{-n_\ell}, \tag{3.31}$$

where n_ℓ is a positive integer, which increases as ℓ increases, and $D_\ell > 0$ is a constant independent of s, T, and ε.

Proof. The numerical scheme (2.1) shows that

$$\left\|\phi^{m+1} - \phi^m\right\|_{H^\ell} = s\left\|\Delta\mu^{m+1/2}\right\|_{H^\ell}. \tag{3.32}$$

By the expansion (2.2) for $\mu^{m+1/2}$, the following estimates could be derived, helped by repeated applications of the Hölder inequality and Sobolev embedding:

$$\begin{aligned}
\left\|\Delta\left(\chi\left(\phi^{m+1},\phi^m\right)\right)\right\|_{H^\ell} &\le C\left\|\chi\left(\phi^{m+1},\phi^m\right)\right\|_{H^{\ell+2}} \\
&\le C\left(\left\|\phi^{m+1}\right\|_{H^{\ell+2}}^3 + \left\|\phi^m\right\|_{H^{\ell+2}}^3\right) \\
&\le CC_{\ell+2,\varepsilon}^3,
\end{aligned} \tag{3.33}$$

$$\begin{aligned}
\left\|\Delta\breve{\phi}^{m+1/2}\right\|_{H^\ell} &\le C\left(\left\|\phi^m\right\|_{H^{\ell+2}} + \left\|\phi^{m-1}\right\|_{H^{\ell+2}}\right) \\
&\le CC_{\ell+2,\varepsilon},
\end{aligned} \tag{3.34}$$

$$\begin{aligned}
\left\|\Delta^2\hat{\phi}^{m+1/2}\right\|_{H^\ell} &\le C\left(\left\|\phi^{m+1}\right\|_{H^{\ell+4}} + \left\|\phi^{m-1}\right\|_{H^{\ell+4}}\right) \\
&\le CC_{\ell+4,\varepsilon},
\end{aligned} \tag{3.35}$$

with the uniform-in-time estimates (3.26) used. Consequently, a substitution of (3.33)–(3.35) into (3.32) yields

$$\left\|\phi^{m+1} - \phi^m\right\|_{H^\ell} \le sD_{\ell,\varepsilon}, \quad D_{\ell,\varepsilon} := C\left(\varepsilon^{-1}\left(C_{\ell+2,\varepsilon}^3 + C_{\ell+2,\varepsilon}\right) + \varepsilon C_{\ell+4,\varepsilon}\right). \tag{3.36}$$

Note that $D_{\ell,\varepsilon}$ depends on ε^{-1} in a polynomial form, since both $C_{\ell+2,\varepsilon}$ and $C_{\ell+4,\varepsilon}$ do as well. This completes the proof of Theorem 3.4. □

In addition, to analyze the second order accurate (in time) scheme, we need the following estimate.

Theorem 3.5. *Assume that the hypotheses of Theorem 3.2 hold. Then we have*

$$\max_{1\le m\le M-1} \left\|\phi^{m+1} - 2\phi^m + \phi^{m-1}\right\|_{H^\ell} \le Q_{\ell,\varepsilon} s^2, \quad Q_{\ell,\varepsilon} := Q_\ell \varepsilon^{-m_\ell}, \tag{3.37}$$

where m_ℓ is a positive integer, which increases as ℓ increases, and $Q_\ell > 0$ is a constant independent of s, T and ε.

Proof. Taking a difference between $\phi^{m+1} - \phi^m$ and $\phi^m - \phi^{m-1}$, we have

$$\left\| \phi^{m+1} - 2\phi^m + \phi^{m-1} \right\|_{H^\ell} = s \left\| \Delta(\mu^{m+1/2} - \mu^{m-1/2}) \right\|_{H^\ell}, \tag{3.38}$$

with

$$\begin{aligned} \mu^{m+1/2} - \mu^{m-1/2} = \varepsilon^{-1}\Big(& \chi\left(\phi^{m+1}, \phi^m\right) - \chi\left(\phi^m, \phi^{m-1}\right) \\ & - \frac{3}{2}(\phi^m - \phi^{m-1}) + \frac{1}{2}(\phi^{m-1} - \phi^{m-2})\Big) \\ & - \varepsilon \Delta \left(\frac{3}{4}(\phi^{m+1} - \phi^m) + \frac{1}{4}(\phi^m - \phi^{m-1}) \right), \end{aligned} \tag{3.39}$$

and

$$\begin{aligned} \chi\left(\phi^{m+1}, \phi^m\right) - \chi\left(\phi^m, \phi^{m-1}\right) = \frac{1}{4}\Big(& ((\phi^{m+1})^2 + (\phi^m)^2)(\phi^{m+1} - \phi^m + \phi^m - \phi^{m-1}) \\ & + (\phi^{m+1} + \phi^m)^2(\phi^{m+1} - \phi^m) \\ & + (\phi^{m+1} + \phi^m)(\phi^m + \phi^{m-1})(\phi^m - \phi^{m-1})\Big). \end{aligned} \tag{3.40}$$

In more detail, we observe that all the right-hand-side terms in (3.39) contain a factor of $\phi^i - \phi^{i-1}$, $m-1 \le i \le m+1$. With the help of (3.26) and (3.31), we are able to derive (3.37) in a similar manner as in Theorem 3.4. The details are skipped for simplicity of presentation. □

Remark 3.6. A uniform bound for $\|\phi^{m+1} - 2\phi^m + \phi^{m-1}\|_{H^\ell}$, given by (3.37), will play an essential role to establish an improved convergence analysis for a second order accurate (in time) scheme, as will be demonstrated in later sections. In comparison, Such a uniform estimate is not needed in the corresponding error analysis for the first order (accurate) in time schemes, as reported in [14–16,54].

