ENERGY STABLE SEMI-IMPLICIT SCHEMES FOR THE 3D ALLEN-CAHN EQUATION

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ABSTRACT. In this work we are interested in a class of numerical schemes for phase field models. It is known that the energy of phase field models decays in time therefore such energy stability is a crucial fidelity check in practical numerical simulations. In recent work [8], several first order semi-implicit schemes for the 2D Allen-Cahn and fractional Cahn-Hilliard equations have been developed and such schemes satisfy the unconditional energy stability (energy decays in time with no requirement on the size of the time steps). In this paper we develop more first and second order semi-implicit schemes to the 3D Allen-Cahn equation with a rigorous proof of similar energy stability.

1. INTRODUCTION

1.1. Introduction to the models and historical review

It is a widely held view that many physical problems can be modeled by partial differential equations (PDEs) in forms of gradient flows. Phase field model, a typical particular gradient flow model, arouses many interest in the area of material sciences, biology and micro-engineering. Throughout this work we focus on a well-known phase field model, the Allen-Cahn (AC) equation. The (AC) model was firstly developed in [1] by Allen and Cahn to study the competition of crystal grain orientations in an annealing process separation of different metals in a binary alloy. The explicit formulation of these two equations are given below:

$$\begin{cases} \partial_t u = \nu \Delta u - f(u), & (x,t) \in \Omega \times (0,\infty) \\ u(x,0) = u_0, \end{cases} \tag{AC} \boxed{\texttt{AC}}$$

Here the solution $u(x,t)$ is a real valued function whose values are taken in $(-1,1)$ representing a mixture of the two phases at position x and time t. In particular -1 represent the pure state of one phase and $+1$ represent the pure state of the other phase. The spatial domain Ω is oftentimes taken to be two or three dimensional periodic domain. Here ν is a small parameter and in the literature sometimes one adopt the following notation $\varepsilon = \sqrt{\nu}$ to represent an average distance over which phases mix. The potential energy term $f(u)$ is often chosen to be

$$f(u) = F'(u) = u^3 - u \ , \ F(u) = \frac{1}{4}(u^2-1)^2.$$

A natural question is the limiting problem of (AC) as the parameter $\varepsilon \to 0$. In fact it is known that such limit is governed by a mean curvature flow and we refer the readers to [18] for scalar and vector-valued AC and a recent work for matrix-valued AC [14], where both asymptotic and rigorous analysis have been investigated. Although the limiting behavior of AC is known, there are related materials science models that are studied only numerically and this current work presents an idea about how to approach these models appropriately. In this paper, we consider the spatial domain Ω to be the three dimensional 2π-periodic torus $\mathbb{T}^3 = (\mathbb{R}/2\pi\mathbb{Z})^3$. In fact, our proof can be applied to more general settings such as Dirichlet and Neumann boundary conditions in a 3D bounded domain. However, considering the periodic domain allows us to use the efficient and accurate Fourier-spectral numerical methods. On top of that, periodic domain is often appropriate for practical questions, which involve the formation of micro-structure away from physical boundaries.

As mentioned earlier, AC is a gradient flow therefore its energy decays in time. Here the associated energy functional of (AC) is given by

$$E(u) = \int_\Omega \left(\frac{1}{2}\nu |\nabla u|^2 + F(u) \right)\, dx. \tag{1.1}$$

energy

Assume that $u(x,t)$ is a smooth solution with zero mean, one can deduce that

$$\frac{d}{dt}E(u(t)) + \int_\Omega |\nu \Delta u - f(u)|^2 \, dx = 0,$$

which implies the decay of the energy: $\frac{d}{dt}E(u(t)) \le 0$. This thus provides an *a priori* H^1-norm bound of the solution u. On the other hand, the scaling analysis shows the scaling-critical space for (AC) is L^2 in 2D and $H^{\frac{1}{2}}$ in 3D, therefore the global well-posedness and regularity of solutions follow from standard arguments. It is also worth mentioning here that unlike the Cahn-Hilliard equation (another classic phase field model introduced in [6] by Cahn and Hilliard to describe the process of phase separation of different metals in a binary alloy), AC does not share the mass conservation property, namely, the mass of the smooth solution of CH is conserved. In other words the solution to CH satisfies $\frac{d}{dt}M(t) \equiv 0$, $M(t) = \int_\Omega u(x,t)\, dx$, which represents the conservation of the two phases in the mixture. This leads to the main difference between AC and CH.

Many different approaches have been developed to study AC and related models both analytically and numerically, cf. [12, 16, 17, 30, 15, 7, 31, 3, 13, 22, 23, 24, 2, 19, 10, 11]. Among which different time stepping methods including fully explicit (forward Euler) scheme, fully implicit (backward Euler) scheme, finite element scheme, convex splitting scheme and operator splitting schemes are adopted. Different strategies have been applied for the spatial discretization including the Fourier-spectral method. All these numerical approximations give accurate results to the values and qualitative features of the solution. One of the key features is the energy dissipation.

Before we introduce our numerical method and stability result, we go through a brief historical review. To start with, Feng and Prohl [15] introduced a semi-discrete in time and fully spatially discrete finite element method for Cahn-Hilliard equation where they obtained an error bound of size of powers of $1/\nu$. Explicit time-stepping schemes require strict time-step restrictions and do not obey energy decay in general. To guarantee the energy decay property and increase the size of time steps, a good alternative is to use semi-implicit schemes in which the linear term is implicit (such as backward time differentiation) and the nonlinear term is treated explicitly. Having only an implicit linear term at every time step has computational advantages, as suggested in [7], Chen and Shen considered a semi-implicit Fourier-spectral scheme for CH. On the other hand, semi-implicit schemes can lose stability for large time steps and thus smaller time steps are needed in practice. To resolve this problem, semi-implicit methods with better stability have been introduced, e.g. [17, 27, 30, 31, 29, 20, 21]. Specifically speaking, [17, 30, 31, 28] give different semi-implicit Fourier-spectral schemes, which involved different stabilizing terms of different “size”, that preserve the energy decay property (we say these schemes are “energy stable”). However, those works either require a strong Lipschitz condition on the nonlinear source term, or require certain L^∞ bounds on the numerical solutions.

In the seminal works [20, 21, 25], Li et al. developed a large time-stepping semi-implicit Fourier-spectral scheme for Cahn-Hilliard equation and proved that it preserves energy decay with no *a priori* assumptions (unconditional stability). The proof uses tools from harmonic analysis in [4, 5], and introduces a novel energy bootstrap scheme in order to obtain a L^∞-bound of the numerical solution. To be more specific, their scheme for (CH) takes the following form:

$$\begin{cases} \dfrac{u^{n+1} - u^n}{\tau} = -\nu \Delta^2 u^{n+1} + A\Delta(u^{n+1} - u^n) + \Delta(f(u^n)) \ , \ n \ge 0 \\ u^0 = u_0 \ . \end{cases} \tag{1.2}$$

{?}

Here τ is the time step and A is a large coefficient for the $O(\tau)$ stabilizing term. The energy decay is guaranteed with a well-chosen large number A, with at least a size of $O(1/\nu |\log(\nu)|^2)$. However, their arguments cannot be applied to the Allen Cahn equation (AC) directly: this is due to the lack of mass conservation. Lately, the work [8] extends previous first order semi-implicit scheme to the Allen-Cahn equation (AC) on $\mathbb{T}^2$. Following the same path the 2D fractional Cahn-Hilliard equation has also been studied as well. To be more specific, in [8] the following stabilized semi-implicit scheme for (AC) is considered:

$$\begin{cases} \dfrac{u^{n+1}-u^n}{\tau} = \nu\Delta u^{n+1} - A(u^{n+1}-u^n) - \Pi_N f(u^n) \\ u^0 = \Pi_N u_0, \end{cases} \tag{1.3}$$ 1stScheme

where τ is the time step and $A > 0$ is the coefficient for the $O(\tau)$ regularization term. Here for $N \geq 2$, Π_N is the truncation operator of Fourier modes $|k| \leq N$. Similarly, the semi-implicit scheme for the fractional Cahn-Hilliard equation is given by the following:

$$\begin{cases} \dfrac{u^{n+1}-u^n}{\tau} = -\nu(-\Delta)^{\alpha+1}u^{n+1} - (-\Delta)^{\alpha}A(u^{n+1}-u^n) - (-\Delta)^{\alpha}\Pi_N f(u^n) \\ u^0 = \Pi_N u_0. \end{cases} \tag{1.4}$$?1stFracscheme?