3.3. Some related estimates for the exact solution

As before, by $\Phi(x, y, z, t)$ we denote as the exact solution of the CH equation (1.2), with sufficiently regular, periodic initial data. The following estimates could be derived by performing a standard energy estimate and Sobolev analysis. The details are skipped for brevity.

Lemma 3.7. *The following estimates are valid for the exact solution Φ:*

$$\|\Phi\|_{L^\infty(0,T;H^\ell)} \le C^*_{\ell,\varepsilon} := C^*_\ell \varepsilon^{-k_\ell}, \quad \forall\, \ell \ge 1, \tag{3.41}$$

$$\|\partial_t \Phi\|_{L^\infty(0,T;H^\ell)} \le D^*_{\ell,\varepsilon} := D^*_\ell \varepsilon^{-n_\ell}, \quad \forall \ell \ge 0, \tag{3.42}$$

$$\left\|\partial_t^2 \Phi\right\|_{L^\infty(0,T;H^\ell)} \le Q^*_{\ell,\varepsilon} := Q^*_\ell \varepsilon^{-m_\ell}, \quad \forall \ell \ge 0, \tag{3.43}$$

where k_ℓ, n_ℓ and m_ℓ are increasing sequences of positive integers – not necessarily the same as those specified before – and C^*_ℓ, D^*_ℓ, and Q^*_ℓ are positive constants that are independent of T, and ε.

Remark 3.8. The derivation of (3.42) and (3.43) is based on applying the original CH equation (1.2) and taking its temporal derivative, combined with the $L^\infty(0, T; H^\ell)$ estimate (3.41), so that the H^ℓ norm of the first and second order temporal derivatives are converted into certain spatial H^m norms of the exact solution.

The following result is a consequence of Lemma 3.7.

Lemma 3.9. *Denote $\Phi^{m+1/2} = \frac{1}{2}(\Phi^{m+1} + \Phi^m)$ and $\hat{\Phi}^{m+1/2} = \Phi(\,\cdot\,, t^{m+1/2})$. The following estimates are valid for the exact solution Φ:*

$$\max_{0\le m\le M-1} \left\|\Phi^{m+1} - \Phi^m\right\|_{H^\ell} \le \hat{D}^*_{\ell,\varepsilon} s, \quad \hat{D}^*_{\ell,\varepsilon} := \hat{D}^*_\ell \varepsilon^{-n_\ell}, \tag{3.44}$$

$$\max_{1\le m\le M-1} \left\|\Phi^{m+1} - 2\Phi^m + \Phi^{m-1}\right\|_{H^\ell} \le \hat{Q}^*_{\ell,\varepsilon} s^2, \quad \hat{Q}^*_{\ell,\varepsilon} := \hat{Q}^*_\ell \varepsilon^{-m_\ell}, \tag{3.45}$$

$$\max_{1\le m\le M-1} \left\|\Phi^{m+1} - 2\hat{\Phi}^{m+1/2} + \Phi^m\right\|_{H^\ell} \le \frac{1}{4}\hat{Q}^*_{\ell,\varepsilon} s^2, \tag{3.46}$$

for any $\ell \ge 1$, where k_ℓ, n_ℓ and m_ℓ are increasing sequences of positive integers – not necessarily the same as those specified before – and $\hat{D}^*_\ell$ and $\hat{Q}^*_\ell$ are positive constants that are independent of T, and ε.

Remark 3.10. The derivation of (3.44)–(3.46) is based on the following Taylor expansions (in time)

$$\Phi^{m+1} - \Phi^m = s\partial_t \Phi(\xi_1), \quad \exists\, \xi_1 \in (t^m, t^{m+1}), \tag{3.47}$$

$$\Phi^{m+1} - 2\Phi^m + \Phi^{m-1} = \frac{s^2}{12}\partial_t^2 \Phi(\xi_2), \quad \exists\, \xi_2 \in (t^{m-1}, t^{m+1}), \tag{3.48}$$

$$\Phi^{m+1} - 2\hat{\Phi}^{m+1/2} + \Phi^m = \frac{s^2}{48}\partial_t^2 \Phi(\xi_3), \quad \exists\, \xi_3 \in (t^m, t^{m+1}), \tag{3.49}$$

combined with the established estimates (3.42) and (3.43).

As a direct consequence, the following L^∞ bound could be derived; this estimate will be used in the improved error analysis in the next section.

Corollary 3.11. *We have the following estimate*

$$\left\|(\Phi^{m+1/2})^2 - (\hat{\Phi}^{m+1/2})^2\right\|_{L^\infty} \le Cs^2 E_{1,\varepsilon}, \quad \text{with } E_{1,\varepsilon} = E_1 \varepsilon^{-j_1}, \tag{3.50}$$

where j_1 is a positive integer and E_1 is a positive constant that is independent of s, T, and ε.

Proof. First, we observe that

$$\begin{aligned}\left\|(\Phi^{m+1/2})^2 - (\hat{\Phi}^{m+1/2})^2\right\|_{L^\infty} &= \left\|(\Phi^{m+1/2} + \hat{\Phi}^{m+1/2})\cdot(\Phi^{m+1/2} - \hat{\Phi}^{m+1/2})\right\|_{L^\infty} \\ &\le \left(\left\|\Phi^{m+1/2}\right\|_{L^\infty} + \left\|\hat{\Phi}^{m+1/2}\right\|_{L^\infty}\right)\cdot\left\|\Phi^{m+1/2} - \hat{\Phi}^{m+1/2}\right\|_{L^\infty}.\end{aligned} \tag{3.51}$$

The first two terms can be controlled via Sobolev inequality:

$$\begin{aligned}\left\|\Phi^{m+1/2}\right\|_{L^\infty} &\le C\left\|\Phi^{m+1/2}\right\|_{H^2} \le CC^*_{2,\varepsilon}, \\ \left\|\hat{\Phi}^{m+1/2}\right\|_{L^\infty} &\le C\left\|\Phi\right\|_{L^\infty(0,T;H^2)} \le CC^*_{2,\varepsilon},\end{aligned} \tag{3.52}$$

with (3.41) recalled. The second term appearing in (3.52) can be analyzed as follows:

$$\begin{aligned}\left\|\Phi^{m+1/2} - \hat{\Phi}^{m+1/2}\right\|_{L^\infty} &\le C\left\|\Phi^{m+1/2} - \hat{\Phi}^{m+1/2}\right\|_{H^2} \\ &= C\left\|\frac{1}{2}(\Phi^{m+1} - 2\Phi(\cdot, t^{m+1/2}) + \Phi^m)\right\|_{H^2} \\ &\le C\left\|\Phi^{m+1} - 2\Phi(\cdot, t^{m+1/2}) + \Phi^m\right\|_{H^2} \\ &\le C\hat{Q}^*_{2,\varepsilon} s^2,\end{aligned} \tag{3.53}$$

with the estimate (3.46) applied. As a result, a substitution of (3.52) and (3.53) implies (3.50), with

$$E_{1,\varepsilon} \ge CC^*_{2,\varepsilon}\hat{Q}^*_{2,\varepsilon},$$

and its dependence on ε^{-1} is clearly in a polynomial pattern. This completes the proof of the corollary. □

4. Error analysis with an improved convergence constant

The numerical error functions are defined as

$$\tilde{\phi}^k := \Phi^k - \phi^k, \quad \tilde{\phi}^{k+1/2} := \frac{1}{2}(\tilde{\phi}^{k+1} + \tilde{\phi}^k), \quad \breve{\tilde{\phi}}^{k+1/2} := \frac{3}{2}\tilde{\phi}^k - \frac{1}{2}\tilde{\phi}^{k-1}. \tag{4.1}$$

Since the exact solution to the CH equation (1.2) is mass conservative, we have

$$\int_\Omega \Phi(\cdot, t)\, d\mathbf{x} = \int_\Omega \Phi(\cdot, 0)\, d\mathbf{x} := \beta_0, \quad \forall\, t > 0. \tag{4.2}$$

On the other hand, the numerical scheme is also mass conservative:

$$\int_\Omega \phi^m\, d\mathbf{x} = \int_\Omega \phi^0\, d\mathbf{x} = \beta_0, \quad \forall\, m \ge 0. \tag{4.3}$$

As a result, we get

$$\int_\Omega \tilde{\phi}^m\, d\mathbf{x} = 0, \quad \forall\, m \ge 0. \tag{4.4}$$

Here we use the notation $H_{\mathrm{per}}^{-1}(\Omega) = \left(H_{\mathrm{per}}^{1}(\Omega)\right)^*$, and $\langle\,\cdot\,,\,\cdot\,\rangle$ is the duality pairing between $H_{\mathrm{per}}^{-1}(\Omega)$ and $H_{\mathrm{per}}^{1}(\Omega)$. We need a norm on a subspace of $H_{\mathrm{per}}^{-1}(\Omega)$. With $L_0^2(\Omega)$ denoting those function in $L^2(\Omega)$ with zero mean, we set

$$\mathring{H}_{\mathrm{per}}^{1}(\Omega) = H_{\mathrm{per}}^{1}(\Omega) \cap L_0^2(\Omega), \quad \mathring{H}_{\mathrm{per}}^{-1}(\Omega) := \left\{ v \in H_{\mathrm{per}}^{-1}(\Omega) \mid \langle v, 1 \rangle = 0 \right\}, \tag{4.5}$$

We define a continuous linear operator $\mathsf{T} : \mathring{H}_{\mathrm{per}}^{-1}(\Omega) \to \mathring{H}_{\mathrm{per}}^{1}(\Omega)$ via the following variational problem: given $\zeta \in \mathring{H}_{\mathrm{per}}^{-1}(\Omega)$, find $\mathsf{T}(\zeta) \in \mathring{H}_{\mathrm{per}}^{1}(\Omega)$ such that

$$(\nabla \mathsf{T}(\zeta), \nabla \chi) = \langle \zeta, \chi \rangle \qquad \forall \chi \in \mathring{H}^1(\Omega). \tag{4.6}$$

T is uniquely defined, as is guaranteed by the Riesz Representation Theorem. The following facts are easily established.

Lemma 4.1. *Let $\zeta, \xi \in \mathring{H}_{\mathrm{per}}^{-1}(\Omega)$ and, for such functions, set*

$$(\zeta, \xi)_{H^{-1}} := (\nabla \mathsf{T}(\zeta), \nabla \mathsf{T}(\xi)) = \langle \zeta, \mathsf{T}(\xi) \rangle = \langle \xi, \mathsf{T}(\zeta) \rangle. \tag{4.7}$$

Then, $(\,\cdot\,,\,\cdot\,)_{H^{-1}}$ defines an inner product on $\mathring{H}_{\mathrm{per}}^{-1}(\Omega)$, and the induced norm is equivalent to the operator norm:

$$\|\zeta\|_{H^{-1}} := \sqrt{(\zeta, \zeta)_{H^{-1}}} = \sup_{0 \neq \chi \in \mathring{H}_{\mathrm{per}}^1} \frac{\langle \zeta, \chi \rangle}{\|\nabla \chi\|_{L^2}}. \tag{4.8}$$

Consequently, for all $\chi \in H_{\mathrm{per}}^{1}(\Omega)$ and all $\zeta \in \mathring{H}_{\mathrm{per}}^{-1}(\Omega)$, $|\langle \zeta, \chi \rangle| \le \|\zeta\|_{H^{-1}} \|\nabla \chi\|_{L^2}$. Furthermore, for all $\zeta \in L_0^2(\Omega)$, we have the Poincare type inequality: for some $C > 0$, $\|\zeta\|_{H^{-1}} \le C \|\zeta\|_{L^2}$.