The results in [8] are obtained via harmonic analysis in borderline spaces and a new bootstrap scheme. Note that with respect to the L^∞ bound, 2D is critical thanks to the energy dissipation which yields an *apriori* H^1 bound. In fact it is well known that H^1 fails to embed into L^∞ in 2D with a logarithm cost (Lemma 3.1 in [8]). On the other hand for 3D case, the H^1 bound is insufficient to yield L^∞ control and more work is needed to achieve energy stability. One of our purposes of this work is to settle the 3D case. To be clearer, we first consider a first-order semi-implicit scheme (1.3) and show the energy of the numerical solution decays in time armed with an L^2 error bound. Secondly, we consider a second-order scheme below:

$$\frac{3u^{n+1}-4u^n+u^{n-1}}{2\tau} = \nu\Delta u^{n+1} - A\tau(u^{n+1}-u^n) - \Pi_N\left(2f(u^n) - f(u^{n-1})\right) \quad , \ n \geq 1 \ , \tag{1.5}$$ 2ndSchemeI

where $\tau > 0$ is the time step and this scheme applies second order backward derivative in time with a second order extrapolation for the nonlinear term. To start the iteration, we need to derive u^1 according to the following first order scheme:

$$\begin{cases} \dfrac{u^1-u^0}{\tau_1} = \nu\Delta u^1 - \Pi_N f(u^0) \quad , \\ u^0 = \Pi_N u_0 \ , \end{cases} \tag{1.6}$$ 2ndSchemeI_1storc

where $\tau_1 = \min\{\tau^{\frac{4}{3}} \ , \ 1\}$. The choice of τ is due to the error analysis which will be shown later. We will show the unconditional energy stability of (1.5) with (1.6) and estimate the L^2 error.

1.2. **Main results**

Our main results state below:

⟨1st_Thm3D⟩ **Theorem 1.1** (3D energy stability for AC)**.** Consider (1.3) with $\nu > 0$ and assume $u_0 \in H^2(\mathbb{T}^3)$. Then there exists a constant β_0 depending only on the initial energy $E_0 = E(u_0)$ such that if

$$A \geq \beta \cdot \left(\|u_0\|_{H^2}^2 + \nu^{-3} + 1\right) \ , \ \beta \geq \beta_0$$

then $E(u^{n+1}) \leq E(u^n)$, $\forall n \geq 0$, where E is defined in (1.1).

⟨1st_3Derror⟩ **Theorem 1.2** (L^2 error estimate of 3D AC)**.** Let $\nu > 0$. Let $u_0 \in H^s$, $s \geq 4$ and $u(t)$ be the solution to Allen-Cahn equation with initial data u_0. Let u^n be the numerical solution to (1.3) with initial data $\Pi_N u_0$. Assume A satisfies the same condition in the stability theorem Theorem 1.1. Define $t_m = m\tau$, $m \geq 1$. Then

$$\|u^m - u(t_m)\|_2 \leq A \cdot e^{C_1 t_m} \cdot C_2 \cdot \left(N^{-s} + \tau\right) \ ,$$

where $C_1 > 0$ depends only on (u_0, ν) and C_2 depends on (u_0, ν, s).

Remark 1.3. Unlike in the 2D case as in [8], our choice of A is independent of τ as long as it has size of $O\left(\nu^{-3}\right)$ at least, which is much larger than $O\left(\nu^{-1}|\log(\nu)|^2\right)$. This results from the loss of log type control for the L^∞ bound.

⟨2ndThm_I⟩ **Theorem 1.4** (Unconditional stability)**.** Consider the scheme (1.5)-(1.6) with $\nu > 0$, $0 < \tau \leq M$ for some arbitrary constant $M > 0$ and we assume in addition $N \geq 2$. Suppose $u_0 \in H^2(\mathbb{T}^3)$. The initial energy is denoted by $E_0 = E(u_0)$. If there exists a constant $\beta_c > 0$ depending only on E_0, $\|u_0\|_{H^2}$ and M, such that

$$A \geq \beta \cdot (1 + \nu^{-8}) \ , \ \beta \geq \beta_c \ ,$$

then

$$\tilde{E}(u^{n+1}) \leq \tilde{E}(u^n) \ , \ n \geq 1 \ ,$$

where $\tilde{E}(u^n)$ for $n \geq 1$ is a modified energy functional and is defined as

$$\tilde{E}(u^n) := E(u^n) + \frac{\nu^{-4} + 1}{4} \|u^n - u^{n-1}\|_2^2 + \frac{1}{4\tau} \|u^n - u^{n-1}\|_2^2 \ .$$

Theorem 1.5 (L^2 error estimate)**.** Let $\nu > 0$ and $u_0 \in H^s$, $s \geq 8$. Let $0 < \tau \leq M$ for some $M > 0$. Let $u(t)$ be the continuous solution to the 3D Allen-Cahn equation with initial data u_0. Let u^1 be defined according to (1.6) with initial data $u^0 = \Pi_N u_0$. Let u^m, $m \geq 2$ be defined in (1.5) with initial data u^0 and u^1. Assume A satisfies the same condition in Theorem 1.4. Define $t_0 = 0$, $t_1 = \tau_1$ and $t_m = \tau_1 + (m-1)\tau$ for $m \geq 2$. Then for any $m \geq 1$,

$$\|u(t_m) - u^m\|_2 \leq C_1 \cdot e^{C_2 t_m} \cdot (N^{-s} + \tau^2) \ ,$$

where C_1 , $C_2 > 0$ are constants depending only on $(u_0,\ \nu,\ s,\ A,\ M)$.

Remark 1.6. Here we require that τ is not arbitrarily large. This is a result of loss of mass conservation as preserved by Cahn-Hilliard equation. However, in practice it is not a big issue as we always use small time steps.

Remark 1.7. By adopting the same strategy, the 3D fractional Cahn-Hilliard model can be handled similarly.

⟨rmk_gen_grad⟩ *Remark* 1.8. More general cases can be discussed. To be more specific by defining a general "gradient" operator $\mathcal{G}$, we can rewrite the equation as :

$$\begin{cases} \partial_t u = \mathcal{G}\left(\nu \Delta u - f(u)\right) \\ u(x,0) = u_0 \end{cases} . \tag{1.7}$$ gradienteq

When $\mathcal{G} = id$, the identity map, (1.7) becomes the Allen-Cahn equation; when $\mathcal{G} = (-\Delta)^\alpha$, (1.7) becomes the fractional Cahn-Hilliard equation as discussed above. And the corresponding semi-implicit scheme is

$$\begin{cases} \dfrac{u^{n+1} - u^n}{\tau} = \mathcal{G}\left(\nu \Delta u^{n+1} - f(u^n)\right) - A\mathcal{G}(u^{n+1} - u^n) \ , \ n \geq 0 \\ u^0 = u_0 \end{cases} . \tag{1.8}$$ gradientscheme

The main result of this paper states that for any fixed time step τ, we can always define a large constant A independent of τ in (1.8), such that the numerical solution will be stable in the sense of satisfying the energy-decay condition for "gradient" cases of AC and fractional CH. In fact our method holds for more general cases such as higher order schemes; we postpone the discussion to the future work.

1.3. **Organization of the presenting paper**

The presenting paper is organized as follows. In Section 2 we list the notation and preliminaries including several useful lemmas. The energy stability of the first order semi-implicit scheme of the 3D Allen-Cahn will be shown in Section 3 while the error estimate is given therein. The second order semi-implicit schemes will be discussed in Section 4.

2. Notation and preliminaries

Throughout this paper, for any two (non-negative in particular) quantities X and Y, we denote $X \lesssim Y$ if $X \le CY$ for some constant $C > 0$. Similarly $X \gtrsim Y$ if $X \ge CY$ for some $C > 0$. We denote $X \sim Y$ if $X \lesssim Y$ and $Y \lesssim X$. The dependence of the constant C on other parameters or constants are usually clear from the context and we will often suppress this dependence. We shall denote $X \lesssim_{Z_1, Z_2, \cdots, Z_k} Y$ if $X \le CY$ and the constant C depends on the quantities $Z_1, \cdots, Z_k$.

For any two quantities X and Y, we shall denote $X \ll Y$ if $X \le cY$ for some sufficiently small constant c. The smallness of the constant c is usually clear from the context. The notation $X \gg Y$ is similarly defined. Note that our use of $\ll$ and $\gg$ here is *different* from the usual Vinogradov notation in number theory or asymptotic analysis.