The zero-mean property (4.4) shows that, the H^{-1} norm for the numerical error function, $\|\tilde{\phi}^k\|_{H^{-1}}$, is well defined.

4.1. Statement of the main theorem

The following theorem is the main result of this paper.

Theorem 4.2. *Suppose that the initial data $\Phi(\,\cdot\,, 0) = \phi_0 \in H_{\mathrm{per}}^{8}(\Omega)$ and that s satisfies the scaling law*

$$s \le C \varepsilon^{J_1}, \tag{4.9}$$

where J_1 is a sufficiently large positive integer and C is some positive constant. Also assume that $\varepsilon \in (0, \varepsilon_0)$, with ε specified in Proposition 4.6. Then the following convergence result is valid:

$$\max_{1 \le m \le M} \left\| \tilde{\phi}^m \right\|_{H^{-1}} \le \hat{R}_\varepsilon^* s^2, \quad \text{with} \quad \hat{R}_\varepsilon^* = \hat{R}^* e^{C_0^* T} \varepsilon^{-J_0}, \tag{4.10}$$

where J_0 is a positive integer, C_0^* and $\hat{R}^*$ are positive constants that are independent of s and ε.

4.2. Consistency analysis and the equation for the error function

With a second order temporal approximation taken, the following consistency estimate could be derived:

$$\frac{\Phi^{m+1} - \Phi^m}{s} = \Delta \left(\varepsilon^{-1} \left((\Phi^{m+1/2})^3 - \Phi^{m+1/2} \right) - \varepsilon \Delta \Phi^{m+1/2} \right) + \tau_2^{m+1/2}, \tag{4.11}$$

where

$$\Phi^{m+1/2} = \frac{1}{2} \left(\Phi^{m+1} + \Phi^m \right), \quad \left\| \tau_2^{m+1/2} \right\|_{H^{-1}} \le C s^2 \varepsilon^{-j_3}.$$

For the numerical scheme (2.1), we rewrite it in an alternate form, to facilitate the error analysis presented later. The following estimate could be derived:

$$\frac{\phi^{m+1} - \phi^m}{s} = \Delta \left(\varepsilon^{-1} \left((\phi^{m+1/2})^3 - \phi^{m+1/2} \right) - \varepsilon \Delta \phi^{m+1/2} \right) + \tau_3^{m+1/2}, \tag{4.12}$$

where

$$\phi^{m+1/2} = \frac{1}{2} \left(\phi^{m+1} + \phi^m \right), \quad \left\| \tau_3^{m+1/2} \right\|_{H^{-1}} \le C s^2 \varepsilon^{-j_4}. \tag{4.13}$$

Remark 4.3. We note that the temporal discretization for both the approximate projection solution (4.11) and the numerical solution (4.12) is very different from the original numerical scheme (2.1). The purpose for these forms is for the simplicity of an error analysis with an improved convergence constant, as will be observed later.

The temporal truncation error estimate (4.11) is based on the following transformations

$$\Phi^{m+1/2} - \Phi(t^{m+1/2}) = \frac{1}{2}\left(\Phi^{m+1} - 2\Phi(t^{m+1/2}) + \Phi^m\right), \tag{4.14}$$

$$(\Phi^{m+1/2})^3 - (\Phi(t^{m+1/2}))^3 = \frac{1}{2}\left(\Phi^{m+1} - 2\Phi(t^{m+1/2}) + \Phi^m\right) \cdot \left((\Phi^{m+1/2})^2 + \Phi^{m+1/2}\Phi_N(t^{m+1/2}) + (\Phi(t^{m+1/2}))^2\right), \tag{4.15}$$

combined with the established estimates (3.41) and (3.46) for Φ.

Similarly, the temporal truncation error estimate (4.12) is based on the following transformations

$$\phi^{m+1/2} - \breve{\phi}^{m+1/2} = \frac{1}{2}\left(\phi^{m+1} - 2\phi^m + \phi^{m-1}\right), \tag{4.16}$$

$$\phi^{m+1/2} - \hat{\phi}^{m+1/2} = -\frac{1}{4}\left(\phi^{m+1} - 2\phi^m + \phi^{m-1}\right), \tag{4.17}$$

$$\chi\left(\phi^{m+1}, \phi^m\right) - (\phi^{m+1/2})^3 = \frac{1}{8}(\phi^{m+1} + \phi^m)(\phi^{m+1} - \phi^m)^2, \tag{4.18}$$

combined with the established estimates (3.26), (3.31) and (3.37) for the numerical solution.

Subtracting (4.11) from the reformulated numerical scheme (4.12) yields

$$\frac{\tilde{\phi}^{m+1} - \tilde{\phi}^m}{s} = \Delta\left(\varepsilon^{-1}\left((\Phi^{m+1/2})^3 - (\phi^{m+1/2})^3 - \tilde{\phi}^{m+1/2}\right) - \varepsilon\Delta\tilde{\phi}^{m+1/2}\right) + \tau^{m+1/2}, \tag{4.19}$$

where

$$\left\|\tau^{m+1/2}\right\|_{H^{-1}} \le Cs^2\varepsilon^{-j_5}. \tag{4.20}$$

4.3. A preliminary estimate for the numerical error term

By a comparison between (3.26) (in Theorem 3.2), (3.31) (in Theorem 3.4), (3.37) (in Theorem 3.5) and (3.41)–(3.46) (for the exact solution) in Lemma 3.7, the following estimates are straightforward.

Lemma 4.4. *For the numerical error function, we have*

$$\max_{0\le n\le M}\left\|\tilde{\phi}^m\right\|_{H^\ell} \le \hat{C}^{**}_{\ell,\varepsilon} := C\varepsilon^{-k_\ell}, \tag{4.21}$$

$$\max_{0\le m\le M-1}\left\|\tilde{\phi}^{m+1} - \tilde{\phi}^m\right\|_{H^\ell} \le D^{**}_{\ell,\varepsilon}s, \quad D^{**}_{\ell,\varepsilon} := C\varepsilon^{-n_\ell}, \tag{4.22}$$

$$\max_{1\le m\le M-1}\left\|\tilde{\phi}^{m+1} - 2\tilde{\phi}^m + \tilde{\phi}^{m-1}\right\|_{H^\ell} \le Q^{**}_{\ell,\varepsilon}s^2, \quad Q^{**}_{\ell,\varepsilon} := C\varepsilon^{-m_\ell}, \tag{4.23}$$

for any $\ell \ge 1$ and $m \ge 0$, where k_ℓ, n_ℓ and m_ℓ are increasing sequences of positive integers and C is a constant independent of s, T and ε.

Remark 4.5. Note that these bounds for the numerical error function do not rely on the error and convergence analysis; all of them are final time independent.

4.4. Review of the spectrum estimate for the linearized Cahn–Hilliard operator

The following linearized spectrum estimate has been established in [14,17–19]. We recall it here.

Proposition 4.6 ([14]). *There exist $0 < \varepsilon_0 \ll 1$ and another positive constant C_0 such that the principle eigenvalue of the linearized Cahn–Hilliard operator satisfies*

$$\lambda_{CH} := \inf_{\substack{\psi\in H^1_{\text{per}}(\Omega)\\ \psi\ne 0}} \frac{\varepsilon^{-1}\left(\left(3\Phi^2(t) - 1\right)\psi, \psi\right) + \varepsilon\left\|\nabla\psi\right\|^2}{\left\|\psi\right\|^2_{H^{-1}}} \ge -C_0, \tag{4.24}$$

for any $t \ge 0$, $\varepsilon \in (0, \varepsilon_0)$, where Φ is the exact solution to the Cahn–Hilliard problem.

Remark 4.7. The spectrum analysis that established the estimate (4.24) was derived for the linearized Cahn–Hilliard operator [17–19], under a homogeneous Neumann boundary condition. An extension of this analysis to the one with the periodic boundary condition is straightforward, and the details are skipped for the sake of brevity.

4.5. Error analysis: Proof of Theorem 4.2

Since both $\tilde{\phi}^{m+1}$ and $\tilde{\phi}^{m}$ have zero-mean, we introduce

$$\tilde{w}^{\ell} := \mathsf{T}\tilde{\phi}^{\ell} = (-\Delta)^{-1}\tilde{\phi}^{\ell}, \quad \ell = m, m+1.$$

Taking an inner product with (4.19) by $\tilde{w}^{m+1/2} = \frac{1}{2}(\tilde{w}^{m+1} + \tilde{w}^{m})$ gives

$$\begin{aligned}&\frac{1}{2}\left(\tilde{\phi}^{m+1} - \tilde{\phi}^{m}, \tilde{w}^{m+1} + \tilde{w}^{m}\right) - \varepsilon^{-1}\left(\left((\Phi^{m+1/2})^3 - (\phi^{m+1/2})^3 - \tilde{\phi}^{m+1/2}\right), \Delta\tilde{w}^{m+1/2}\right)\\ &\quad+\varepsilon\left(\Delta\tilde{\phi}^{m+1/2}, \Delta\tilde{w}^{m+1/2}\right) = \left(\tau^{m+1/2}, \tilde{w}^{m+1/2}\right),\end{aligned} \tag{4.25}$$

with the integration-by-parts formula applied.

The subsequent estimates are standard:

$$\begin{aligned}\left(\tilde{\phi}^{m+1} - \tilde{\phi}^{m}, \tilde{w}^{m+1} + \tilde{w}^{m}\right) &= -\left(\Delta(\tilde{w}^{m+1} - \tilde{w}^{m}), \tilde{w}^{m+1} + \tilde{w}^{m}\right)\\ &= \left(\nabla(\tilde{w}^{m+1} - \tilde{w}^{m}), \nabla(\tilde{w}^{m+1} + \tilde{w}^{m})\right)\\ &= \left\|\nabla\tilde{w}^{m+1}\right\|^2 - \left\|\nabla\tilde{w}^{m}\right\|^2\\ &= \left\|\tilde{\phi}^{m+1}\right\|_{H^{-1}}^2 - \left\|\tilde{\phi}^{m}\right\|_{H^{-1}}^2,\end{aligned} \tag{4.26}$$

$$\left(\tilde{\phi}^{m+1/2}, \Delta\tilde{w}^{m+1/2}\right) = -\left(\phi^{m+1/2}, \tilde{\phi}^{m+1/2}\right) = -\left\|\tilde{\phi}^{m+1/2}\right\|^2, \tag{4.27}$$

$$\begin{aligned}&-\left(\left((\Phi^{m+1/2})^3 - (\phi^{m+1/2})^3\right), \Delta\tilde{w}^{m+1/2}\right)\\ &\qquad= \left(\left((\Phi^{m+1/2})^3 - (\phi^{m+1/2})^3\right), \tilde{\phi}^{m+1/2}\right)\\ &\qquad= \left(\left((\Phi^{m+1/2})^2 + \Phi^{m+1/2}\phi^{m+1/2} + (\phi^{m+1/2})^2\right), (\tilde{\phi}^{m+1/2})^2\right),\end{aligned} \tag{4.28}$$

$$\left(\Delta\tilde{\phi}^{m+1/2}, \Delta\tilde{w}^{m+1/2}\right) = -\left(\Delta\phi^{m+1/2}, \tilde{\phi}^{m+1/2}\right) = \left\|\nabla\tilde{\phi}^{m+1/2}\right\|^2, \tag{4.29}$$

and, finally,

$$\begin{aligned}-(\tau^{m+1/2}, \tilde{w}^{m+1/2}) &\le \left\|\tau^{m+1/2}\right\|_{H^{-1}} \cdot \left\|\nabla\tilde{w}^{m+1/2}\right\|_2\\ &\le \left\|\tau^{m+1/2}\right\|_{H^{-1}} \cdot \left\|\tilde{\phi}^{m+1/2}\right\|_{H^{-1}}\\ &\le \frac{1}{2}\|\tau^{m+1/2}\|_{H^{-1}}^2 + \frac{1}{4}\left(\|\phi^{m+1}\|_{H^{-1}}^2 + \|\tilde{\phi}^{m}\|_{H^{-1}}^2\right).\end{aligned} \tag{4.30}$$

The rest work is focused on the nonlinear estimates. The following a-priori assumption is made.