For a real-valued function $u : \Omega \to \mathbb{R}$ we denote its usual Lebesgue L^p-norm by

$$\|u\|_p = \|u\|_{L^p(\Omega)} = \begin{cases} \left(\int_\Omega |u|^p \, dx\right)^{\frac{1}{p}}, & 1 \le p < \infty; \\ \operatorname{esssup}_{x \in \Omega} |u(x)|, & p = \infty. \end{cases} \tag{2.1}$$ {?}

Similarly, we use the weak derivative in the following sense: For u, $v \in L^1_{loc}(\Omega)$, (i.e they are locally integrable); $\forall \phi \in C_0^\infty(\Omega)$, i.e ϕ is infinitely differentiable (smooth) and compactly supported; and

$$\int_\Omega u(x) \, \partial^\alpha \phi(x) \, dx = (-1)^{\alpha_1 + \cdots + \alpha_n} \int_\Omega v(x) \, \phi(x) \, dx,$$

then v is defined to be the weak partial derivative of u, denoted by $\partial^\alpha u$. Suppose $u \in L^p(\Omega)$ and all weak derivatives $\partial^\alpha u$ exist for $|\alpha| = \alpha_1 + \cdots + \alpha_n \le k$, such that $\partial^\alpha u \in L^p(\Omega)$ for $|\alpha| \le k$, then we denote $u \in W^{k,p}(\Omega)$ to be the standard Sobolev space. The corresponding norm of $W^{k,p}(\Omega)$ is :

$$\|u\|_{W^{k,p}(\Omega)} = \left(\sum_{|\alpha| \le k} \int_\Omega |\partial^\alpha u|^p \, dx \right)^{\frac{1}{p}} .$$

For $p = 2$ case, we use the convention $H^k(\Omega)$ to denote the space $W^{k,2}(\Omega)$. We often use $D^m u$ to denote any differential operator $D^\alpha u$ for any $|\alpha| = m$: D^2 denotes $\partial^2_{x_i x_j} u$ for $1 \le i, j \le d$, as an example.

In this paper we use the following convention for Fourier expansion on $\mathbb{T}^d$:

$$f(x) = \frac{1}{(2\pi)^d} \sum_{k \in \mathbb{Z}^d} \hat{f}(k) e^{ik \cdot x} \ , \ \hat{f}(k) = \int_\Omega f(x) e^{-ik \cdot x} \, dx \ .$$

Taking advantage of the Fourier expansion, we use the well-known equivalent H^s-norm and $\dot{H}^s$-semi-norm of function f by

$$\|f\|_{H^s} = \frac{1}{(2\pi)^{d/2}} \left(\sum_{k \in \mathbb{Z}^d} (1 + |k|^{2s}) |\hat{f}(k)|^2 \right)^{\frac{1}{2}} \ , \ \|f\|_{\dot{H}^s} = \frac{1}{(2\pi)^{d/2}} \left(\sum_{k \in \mathbb{Z}^d} |k|^{2s} |\hat{f}(k)|^2 \right)^{\frac{1}{2}} .$$

⟨Sobolevineq⟩ **Lemma 2.1** (Sobolev inequality on $\mathbb{T}^d$)**.** Let $0 < s < d$ and $f \in L^q(\mathbb{T}^d)$ for any $\frac{d}{d-s} < p < \infty$, then

$$\| \langle \nabla \rangle^{-s} f \|_{L^p(\mathbb{T}^d)} \lesssim_{s,p,d} \|f\|_{L^q(\mathbb{T}^d)} \ , \text{ where } \frac{1}{q} = \frac{1}{p} + \frac{s}{d} \ ,$$

where $\langle \nabla \rangle^{-s}$ denotes $(1 - \Delta)^{-\frac{s}{2}}$ and $A \lesssim_{s,p,d} B$ is defined as $A \le C_{s,p,d} \, B$ where $C_{s,p,d}$ is a constant dependent on s, p and d.

Remark 2.2. Note that the this Sobolev inequality is a variety of the standard version. Note that on the Fourier side the symbol of $\langle \nabla \rangle^{-s}$ is given by $(1 + |k|^2)^{-\frac{s}{2}}$. In particular, $\|f\|_{\infty(\mathbb{T}^d)} \lesssim \|f\|_{H^2(\mathbb{T}^d)}$, known as Morrey's inequality.

⟨DiscreteGronwall⟩ **Lemma 2.3** (Discrete Grönwall's inequality)**.** Let $\tau > 0$ and $y_n \ge 0$, $\alpha_n \ge 0$, $\beta_n \ge 0$ for $n = 1, 2, 3 \cdots$. Suppose

$$\frac{y_{n+1} - y_n}{\tau} \le \alpha_n y_n + \beta_n \ , \ \forall \ n \ge 0 \ .$$

Then for any $m \geq 1$, we have

$$y_m \leq \exp\left(\tau \sum_{n=0}^{m-1} \alpha_n\right)\left(y_0 + \sum_{k=0}^{m-1} \beta_k\right) .$$

Proof. We sketch the proof here. By the assumption, it follows that for $n \geq 0$,

$$y_{n+1} \leq (1+\alpha_n \tau) y_n + \tau\beta_n \leq e^{\tau\alpha_n} y_n + \tau\beta_n ;$$

therefore one can derive that

$$\exp\left(-\tau \sum_{j=0}^{n} \alpha_j\right) y_{n+1} \leq \exp\left(-\tau \sum_{j=0}^{n-1} \alpha_j\right) y_n + \exp\left(-\tau \sum_{j=0}^{n} \alpha_j\right) \beta_n .$$

We thus obtain the desired result by performing a telescoping summation. ☐

⟨MP_ac⟩ **Lemma 2.4** (Maximum principle for smooth solutions to the Allen-Cahn equation)**.** Let $T > 0$, $d \leq 3$ and assume $u \in C_x^2 C_t^1(\mathbb{T}^d \times [0,T])$ is a classical solution to Allen-Cahn equation with initial data u_0. Then

$$\|u(.\ ,\ t)\|_\infty \leq \max\{\|u_0\|_\infty\ ,\ 1\}\ ,\ \forall\ 0 \leq t \leq T\ .$$

Proof. We refer the readers to Lemma 4.2 in [8] for the proof. ☐

⟨H^kregularity_AC⟩ **Lemma 2.5** (H^k boundedness of the exact solution to the Allen-Cahn equation)**.** Assume $u(x,t)$ is a smooth solution to the Allen-Cahn equation in $\mathbb{T}^d$ with $d \leq 3$ and the initial data $u_0 \in H^k(\mathbb{T}^d)$ for $k \geq 2$. Then,

$$\sup_{t\geq 0} \|u(t)\|_{H^k(\mathbb{T}^d)} \lesssim_k 1 \tag{2.2}$$ {?}

where we omit the dependence on ν and u_0.

Proof. All cases $d = 1, 2, 3$ have been proved and we refer the readers to Lemma 4.4 in [8] for the proof. ☐

3. Stability of a first order semi-implicit scheme for the 3D Allen-Cahn equation

In this section, we consider the three dimensional AC. It is worth mentioning the work [8] in the 2D case. What makes a difference is that the log-interpolation lemma (Lemma 3.1 in [8]) does not hold. To clarify, the $\dot{H}^1$-norm should be replaced by the $\dot{H}^{\frac{3}{2}}$-norm, as a result of scaling invariance. However, the $\dot{H}^{\frac{3}{2}}$-norm will not help to prove the 3D theorem as there is no *a priori* energy bound for the $\dot{H}^{\frac{3}{2}}$-norm. To solve this issue, we will try an alternate interpolation inequality. For simplicity, we only consider Allen-Cahn equation in 3D periodic domain $\mathbb{T}^3 = (\mathbb{R}/2\pi\mathbb{Z})^3$ in this section as other Cahn-Hilliard type equations can be handled similarly. To begin with, we recall the numerical scheme (1.3) for Allen-Cahn equation.

$$\begin{cases} \dfrac{u^{n+1}-u^n}{\tau} = \nu\Delta u^{n+1} - A(u^{n+1}-u^n) - \Pi_N f(u^n) \\ u^0 = \Pi_N u_0 \end{cases} . \tag{3.1}$$?1stScheme3D?

where τ is the time step and $A > 0$ is the coefficient for the $O(\tau)$ regularization term. As usual, for $N \geq 2$, define

$$X_N = \mathrm{span}\left\{\cos(k\cdot x)\ , \sin(k\cdot x):\quad k = (k_1,k_2,k_3) \in \mathbb{Z}^3\ ,\ |k|_\infty = \max\{|k_1|,|k_2|,|k_3|\} \leq N\right\}\ .$$

In this section we show Theorem 1.1. First we recall the statement of Theorem 1.1.

Theorem 3.1 (3D energy stability for AC)**.** Consider (1.3) with $\nu > 0$ and assume $u_0 \in H^2(\mathbb{T}^3)$. Then there exists a constant β_0 depending only on the initial energy $E_0 = E(u_0)$ such that if

$$A \geq \beta \cdot \left(\|u_0\|_{H^2}^2 + \nu^{-3} + 1\right)\ ,\ \beta \geq \beta_0$$

then $E(u^{n+1}) \leq E(u^n)$, $\forall n \geq 0$, where E is defined before.

Before proving Theorem 1.1, we will prove a new interpolation lemma here.