An a-priori assumption up to time step t^m. We assume a-priori that the numerical error function has the desired convergence as given by (4.10), at time steps up to t^m.

$$\|\tilde{\phi}^{\ell}\|_{H^{-1}} \le \hat{R}_{\varepsilon}^{*}s^2, \qquad \hat{R}_{\varepsilon}^{*} = Ce^{C_0^{*}T}\varepsilon^{-J_0}, \quad \ell \le m. \tag{4.31}$$

For the nonlinear inner product (4.28), we begin with the following identity:

$$\begin{aligned}&(\Phi^{m+1/2})^2 + \Phi^{m+1/2}\phi^{m+1/2} + (\phi^{m+1/2})^2\\ &\qquad= 3(\Phi^{m+1/2})^2 - 3\Phi^{m+1/2}\tilde{\phi}^{m+1/2} + (\tilde{\phi}^{m+1/2})^2.\end{aligned} \tag{4.32}$$

As a result, we get

$$\begin{aligned}I_1 &:= \left(\left((\Phi^{m+1/2})^2 + \Phi^{m+1/2}\phi^{m+1/2} + (\phi^{m+1/2})^2\right), (\tilde{\phi}^{m+1/2})^2\right)\\ &\ge 3\left((\Phi^{m+1/2})^2, (\tilde{\phi}^{m+1/2})^2\right) - 3\left(\Phi^{m+1/2}\tilde{\phi}^{m+1/2}, (\tilde{\phi}^{m+1/2})^2\right)\\ &= 3\left((\hat{\Phi}^{m+1/2})^2, (\tilde{\phi}^{m+1/2})^2\right) + \mathcal{E}_1 + \mathcal{E}_2,\end{aligned} \tag{4.33}$$

where

$$\mathcal{E}_1 := 3\left((\Phi^{m+1/2})^2 - (\hat{\Phi}^{m+1/2})^2, (\tilde{\phi}^{m+1/2})^2\right),$$

$$\mathcal{E}_2 := -3\int_{\Omega}\Phi^{m+1/2}(\tilde{\phi}^{m+1/2})^3 d\boldsymbol{x}.$$

The first term can be controlled as follows.

$$\begin{aligned} |\mathcal{E}_1| &\le 3\left\|(\Phi^{m+1/2})^2-(\hat{\Phi}^{m+1/2})^2\right\|_{L^\infty}\cdot\left\|\tilde{\phi}^{m+1/2}\right\|^2\\ &\le Cs^2\hat{E}_{1,\varepsilon}\left\|\tilde{\phi}^{m+1/2}\right\|^2, \end{aligned}\tag{4.34}$$

$$\left\|\tilde{\phi}^{m+1/2}\right\|^2 \le \left\|\tilde{\phi}^{m+1/2}\right\|_{H^1}\cdot\left\|\tilde{\phi}^{m+1/2}\right\|_{H^{-1}} \le C\hat{C}^{**}_{1,\varepsilon}\left\|\tilde{\phi}^{m+1/2}\right\|_{H^{-1}},\tag{4.35}$$

$$\begin{aligned} |\mathcal{E}_1| &\le Cs^2\hat{C}^{**}_{1,\varepsilon}\hat{E}_{1,\varepsilon}\left\|\tilde{\phi}^{m+1/2}\right\|_{H^{-1}}\\ &\le \hat{R}^*_{1,\varepsilon}s^4+\varepsilon\left(\|\tilde{\phi}^{m+1}\|^2_{H^{-1}}+\|\tilde{\phi}^m\|^2_{H^{-1}}\right), \end{aligned}\tag{4.36}$$

with $\hat{R}^*_{1,\varepsilon}=C\varepsilon^{-1}\left(\hat{C}^{**}_{1,\varepsilon}\hat{E}_{1,\varepsilon}\right)^2$, in which the L^∞ estimate (3.50) (in Corollary 3.11) was applied in the second step of (4.34).

For the second nonlinear error term appearing in (4.33), we begin with

$$\begin{aligned} |\mathcal{E}_2| &\le 3\left\|\Phi^{m+1/2}\right\|_{L^\infty}\cdot\left\|\tilde{\phi}^{m+1/2}\right\|^3_{L^3} \le C\left\|\Phi^{m+1/2}\right\|_{H^2}\cdot\left\|\tilde{\phi}^{m+1/2}\right\|^3_{L^3}\\ &\le CC^*_{2,\varepsilon}\left\|\tilde{\phi}^{m+1/2}\right\|^3_{L^3}, \end{aligned}\tag{4.37}$$

with the estimate (3.41) applied in the last step. Meanwhile, the following observation is made:

$$\begin{aligned} \tilde{\phi}^{m+1/2} &= \breve{\tilde{\phi}}^{m+1/2}+\frac{1}{2}(\tilde{\phi}^{m+1}-2\tilde{\phi}^m+\tilde{\phi}^{m-1}),\quad \text{so that}\\ \|\tilde{\phi}^{m+1/2}\|^3_{L^3} &\le C\left(\|\breve{\tilde{\phi}}^{m+1/2}\|^3_{L^3}+\|\tilde{\phi}^{m+1}-2\tilde{\phi}^m+\tilde{\phi}^{m-1}\|^3_{L^3}\right)\\ &\le C\left(\|\breve{\tilde{\phi}}^{m+1/2}\|^3_{L^3}+\|\tilde{\phi}^{m+1}-2\tilde{\phi}^m+\tilde{\phi}^{m-1}\|^3_{H^1}\right)\\ &\le C\left(\|\breve{\tilde{\phi}}^{m+1/2}\|^3_{L^3}+s^6(\hat{Q}^{**}_{1,\varepsilon})^3\right), \end{aligned}\tag{4.38}$$

with the preliminary estimate (4.23) applied in the last step. Moreover, the Sobolev inequalities indicate that

$$\begin{aligned} \left\|\breve{\tilde{\phi}}^{m+1/2}\right\|_{L^3} &\le C\left\|\breve{\tilde{\phi}}^{m+1/2}\right\|_{H^{1/2}} \le C\left\|\breve{\tilde{\phi}}^{m+1/2}\right\|^{\frac{3}{4}}_{H^{-1}}\cdot\left\|\breve{\tilde{\phi}}^{m+1/2}\right\|^{\frac{1}{4}}_{H^5}\\ &\le C(\hat{C}^{**}_{5,\varepsilon})^{\frac{1}{4}}\left(\|\tilde{\phi}^m\|_{H^{-1}}+\|\tilde{\phi}^{m-1}\|_{H^{-1}}\right)^{\frac{3}{4}}\\ &\le C(\hat{C}^{**}_{5,\varepsilon})^{\frac{1}{4}}(\hat{R}^*)^{\frac{3}{4}}s^{\frac{3}{2}}. \end{aligned}\tag{4.39}$$

The preliminary estimate (4.21) was applied in the third step and the a-priori assumption (4.31) was recalled in the last step, due to the fact that $\breve{\tilde{\phi}}^{m+1/2}$ is only involved with the error function at t^m and t^{m-1}. Subsequently, a substitution of (4.38) and (4.39) into (4.37) yields

$$|\mathcal{E}_2| \le \hat{R}^*_{2,\varepsilon}s^{9/2}+\hat{R}^*_{3,\varepsilon}s^6,\tag{4.40}$$

with

$$\hat{R}^*_{2,\varepsilon}=CC^*_{2,\varepsilon}(\hat{C}^{**}_{5,\varepsilon})^{\frac{3}{4}}(\hat{R}^*)^{\frac{9}{4}},\quad \hat{R}^*_{3,\varepsilon}=CC^*_{2,\varepsilon}(\hat{Q}^{**}_{1,\varepsilon})^3.$$

Therefore, a combination of (4.33), (4.36) and (4.40) results in

$$\begin{aligned} I_1 \ge\ & 3\left((\hat{\Phi}^{m+1/2})^2,(\tilde{\phi}^{m+1/2})^2\right)-\varepsilon\left(\|\tilde{\phi}^{m+1}\|^2_{H^{-1}}+\|\tilde{\phi}^m\|^2_{H^{-1}}\right)\\ &-\hat{R}^*_{1,\varepsilon}s^4-\hat{R}^*_{2,\varepsilon}s^{9/2}-\hat{R}^*_{3,\varepsilon}s^6. \end{aligned}\tag{4.41}$$

Finally, a combination of (4.25)–(4.30), (4.33) and (4.41) leads to

$$\begin{aligned} &\|\tilde{\phi}^{m+1}\|^2_{H^{-1}}-\|\tilde{\phi}^m\|^2_{H^{-1}}+2\varepsilon^{-1}s\left(3(\hat{\Phi}^{m+1/2})^2-1,(\tilde{\phi}^{m+1/2})^2\right)+2\varepsilon s\|\nabla\tilde{\phi}^{m+1/2}\|^2\\ &\quad\le 3s\left(\|\tilde{\phi}^{m+1}\|^2_{H^{-1}}+\|\tilde{\phi}^m\|^2_{H^{-1}}\right)+Csh^4\left((\hat{C}^{**}_{5,\varepsilon})^2+\varepsilon^{-4k_4}\right)+s\|\tau^{m+1/2}\|^2_{H^{-1}}\\ &\qquad+2\hat{R}^*_{1,\varepsilon}\varepsilon^{-1}s^5+2\hat{R}^*_{2,\varepsilon}\varepsilon^{-1}s^{11/2}+2\hat{R}^*_{3,\varepsilon}\varepsilon^{-1}s^7. \end{aligned}\tag{4.42}$$

By the linearized spectrum estimate (4.24) (reviewed in Proposition 4.6, by [14]), we conclude that

$$\begin{aligned} &2\varepsilon^{-1}\left(3(\hat{\Phi}^{m+1/2})^2-1,(\tilde{\phi}^{m+1/2})^2\right)+2\varepsilon\|\nabla\tilde{\phi}^{m+1/2}\|^2\\ &\qquad\ge 2C_0\|\tilde{\phi}^{m+1/2}\|^2_{H^{-1}}\\ &\qquad\ge C_0\left(\|\tilde{\phi}^{m+1}\|^2_{H^{-1}}+\|\tilde{\phi}^m\|^2_{H^{-1}}\right). \end{aligned}\tag{4.43}$$

Going back to (4.42), we arrive at

$$\|\tilde{\phi}^{m+1}\|_{H^{-1}}^2 - \|\tilde{\phi}^m\|_{H^{-1}}^2 \le (C_0+3)s\left(\|\tilde{\phi}^{m+1}\|_{H^{-1}}^2 + \|\tilde{\phi}^m\|_{H^{-1}}^2\right) + \hat{R}_{4,\varepsilon}^* s^5 + 2\hat{R}_{2,\varepsilon}^* \varepsilon^{-1} s^{11/2}, \tag{4.44}$$

with

$$\hat{R}_{4,\varepsilon}^* = C\left((\hat{C}_{5,\varepsilon}^{**})^2 + \varepsilon^{-4k_4} + \varepsilon^{-2j_5} + 2\hat{R}_{1,\varepsilon}^*\varepsilon^{-1} + 2\hat{R}_{3,\varepsilon}^*\varepsilon^{-1}\right). \tag{4.45}$$