⟨3DInterpolation⟩ **Lemma 3.2.** For all $f \in H^2(\mathbb{T}^3)$, one has

$$\|f\|_\infty \lesssim \|f\|_{\dot{H}^1}^{\frac{1}{2}} \|f\|_{\dot{H}^2}^{\frac{1}{2}} + |\hat{f}(0)| \ .$$

Proof. To start with we write $f(x) = \frac{1}{(2\pi)^3} \sum_{k\in\mathbb{Z}^3} \hat{f}(k)\ e^{ik\cdot x}$, the Fourier series of f in $\mathbb{T}^3$. So,

$$\begin{aligned}
\|f\|_\infty &\le \frac{1}{(2\pi)^3} \sum_{k\in\mathbb{Z}^3} |\hat{f}(k)| \\
&\le \frac{1}{(2\pi)^3} |\hat{f}(0)| + \frac{1}{(2\pi)^3} \left(\sum_{0<|k|\le N} |\hat{f}(k)| + \sum_{|k|>N} |\hat{f}(k)| \right) \\
&\lesssim |\hat{f}(0)| + \sum_{0<|k|\le N} (|\hat{f}(k)| |k| \cdot |k|^{-1}) + \sum_{|k|>N} (|\hat{f}(k)| |k|^2 \cdot |k|^{-2}) \\
&\lesssim |\hat{f}(0)| + \left(\sum_{0<|k|\le N} |\hat{f}(k)|^2 |k|^2 \right)^{\frac{1}{2}} \cdot \left(\sum_{0<|k|\le N} |k|^{-2} \right)^{\frac{1}{2}} + \left(\sum_{|k|>N} |\hat{f}(k)|^2 |k|^4 \right)^{\frac{1}{2}} \cdot \Big(\sum_{|k|>N} |k|^{-4} \Big)^{\frac{1}{2}} \\
&\lesssim |\hat{f}(0)| + \left(\sum_{|k|>N} |\hat{f}(k)|^2 |k|^4 \right)^{\frac{1}{2}} \cdot \left(\int_N^\infty \frac{\pi r^2}{r^4}\ dr \right)^{\frac{1}{2}} + \left(\sum_{0<|k|\le N} |\hat{f}(k)|^2 |k|^2 \right)^{\frac{1}{2}} \cdot \left(\int_1^N \frac{\pi r^2}{r^2}\ dr \right)^{\frac{1}{2}} \\
&\lesssim |\hat{f}(0)| + \|f\|_{\dot{H}^2} \cdot N^{-\frac{1}{2}} + \|f\|_{\dot{H}^1} \cdot N^{\frac{1}{2}} \ .
\end{aligned}$$

We optimize N and hence derive

$$\|f\|_\infty \lesssim |\hat{f}(0)| + \|f\|_{\dot{H}^1}^{\frac{1}{2}} \|f\|_{\dot{H}^2}^{\frac{1}{2}} \ .$$

□

3.1. **Proof of the 3D stability theorem**

We will prove Theorem 1.1 by induction. To start with, let us recall the numerical scheme (1.3):

$$\frac{u^{n+1} - u^n}{\tau} = \nu \Delta u^{n+1} - A(u^{n+1} - u^n) - \Pi_N f(u^n).$$

As usual here Π_N is truncation of Fourier modes of L^2 functions to $|k|_\infty \le N$. Multiply the equation by $(u^{n+1} - u^n)$ and integrate over Ω, one has

$$\frac{1}{\tau} \int_{\mathbb{T}^3} |u^{n+1} - u^n|^2 = \nu \int_{\mathbb{T}^3} \Delta u^{n+1} (u^{n+1} - u^n) - A \int_{\mathbb{T}^3} |u^{n+1} - u^n|^2 - \big(\Pi_N f(u^n), u^{n+1} - u^n\big) \ .$$

Then by integration by parts we arrive at

$$\left(\frac{1}{\tau} + A\right) \int_{\mathbb{T}^3} |u^{n+1} - u^n|^2 + \nu \int_{\mathbb{T}^3} \nabla u^{n+1} \nabla (u^{n+1} - u^n) = - \big(\Pi_N f(u^n), u^{n+1} - u^n\big) \ .$$

Note $\nabla u^{n+1} \nabla (u^{n+1} - u^n) = \frac{1}{2} \left(|\nabla u^{n+1}|^2 - |\nabla u^n|^2 + |\nabla (u^{n+1} - u^n)|^2 \right)$, we have

$$\left(\frac{1}{\tau} + A\right) \int_{\mathbb{T}^3} |u^{n+1} - u^n|^2 + \frac{\nu}{2} \int_{\mathbb{T}^3} |\nabla u^{n+1}|^2 - |\nabla u^n|^2 + |\nabla (u^{n+1} - u^n)|^2 = - \big(\Pi_N f(u^n), u^{n+1} - u^n\big) \ .$$

Moreover, for every $u^n \in X_N$, we have

$$\left(\frac{1}{\tau} + A\right) \int_{\mathbb{T}^3} |u^{n+1} - u^n|^2 + \frac{\nu}{2} \int_{\mathbb{T}^3} |\nabla u^{n+1}|^2 - |\nabla u^n|^2 + |\nabla (u^{n+1} - u^n)|^2 = - \big(f(u^n), u^{n+1} - u^n\big) \ .$$

It then follows by the fundamental theorem of calculus and integration by parts,

$$\begin{aligned}
F(u^{n+1}) - F(u^n) &= f(u^n)(u^{n+1}-u^n) + \int_{u^n}^{u^{n+1}} f'(s)(u^{n+1}-s)\ ds \\
&= f(u^n)(u^{n+1}-u^n) + \int_{u^n}^{u^{n+1}} (3s^2-1)(u^{n+1}-s)\ ds \\
&= f(u^n)(u^{n+1}-u^n) + \frac{1}{4}(u^{n+1}-u^n)^2\left(3(u^n)^2+(u^{n+1})^2+2u^nu^{n+1}-2\right)\ .
\end{aligned}$$

Combining the two equations above and denoting $E(u^n)$ by E^n, we then have

$$\begin{aligned}
&\left(\frac{1}{\tau}+A\right)\|u^{n+1}-u^n\|_{L^2}^2 + \frac{\nu}{2}\|\nabla(u^{n+1}-u^n)\|_{L^2}^2 + \frac{\nu}{2}\|\nabla u^{n+1}\|_{L^2}^2 - \frac{\nu}{2}\|\nabla u^n\|_{L^2}^2 \\
&+\int_{\mathbb{T}^3} F(u^{n+1}) - F(u^n) = \frac{1}{4}\left((u^{n+1}-u^n)^2, 3(u^n)^2+(u^{n+1})^2+2u^nu^{n+1}-2\right) \\
&\text{Note that}\quad \frac{\nu}{2}\|\nabla u^{n+1}\|_{L^2}^2 + \int_{\mathbb{T}^3} F(u^{n+1}) = E(u^{n+1}) = E^{n+1} \\
&\implies \left(\frac{1}{\tau}+A+\frac{1}{2}\right)\|u^{n+1}-u^n\|_{L^2}^2 + \frac{\nu}{2}\|\nabla(u^{n+1}-u^n)\|_{L^2}^2 + E^{n+1}-E^n \\
&= \frac{1}{4}\left((u^{n+1}-u^n)^2, 3(u^n)^2+(u^{n+1})^2+2u^nu^{n+1}\right) \\
&\le \|u^{n+1}-u^n\|_{L^2}^2\left(\|u^n\|_\infty^2 + \frac{1}{2}\|u^{n+1}\|_\infty^2\right)\ .
\end{aligned}$$

Clearly, in order to show $E^{n+1} \le E^n$, it suffices to show

$$\frac{1}{\tau}+A+\frac{1}{2} \ge \frac{3}{2}\max\left\{\|u^n\|_\infty^2\ ,\ \|u^{n+1}\|_\infty^2\right\}\ . \tag{3.2}$$ 3Dcondition

Now we rewrite the scheme (1.3) as the following:

$$u^{n+1} = \frac{1+A\tau}{1+A\tau-\nu\tau\Delta}u^n - \frac{\tau}{1+A\tau-\nu\tau\Delta}\Pi_N[f(u^n)].$$

Recall that

$$\|u^{n+1}\|_\infty \lesssim |\widehat{u^{n+1}}(0)| + \|u^{n+1}\|_{\dot H^1}^{\frac12}\|u^{n+1}\|_{\dot H^2}^{\frac12}\ .$$

Clearly, we need to estimate $|\widehat{u^{n+1}}(0)|$, $\|u^{n+1}\|_{\dot H^1}$ and $\|u^{n+1}\|_{\dot H^2}$. By the same argument,

$$|\widehat{u^{n+1}}(0)| \lesssim 1+\sqrt{E^n}\ .$$

Note that

$$\begin{cases}
\dfrac{(1+A\tau)|k|}{1+A\tau+\nu\tau|k|^2} \le |k| \\[2mm]
\dfrac{\tau|k|}{1+A\tau+\nu\tau|k|^2} \le \dfrac{\tau|k|}{2\tau\sqrt{A\nu}|k|} \lesssim \dfrac{1}{\sqrt{A\nu}}\ .
\end{cases}$$

Hence we have

$$\begin{aligned}
\|u^{n+1}\|_{\dot H^1} &\lesssim \|u^n\|_{\dot H^1} + \frac{1}{\sqrt{A\nu}}\|f(u^n)\|_{L^2} \\
&\lesssim \|u^n\|_{\dot H^1} + \frac{1}{\sqrt{A\nu}}(\|(u^n)^3\|_{L^2}+1)\ .
\end{aligned}$$

Similarly, we have

$$\begin{cases}
\dfrac{(1+A\tau)|k|^2}{1+A\tau+\nu\tau|k|^2} \lesssim \left(\dfrac{1}{\tau\sqrt{A\nu}}+\sqrt{\dfrac{A}{\nu}}\right)|k| \\[2mm]
\dfrac{\tau|k|^2}{1+A\tau+\nu\tau|k|^2} \le \dfrac{1}{\nu}\ .
\end{cases}$$

This implies

$$\|u^{n+1}\|_{\dot H^2} \lesssim \left(\frac{1}{\tau\sqrt{A\nu}} + \sqrt{\frac{A}{\nu}}\right)\|u^n\|_{\dot H^1} + \frac{1}{\nu}\|f(u^n)\|_{L^2}$$
$$\lesssim \left(\frac{1}{\tau\sqrt{A\nu}} + \sqrt{\frac{A}{\nu}}\right)\|u^n\|_{\dot H^1} + \frac{1}{\nu}\left(\|(u^n)^3\|_{L^2} + 1\right) .$$

Note that by a standard Sobolev inequality,

$$\|(u^n)^3\|_{L^2} = \|u^n\|_{L^6}^3 \lesssim \|u^n\|_{H^1}^3 \lesssim \|\nabla u^n\|_{L^2}^3 + \|u^n\|_{L^2}^3 \lesssim \|u^n\|_{\dot H^1}^3 + 1 + (E^n)^{\frac{3}{2}} .$$

As a result, we get

$$\begin{cases} \|u^{n+1}\|_{\dot H^1} \lesssim \|u^n\|_{\dot H^1} + \dfrac{1}{\sqrt{A\nu}}\left(\|(u^n)\|_{\dot H^1}^3 + 1 + (E^n)^{\frac{3}{2}}\right) \\ \|u^{n+1}\|_{\dot H^2} \lesssim \left(\dfrac{1}{\tau\sqrt{A\nu}} + \sqrt{\dfrac{A}{\nu}}\right)\|u^n\|_{\dot H^1} + \dfrac{1}{\nu}\left(\|(u^n)\|_{\dot H^1}^3 + 1 + (E^n)^{\frac{3}{2}}\right) \end{cases} . \quad (3.3) \text{ eq\_3DHs}$$

We prove the 3D stability theorem inductively as in the 2D case in [8].

Step 1: The induction $n \to n+1$ step. Assume $E^n \le E^{n-1} \le \cdots \le E^0$ and $E^n \le \sup_N\ E(\Pi_N u_0)$, we show $E^{n+1} \le E^n$. This implies $\|u^n\|_{\dot H^1}^2 = \|\nabla u^n\|_{L^2}^2 \le \frac{2E^n}{\nu} \le \frac{2E^0}{\nu}$. Recall $\sup_N\ E(\Pi_N u_0) \lesssim E_0 + 1$ as well. Hence we derive from (3.3) that

$$\begin{cases} \|u^{n+1}\|_{\dot H^1} \lesssim_{E_0} \nu^{-\frac{1}{2}} + A^{-\frac{1}{2}}\nu^{-\frac{1}{2}}\left(\nu^{-\frac{3}{2}} + 1\right) \lesssim_{E_0} \nu^{-\frac{1}{2}} + A^{-\frac{1}{2}}\nu^{-2} \\ \|u^{n+1}\|_{\dot H^2} \lesssim_{E_0} A^{\frac{1}{2}}\nu^{-1} + \nu^{-\frac{5}{2}} + \tau^{-1}A^{-\frac{1}{2}}\nu^{-1} \end{cases} .$$

Applying Lemma 3.2, we get

$$\|u^{n+1}\|_\infty^2 \lesssim_{E_0} \left(\nu^{-\frac{1}{2}} + A^{-\frac{1}{2}}\nu^{-2}\right)\cdot\left(A^{\frac{1}{2}}\nu^{-1} + \nu^{-\frac{5}{2}} + \tau^{-1}A^{-\frac{1}{2}}\nu^{-1}\right) + 1$$
$$\lesssim_{E_0} A^{\frac{1}{2}}\nu^{-\frac{3}{2}} + \nu^{-3} + A^{-\frac{1}{2}}\nu^{-\frac{9}{2}} + \tau^{-1}A^{-\frac{1}{2}}\nu^{-\frac{3}{2}} + \tau^{-1}A^{-1}\nu^{-3} + 1 .$$

To satisfy the sufficient condition (3.2),

$$A^{\frac{1}{2}}\nu^{-\frac{3}{2}} + \nu^{-3} + A^{-\frac{1}{2}}\nu^{-\frac{9}{2}} + \tau^{-1}A^{-\frac{1}{2}}\nu^{-\frac{3}{2}} + \tau^{-1}A^{-1}\nu^{-3} \lesssim_{E_0} A + \frac{1}{\tau} ,$$

it suffices to take

$$A \ge C_{E_0}\nu^{-3} , \quad (3.4) \{?\}$$

for a large enough constant C_{E_0} depending only on E_0.

Step 2: Check the induction base step $n = 1$. It is clear that we only need to check

$$A + \frac{1}{2} + \frac{1}{\tau} \ge \frac{3}{2}\|\Pi_N u_0\|_\infty^2 + \frac{3}{2}\|u^1\|_\infty^2.$$

By standard Sobolev inequality in $\mathbb{T}^3$, we get

$$\|\Pi_N u_0\|_\infty^2 \lesssim \|\Pi_N u_0\|_{H^2}^2 \lesssim \|u_0\|_{H^2}^2 .$$

On the other hand, by Lemma 3.2 it suffices to take

$$A + \frac{1}{\tau} \ge c_1\|u_0\|_{H^2}^2 + \alpha_{E_0}\left(A^{\frac{1}{2}}\nu^{-\frac{3}{2}} + \nu^{-3} + A^{-\frac{1}{2}}\nu^{-\frac{9}{2}} + \tau^{-1}A^{-\frac{1}{2}}\nu^{-\frac{3}{2}} + \tau^{-1}A^{-1}\nu^{-3}\right) ,$$

where c_1 is an absolute constant and α_{E_0} is a constant only depending on E_0. Hence it suffices to take

$$A \ge C_{E_0}\left(\|u_0\|_{\dot H^2}^2 + \nu^{-3} + 1\right) , \quad (3.5) \{?\}$$

for a large constant C_{E_0} only depending on E_0. This completes the proof. A numerical result is given in Figure 1 where we choose $\nu = 0.1$, A=1, $u_0 = \sin(x)\sin(y)$, $\tau = 0.01$, $N_x = N_y = 256$.

To close the case, it remains to estimate the L^2 error.

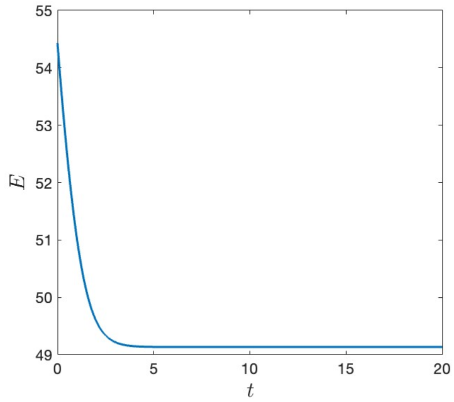

FIGURE 1. Dynamics of 3D Allen-Cahn equation using semi-implicit scheme where $\nu = 0.1$, A=1, $u_0 = \sin(x)\sin(y)\sin(z)$, $\tau = 0.01$, $N_x = N_y = 256$.

⟨fig:3dAC⟩

3.2. L^2 error estimate of 3D Allen-Cahn equation

Recall the statement of Theorem 1.2 is as follows.

Theorem 3.3. Let $\nu > 0$. Let $u_0 \in H^s$, $s \geq 4$ and $u(t)$ be the solution to Allen-Cahn equation with initial data u_0. Let u^n be the numerical solution with initial data $\Pi_N u_0$. Assume A satisfies the same condition in the stability theorem. Define $t_m = m\tau$, $m \geq 1$. Then

$$\|u^m - u(t_m)\|_2 \leq A \cdot e^{C_1 t_m} \cdot C_2 \cdot \left(N^{-s} + \tau\right) \ ,$$

where $C_1 > 0$ depends only on (u_0, ν) and C_2 depends on (u_0, ν, s).

Proof. We consider the semi-implicit scheme together with the exact Allen-Cahn equation

$$\begin{cases} \dfrac{u^{n+1} - u^n}{\tau} = \nu \Delta u^{n+1} - \Pi_N f(u^n) - A(u^{n+1} - u^n) \\ \partial_t u = \nu \Delta u - f(u) \\ u^0 = \Pi_N u_0 \ , \ u(0) = u_0 \ . \end{cases} \tag{3.6}$$ {?}

As is proved in [8], the auxiliary L^2 estimate lemma and all boundedness lemma work for 3D case. This leads to the conclusion of Theorem 1.2 by the same argument, therefore we refer the readers to Section 4 in [8].