Under the condition that

$$\hat{R}_{2,\varepsilon}^*\varepsilon^{-1}s^{1/2} \le \frac{1}{4}, \quad \text{i.e.} \quad s \le \frac{\varepsilon^2}{16}(\hat{R}_{2,\varepsilon}^*)^{-2}, \tag{4.46}$$

we get

$$\|\tilde{\phi}^{m+1}\|_{H^{-1}}^2 - \|\tilde{\phi}^m\|_{H^{-1}}^2 \le (C_0+3)s\left(\|\tilde{\phi}^{m+1}\|_{H^{-1}}^2 + \|\tilde{\phi}^m\|_{H^{-1}}^2\right) + \hat{R}_{5,\varepsilon}^* s^5, \tag{4.47}$$

where

$$\hat{R}_{5,\varepsilon}^* = \hat{R}_{4,\varepsilon}^* + 1.$$

Note that C_0+3 is a constant independent of ε, and $\hat{R}_{5,\varepsilon}^*$ is independent on $\hat{R}^*$ appearing in (4.31). Clearly, $\hat{R}_{5,\varepsilon}^*$ depends on ε^{-1} in a polynomial form. An application of discrete Gronwall inequality to (4.47) yields the desired error analysis:

$$\|\tilde{\phi}^{m+1}\|_{H^{-1}}^2 \le C e^{(2C_0+7)T}\hat{R}_{5,\varepsilon}^* s^4. \tag{4.48}$$

Recovery of the a-priori assumption (4.31) In turn, we can take $C_0^* = C_0 + \frac{7}{2}$, and the integer index J_0 could be chosen according to the form of $\hat{R}_{5,\varepsilon}^*$, to recover the a-priori assumption (4.31) at time step t^{m+1}.

Moreover, $\hat{R}^*$ is determined by this convergence result, so is $\hat{R}_{2,\varepsilon}^*$, given by $\hat{R}_{2,\varepsilon}^* = CC_{2,\varepsilon}^*(\hat{C}_{5,\varepsilon}^{**})^{\frac{3}{4}}(\hat{R}^*)^{\frac{9}{4}}$. As a result, the condition (4.46) for s could be converted into the form of (4.9). The proof of Theorem 4.2 is complete.

Remark 4.8. The H_{per}^8 regularity requirement for the initial data, as stated in Theorem 4.2, is quite strong. Meanwhile, the Cahn–Hilliard flow is a parabolic equation with a very strong smoothing property; it has been proved in an earlier work [55] that, any H_{per}^1 initial data would lead to a real analytic solution for the Cahn–Hilliard equation, with a global-in-time Gevrey regularity. In other words, even if the initial data is not in the class of H_{per}^8, the PDE solution will become real analytic (henceforth C_{per}^∞) at any finite time. This article is more concerned with the Cahn–Hilliard flow with certain structures; in fact, the linearized spectrum analysis (4.24) in Proposition 4.6 has to be based on such a structure for the exact solution Φ, and it may not be valid for a rough initial data. As a result, we could take the real analytic initial data, after a positive time evolution of the Cahn–Hilliard flow. Moreover, this initial data regularity requirement does not cause any conflict with the spatial discretization. For a fully discrete scheme, with either finite difference or finite element spatial approximation, the corresponding analysis could be carried out in a similar fashion. The technical details are left to interested readers.

Remark 4.9. The time step has to satisfy the scaling law as indicated in (4.9): $s \le C\varepsilon^{J_1}$. A preliminary calculation shows that J_1 has to be greater than 40 for the 3-D CH flow, to make the theoretical analysis available.

Note that these two integer numbers have larger values than the ones reported in [14,15], for a few reasons. The Allen–Cahn model covered in [15] has a well-known maximum principle, which in turn would greatly simplify the corresponding analysis. The numerical scheme for the Cahn–Hilliard model analyzed in [14] is first order accurate; in comparison, a second order accurate (in time) scheme is considered in our work, so that higher order temporal derivatives have to be involved in the analysis, which in turn leads to much higher spatial norms to be uniform-in-time bounded.

On the other hand, such a restrictive requirement for s is only associated with a theoretical justification of the improved convergence estimate. In the practical computations, as have been reported in [22], this scaling law requirement is not needed for small ε. And also, for the 2-D case, the scaling law index J_1 could be much more reduced, to approximately 15.

Remark 4.10. The techniques presented in this article could be similarly applied to many other second order accurate energy stable schemes for 2-D and 3-D Cahn–Hilliard models, such as the finite element method [42], the Fourier pseudo-spectral version [56], an alternate second order scheme based on the BDF temporal stencil [47,48], *et cetera*. The technical details are expected to be very involved and are left to interested readers.

5. Concluding remarks

An improved error analysis is provided for a second order accurate in time, energy stable numerical scheme to the 2-D and 3-D Cahn–Hilliard equation. A uniform-in-time H^{m_0} bound of the numerical solution, for any $m_0 \ge 3$, is obtained through Sobolev estimates at a discrete level. Moreover, to analyze the second order scheme with an improved constant, we have also obtained uniform-in-time H^{m_0} bounds for the first and second order temporal difference stencil, namely $\|\phi^{m+1} - \phi^m\|_{H^\ell}$ and $\|\phi^{m+1} - 2\phi^m + \phi^{m-1}\|_{H^\ell}$, respectively. In the error estimate, we apply a spectrum estimate for the linearized Cahn–Hilliard operator, so that an application of the discrete Gronwall inequality avoids a convergence constant of the form $\exp(CT\varepsilon^{-m_0})$; instead, the constant turns out to be dependent on ε^{-1} only in a polynomial order.

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