□

4. SECOND ORDER SEMI-IMPLICIT SCHEMES FOR THE 3D ALLEN-CAHN EQUATION

In the previous section we introduce a first order semi-implicit scheme for the Allen-Cahn equation in the three dimensional periodic domain. For the sake of completeness, we study the second order schemes in this section. As a representative case, we only consider the 3D Allen-Cahn equation here and other cases can be analyzed similarly. We recall the second order scheme (1.5)-(1.6) and prove the unconditional energy stability.

4.1. Unconditional stability of second-order scheme (1.5) and (1.6)

Recall that the second order semi-implicit Fourier spectral scheme is given by:

$$\frac{3u^{n+1} - 4u^n + u^{n-1}}{2\tau} = \nu \Delta u^{n+1} - A\tau(u^{n+1} - u^n) - \Pi_N \left(2f(u^n) - f(u^{n-1})\right) \ , \ n \geq 1 \ , \tag{4.1}$$ {?}

where $\tau > 0$ is the time step and this scheme applies second order backward derivative in time with a second order extrapolation for the nonlinear term. Recall that u^1 is defined according to the following first order scheme:

$$\begin{cases} \dfrac{u^1 - u^0}{\tau_1} = \nu\Delta u^1 - \Pi_N f(u^0) \ , \\ u^0 = \Pi_N u_0 \ , \end{cases} \tag{4.2}$$ {?}

where $\tau_1 = \min\{\tau^{\frac{4}{3}} \ , \ 1\}$. The choice of τ_1 is due to the error analysis which will be shown later. Roughly speaking,

$$\|u^1 - u(\tau_1)\|_2 \lesssim N^{-s} + \tau_1^{\frac{3}{2}} \ ,$$

where $u(\tau_1)$ denotes the exact PDE solution at τ_1. As expected in L^2 error analysis of the second order scheme, we require that $\tau_1^{\frac{3}{2}} \lesssim \tau^2$ or $\tau_1 \lesssim \tau^{\frac{4}{3}}$.

4.1.1. **Estimate of the first order scheme (1.6)**

In this section we will estimate some bounds for u^1 which will be used to prove the stability and L^2 error estimate of the second order scheme.

⟨2ndSchemem_I_lem1⟩ **Lemma 4.1.** Consider the scheme (1.6). Assume $u_0 \in H^2(\mathbb{T}^3)$, then

$$\|u^1\|_\infty + \frac{\|u^1 - u^0\|_2^2}{\tau_1} + \frac{\nu}{2}\|\nabla u^1\|_2^2 \lesssim_{E(u_0)\ ,\ \|u_0\|_{H^2}} 1 \ .$$

Proof. Firstly, we consider $\|u^1\|_\infty$. We write

$$u^1 = \frac{1}{1 - \tau_1\nu\Delta}u^0 - \frac{\tau_1\Pi_N}{1 - \tau_1\nu\Delta}f(u^0) \ .$$

Note that

$$\frac{1}{1 + \tau_1\nu|k|^2} \le 1 \ , \ \tau_1 \le 1 \ ,$$

thus we have

$$\begin{aligned} \|u^1\|_\infty \lesssim \|u^1\|_{H^2} &\lesssim \|u^0\|_{H^2} + \|f(u^0)\|_{H^2} \\ &\lesssim \|u^0\|_{H^2} + \|(u^0)^3\|_{H^2} \\ &\lesssim_{\|u_0\|_{H^2}} 1 \ , \end{aligned}$$

as $\|u^0\|_\infty \lesssim 1$ by Morrey's inequality.

Secondly, we take L^2 inner product with $u^1 - u^0$ on both sides of (1.6).

$$\begin{aligned} &\frac{\|u^1 - u^0\|_2^2}{\tau_1} + \frac{\nu}{2}\left(\|\nabla u^1\|_2^2 - \|\nabla u^0\|_2^2 + \|\nabla(u^1 - u^0)\|_2^2\right) \\ &= -(f(u^0)\ ,\ u^1 - u^0) \\ &\le \|f(u^0)\|_{\frac{4}{3}}\|u^1 - u^0\|_4 \\ &\lesssim_{E(u^0)} 1 \ , \end{aligned}$$

by $\|u^0\|_\infty \ , \ \|u^1\|_\infty \lesssim 1$. As a result, $\|u^1\|_\infty + \frac{\|u^1-u^0\|_2^2}{\tau_1} + \frac{\nu}{2}\|\nabla u^1\|_2^2 \lesssim_{E(u_0)\ ,\ \|u_0\|_{H^2}} 1$.

□

⟨2ndSchemem_I_lem2⟩ **Lemma 4.2** (Error estimate for u^1)**.** Consider the system for first time step u^1:

$$\begin{cases} \dfrac{u^1 - u^0}{\tau_1} = \nu\Delta u^1 - \Pi_N f(u^0) \\ \partial_t u = \nu\Delta u - f(u) \\ u^0 = \Pi_N u_0 \ , \ u(0) = u_0 \ . \end{cases} \tag{4.3}$$ 4.3a

Let $u_0 \in H^s$, $s \ge 6$. There exists a constant $D_1 > 0$ depending only on (u_0, ν, s), such that $\|u(\tau_1) - u^1\|_2 \le D_1 \cdot (N^{-s} + \tau_1^{\frac{3}{2}})$.

Proof. We start the proof in three steps:

Step 1: We discretize the exact solution u in time. Write the continuous time PDE in time interval $[0,\tau_1]$. Note that for a one-variable function $h(s)$,

$$\begin{aligned} h(0) &= h(\tau_1) + \int_{\tau_1}^{0} h'(s)\ ds \\ &= h(\tau_1) - h'(\tau_1)\tau_1 + \int_0^{\tau_1} h''(s)\cdot s\ ds\ . \end{aligned}$$

By applying this formula, we have

$$\begin{aligned} \frac{u(\tau_1)-u(0)}{\tau_1} &= \partial_t u(\tau_1) - \frac{1}{\tau_1}\int_0^{\tau_1} (\partial_{tt}u)\cdot s\ ds \\ &= \nu\Delta u(\tau_1) - f(u(\tau_1)) - \frac{1}{\tau_1}\int_0^{\tau_1} (\partial_{tt}u)\cdot s\ ds \\ &= \nu\Delta u(\tau_1) - \Pi_N f(u(0)) - \Pi_{>N} f(u(0)) - [f(u(\tau_1) - f(u(0))] \\ &\quad - \frac{1}{\tau_1}\int_0^{\tau_1} (\partial_{tt}u)\cdot s\ ds\ , \end{aligned}$$

where $\Pi_{>N} = id - \Pi_N$. Therefore, we get

$$\frac{u(\tau_1)-u(0)}{\tau_1} = \nu\Delta u(\tau_1) - \Pi_N f(u(0)) + G^0\ , \tag{4.4}$$ 4.3

where

$$\begin{aligned} G^0 &= -\Pi_{>N} f(u(0)) - [f(u(\tau_1) - f(u(0))] - \frac{1}{\tau_1}\int_0^{\tau_1} (\partial_{tt}u)\cdot s\ ds \\ &= -\Pi_{>N} f(u(0)) - [f(u(\tau_1) - f(u(0))] - \frac{1}{\tau_1}\int_0^{\tau_1} (\nu\Delta\partial_t u - f'(u)\partial_t u)\cdot s\ ds \end{aligned} \tag{4.5}$$ 4.3b

Step 2: Estimate $\|u(\tau_1)-u^1\|_2$. We rewrite the system (4.3),(4.4) and (4.5) as follows:

$$\begin{cases} \dfrac{u(\tau_1)-u(0)}{\tau_1} = \nu\Delta u(\tau_1) - \Pi_N f(u(0)) + G^0 \\ \dfrac{u^1-u^0}{\tau_1} = \nu\Delta u^1 - \Pi_N f(u^0) \\ u^0 = \Pi_N u_0\ ,\ u(0) = u_0\ . \end{cases}$$

Define $e^1 = u(\tau_1) - u^1$ and $e^0 = u(0) - u^0$. Then we arrive at

$$\frac{e^1-e^0}{\tau_1} = \nu\Delta e^1 - \Pi_N\left(f(u(0)) - f(u^0)\right) + G^0\ . \tag{4.6}$$ 4.6

Taking the L^2 inner product with e^1 on both sides of (4.6), we can obtain that

$$\begin{aligned} &\frac{1}{2\tau_1}\left(\|e^1\|_2^2 - \|e^0\|_2^2 + \|e^1-e^0\|_2^2\right) + \nu\|\nabla e^1\|_2^2 \\ &\le \|f(u(0)) - f(u^0)\|_2\cdot\|e^1\|_2 + \|G^0\|_2\cdot\|e^1\|_2 \\ &\lesssim \left(\|e^0\|_2 + \|G^0\|_2\right)\|e^1\|_2 \\ &\lesssim \left(\|e^0\|_2^2 + \|G^0\|_2^2\right) + \frac{1}{4}\|e^1\|_2^2\ . \end{aligned}$$

As a result, we have

$$\left(1-\frac{\tau_1}{2}\right)\|e^1\|_2^2 \le 2\tau_1\left(\|e^0\|_2^2 + \|G^0\|_2^2\right) + \|e^0\|_2^2\ .$$

Note that $\tau_1 \le 1$, so $1-\frac{\tau_1}{2} \ge \frac{1}{2}$ and

$$\|e^1\|_2^2 \lesssim (1+\tau_1)\|e^0\|_2^2 + \tau_1\|G^0\|_2^2\ .$$

Step 3: Estimate $\|e^0\|_2^2$ and $\|G^0\|_2^2$. Note that $\|e^0\|_2^2 = \|u(0) - u^0\|_2^2 = \|u_0 - \Pi_N u_0\|_2^2 = \|\Pi_{>N} u_0\|_2^2$. On the other hand, we see that

$$\begin{aligned}\|\Pi_{>N} u_0\|_2^2 &= \sum_{|k|>N} |\hat{u_0}(k)|^2 \\ &\le \sum_{|k|>N} |k|^{2s} |\hat{u_0}(k)|^2 \cdot |k|^{-2s} \\ &\lesssim N^{-2s} \cdot \sum_{|k|>N} |k|^{2s} |\hat{u_0}(k)|^2 \\ &\lesssim N^{-2s} \cdot \|u_0\|_{H^s}^2 .\end{aligned} \tag{4.7}$$

4.7

Similarly for $\|G^0\|_2$ we can derive that $\|\Pi_{>N} f(u(0))\|_2 \lesssim N^{-s}$, by the maximum principle (Lemma 2.4) and (4.7) above. On the other hand, by the classic mean value theorem we have

$$f(u(\tau_1)) - f(u(0)) = f'(\xi)(u(\tau_1) - u(0)) ,$$

where ξ is a number between $u(\tau_1)$ and $u(0)$. Again by the maximum principle (Lemma 2.4),

$$\|f(u(\tau_1)) - f(u(0))\|_2 \lesssim \|u(\tau_1) - u(0)\|_2 \lesssim \tau_1 \|\partial_t u\|_{L_t^\infty L_x^2([0,\ \tau_1]\times\mathbb{T}^3)} \lesssim \tau_1 ,$$

by the Sobolev bound of the exact solution Lemma 2.5. Finally using Lemma 2.5 we end up with

$$\begin{aligned}&\left\| \frac{1}{\tau_1} \int_0^{\tau_1} (\nu\Delta\partial_t u - f'(u)\partial_t u) \cdot s \, ds \right\|_2 \\ &\lesssim \left\| \int_0^{\tau_1} \nu\Delta\partial_t u - f'(u)\partial_t u \, ds \right\|_2 \\ &\lesssim \int_0^{\tau_1} \|\nu\Delta\partial_t u\|_2 \, ds + \int_0^{\tau_1} \|f'(u)\partial_t u\|_2 \, ds \\ &\lesssim \tau_1 .\end{aligned}$$

This implies $\|G^0\|_2^2 \lesssim N^{-2s} + \tau_1^2$. Therefore we get

$$\|e^1\|_2^2 \lesssim (1+\tau_1)N^{-2s} + \tau_1(N^{-2s} + \tau_1^2) \lesssim N^{-2s} + \tau_1^3 .$$

As a result, we obtain that

$$\|e^1\|_2 \lesssim N^{-s} + \tau_1^{\frac{3}{2}} . \tag{4.8}$$

?2ndorderSchI:e1?

This completes the proof. □

4.1.2. **Unconditional stability of the second order scheme (1.5) & (1.6)**

In this section we will prove a unconditional stability theorem for the second order scheme (1.5) combining (1.6). To start with, we recall the theorem first.

Theorem 4.3 (Unconditional stability)**.** Consider the scheme (1.5)-(1.6) with $\nu > 0$, $0 < \tau \le M$ for some arbitrary constant $M > 0$ and we assume in addition $N \ge 2$. Suppose $u_0 \in H^2(\mathbb{T}^3)$. The initial energy is denoted by $E_0 = E(u_0)$. If there exists a constant $\beta_c > 0$ depending only on E_0, $\|u_0\|_{H^2}$ and M, such that

$$A \ge \beta \cdot (1 + \nu^{-8}) \ , \ \beta \ge \beta_c \ ,$$

then

$$\tilde{E}(u^{n+1}) \le \tilde{E}(u^n) \ , \ n \ge 1 \ ,$$

where $\tilde{E}(u^n)$ for $n \ge 1$ is a modified energy functional and is defined as

$$\tilde{E}(u^n) := E(u^n) + \frac{\nu^{-4}+1}{4}\|u^n - u^{n-1}\|_2^2 + \frac{1}{4\tau}\|u^n - u^{n-1}\|_2^2 .$$

Before proving this stability theorem, we begin with several lemmas.

⟨2ndScheme_I_lem3⟩ **Lemma 4.4.** Consider (1.5) for $n \geq 1$. Suppose $E(u^n) \leq B$ and $E(u^{n-1}) \leq B$ for some $B > 0$. Then

$$\|u^{n+1}\|_\infty \leq \alpha_B \cdot \left\{ \left(\nu^{-\frac{1}{2}} + \sqrt{\frac{\tau}{\nu}}(1+\nu^{-\frac{3}{2}}) \right)^{\frac{1}{2}} \cdot \left(\nu^{-1}\tau^{-\frac{1}{2}} + \sqrt{A}\nu^{-1}\tau^{\frac{1}{2}} + \nu^{-\frac{5}{2}} + \nu^{-1} \right)^{\frac{1}{2}} + \tau + 1 \right\}, \tag{4.9}$$ 4.4a

for some $\alpha_B > 0$ only depending on B.

Proof. For simplicity we write $\lesssim$ instead of $\lesssim_B$. Recall that (1.5)

$$\frac{3u^{n+1} - 4u^n + u^{n-1}}{2\tau} = \nu\Delta u^{n+1} - A\tau(u^{n+1} - u^n) - \Pi_N \left(2f(u^n) - f(u^{n-1}) \right) .$$

We rewrite (1.5) as

$$\begin{aligned} u^{n+1} =& \frac{4 + 2A\tau^2}{3 - 2\nu\tau\Delta + 2A\tau^2} u^n - \frac{1}{3 - 2\nu\tau\Delta + 2A\tau^2} u^{n-1} \\ &- \frac{2\tau\Pi_N}{3 - 2\nu\tau\Delta + 2A\tau^2} \left(2f(u^n) - f(u^{n-1}) \right) . \end{aligned} \tag{4.10}$$ 4.9

We then consider (4.10) on the Fourier side. To start with, for the 0-th mode, namely when $k = 0$, we have

$$\begin{cases} \dfrac{4 + 2A\tau^2}{3 + 2A\tau^2} \lesssim 1 \\ \dfrac{1}{3 + 2A\tau^2} \lesssim 1 \\ \dfrac{2}{3 + 2A\tau^2} \lesssim \tau \ . \end{cases}$$

We thus have

$$|\widehat{u^{n+1}}(0)| \lesssim \tau + 1 \ .$$

Note that for the case when $|k| \geq 1$,

$$\begin{cases} \dfrac{4 + 2A\tau^2}{3 + 2\nu\tau|k|^2 + 2A\tau^2} \lesssim 1 \\ \dfrac{1}{3 + 2\nu\tau|k|^2 + 2A\tau^2} \lesssim 1 \\ \dfrac{2\tau|k|}{3 + 2\nu\tau|k|^2 + 2A\tau^2} \lesssim \dfrac{\tau|k|}{\sqrt{\nu\tau}|k|} \lesssim \sqrt{\dfrac{\tau}{\nu}} \ . \end{cases}$$

Therefore we get

$$\begin{aligned} \|u^{n+1}\|_{\dot{H}^1} &\lesssim \|u^n\|_{\dot{H}^1} + \|u^{n-1}\|_{\dot{H}^1} + \sqrt{\frac{\tau}{\nu}}\|2f(u^n) - f(u^{n-1})\|_2 \\ &\lesssim \nu^{-\frac{1}{2}} + \sqrt{\frac{\tau}{\nu}}(\|(u^n)^3\|_2 + \|(u^{n-1})^3\|_2 + \|u^n\|_2 + \|u^{n-1}\|_2) \\ &\lesssim \nu^{-\frac{1}{2}} + \sqrt{\frac{\tau}{\nu}}(1 + \nu^{-\frac{3}{2}}) \ , \end{aligned} \tag{4.11}$$?4.10?

after applying Sobolev inequality Lemma 2.1 and the energy bound $E(u^n), E(u^{n-1}) \leq B$. Similarly, we can derive that

$$\begin{cases} \dfrac{|k|^2(4 + 2A\tau^2)}{3 + 2\nu\tau|k|^2 + 2A\tau^2} \lesssim \left(\dfrac{1}{\sqrt{\nu\tau}} + \sqrt{\dfrac{A\tau}{\nu}} \right) |k| \\ \dfrac{|k|^2}{3 + 2\nu\tau|k|^2 + 2A\tau^2} \lesssim \dfrac{|k|}{\sqrt{\nu\tau}} \\ \dfrac{2\tau|k|^2}{3 + 2\nu\tau|k|^2 + 2A\tau^2} \lesssim \dfrac{\tau|k|^2}{\nu\tau|k|^2} \lesssim \dfrac{1}{\nu} \ . \end{cases} \tag{4.12}$$ 4.11

Then combining (4.12) together with the Sobolev inequality Lemma 2.1 we arrive at

$$\begin{aligned}
\|u^{n+1}\|_{\dot{H}^2} &\lesssim \left(\frac{1}{\sqrt{\nu\tau}}+\sqrt{\frac{A}{\nu}}\tau^{\frac12}\right)\|u^n\|_{\dot{H}^1}+\frac{1}{\sqrt{\nu\tau}}\|u^{n-1}\|_{\dot{H}^1}+\frac{1}{\nu}\|2f(u^n)-f(u^{n-1})\|_2\\
&\lesssim \left(\frac{1}{\sqrt{\nu\tau}}+\sqrt{\frac{A}{\nu}}\tau^{\frac12}\right)\nu^{-\frac12}+\frac{1}{\nu}\left(\|u^n\|_6^3+\|u^{n-1}\|_6^3+\|u^n\|_2+\|u^{n-1}\|_2\right)\\
&\lesssim \left(\frac{1}{\sqrt{\nu\tau}}+\sqrt{\frac{A}{\nu}}\tau^{\frac12}\right)\nu^{-\frac12}+\frac{1}{\nu}\left(\|u^n\|_{H^1}^3+\|u^{n-1}\|_{H^1}^3+1\right)\\
&\lesssim \nu^{-1}\tau^{-\frac12}+\sqrt{A}\nu^{-1}\tau^{\frac12}+\nu^{-\frac52}+\nu^{-1}\ .
\end{aligned} \tag{4.13}$$

?4.12?

Finally by applying Lemma 3.2, we can show (4.9):

$$\begin{aligned}
\|u^{n+1}\|_\infty &\lesssim \|u^{n+1}\|_{\dot{H}^1}^{\frac12}\|u^{n+1}\|_{\dot{H}^2}^{\frac12}+|\widehat{u^{n+1}(0)}|\\
&\lesssim \left(\nu^{-\frac12}+\sqrt{\frac{\tau}{\nu}}(1+\nu^{-\frac32})\right)^{\frac12}\cdot\left(\nu^{-1}\tau^{-\frac12}+\sqrt{A}\nu^{-1}\tau^{\frac12}+\nu^{-\frac52}+\nu^{-1}\right)^{\frac12}+\tau+1\ .
\end{aligned}$$

□

4.1.3. **Proof of unconditional stability Theorem 1.4**

Before proving Theorem 1.4, we introduce some notation. We denote $\delta u^{n+1} := u^{n+1}-u^n$ and $\delta^2 u^{n+1} := u^{n+1}-2u^n+u^{n-1}$. Clearly,

$$\begin{cases}
3u^{n+1}-4u^n+u^{n-1} = 2\delta u^{n+1}+\delta^2 u^{n+1}\\
\delta^2 u^{n+1}-\delta u^{n+1} = -\delta u^n\\
\delta u^n\cdot u^n = (u^n-u^{n-1})u^n = \dfrac12\left(|u^n|^2-|u^{n-1}|^2+|\delta u^n|^2\right)\ .
\end{cases}$$

As a result, we have

$$\begin{aligned}
&\left(3u^{n+1}-4u^n+u^{n-1}\ ,\ u^{n+1}-u^n\right)\\
&=\left(2\delta u^{n+1}+\delta^2 u^{n+1}\ ,\ \delta u^{n+1}\right)\\
&=2\|\delta u^{n+1}\|_2^2+\left(\delta u^{n+1}-\delta u^n\ ,\ \delta u^{n+1}\right)\\
&=2\|\delta u^{n+1}\|_2^2+\frac12\left(\|\delta u^{n+1}\|_2^2-\|\delta u^n\|_2^2+\|\delta^2 u^{n+1}\|_2^2\right)\ .
\end{aligned}$$

Now recall the scheme (1.5)

$$\frac{3u^{n+1}-4u^n+u^{n-1}}{2\tau} = \nu\Delta u^{n+1}-A\tau(u^{n+1}-u^n)-\Pi_N\left(2f(u^n)-f(u^{n-1})\right)\ .$$

Taking the L^2 inner product with $\delta u^{n+1}=u^{n+1}-u^n$ on both sides of (1.5), we have

$$\begin{aligned}
\frac{1}{\tau}\|\delta u^{n+1}\|_2^2+\frac{1}{4\tau}\left(\|\delta u^{n+1}\|_2^2-\|\delta u^n\|_2^2+\|\delta^2 u^{n+1}\|_2^2\right)&\\
+\frac{\nu}{2}\left(\|\nabla u^{n+1}\|_2^2-\|\nabla u^n\|_2^2+\|\delta\nabla u^{n+1}\|_2^2\right)&\\
+A\tau\|\delta u^{n+1}\|_2^2 = -\left(\Pi_N(2f(u^n)-f(u^{n-1}))\ ,\ \delta u^{n+1}\right)&\ .
\end{aligned}$$

To analyze $\left(2f(u^n)-f(u^{n-1})\ ,\ \delta u^{n+1}\right)$, we consider

$$2f(u^n)-f(u^{n-1}) = f(u^n)+\left(f(u^n)-f(u^{n-1})\right).$$

Note that $F' = f$, hence by the fundamental theorem of calculus,

$$\begin{aligned}
&F(u^{n+1}) - F(u^n) \\
=&f(u^n)\delta u^{n+1} + \int_0^1 f'(u^n + s\delta u^{n+1})(1-s)\ ds \cdot (\delta u^{n+1})^2 \\
=&f(u^n)\delta u^{n+1} + \int_0^1 \tilde{f}(u^n + s\delta u^{n+1})(1-s)\ ds \cdot (\delta u^{n+1})^2 - \frac{1}{2}(\delta u^{n+1})^2\ ,
\end{aligned}$$

where $\tilde{f}(x) = 3x^2$, as $f'(x) = 3x^2 - 1$. Therefore, we can get

$$f(u^n)\delta u^{n+1} \geq F(u^{n+1}) - F(u^n) + \frac{1}{2}(\delta u^{n+1})^2 - \frac{3}{2}\left(\|u^n\|_\infty^2 + \|u^{n+1}\|_\infty^2\right) \cdot (\delta u^{n+1})^2\ .$$

On the other hand by the mean value theorem,

$$f(u^n) - f(u^{n-1}) = f'(\xi)\delta u^n\ ,$$

and hence we have

$$\begin{aligned}
&\int_{\mathbb{T}^3} (f(u^n) - f(u^{n-1})) \cdot \delta u^{n+1} \geq -\left(3\|u^n\|_\infty^2 + 3\|u^{n-1}\|_\infty^2 + 1\right) \cdot \|\delta u^n\|_2 \cdot \|\delta u^{n+1}\|_2 \\
&\geq -\frac{\left(1 + 3\|u^n\|_\infty^2 + 3\|u^{n-1}\|_\infty^2\right)^2}{\nu^{-4}+1} \cdot \|\delta u^n\|_2^2 - \frac{\nu^{-4}+1}{4}\|\delta u^{n+1}\|_2^2\ .
\end{aligned}$$

Then the estimate of the nonlinear term is as following:

$$\begin{aligned}
&-\left(\Pi_N(2f(u^n) - f(u^{n-1}))\ ,\ \delta u^{n+1}\right) \\
=&-\left(2f(u^n) - f(u^{n-1})\ ,\ \delta u^{n+1}\right) \\
\leq&-\int_{\mathbb{T}^3} F(u^{n+1})\ dx + \int_{\mathbb{T}^3} F(u^n)\ dx - \frac{1}{2}\|\delta u^{n+1}\|_2^2 \\
&+\frac{3}{2}\left(\|u^n\|_\infty^2 + \|u^{n+1}\|_\infty^2\right) \cdot \|\delta u^{n+1}\|_2^2 \\
&+\frac{\left(1 + 3\|u^n\|_\infty^2 + 3\|u^{n-1}\|_\infty^2\right)^2}{\nu^{-4}+1} \cdot \|\delta u^{n+1}\|_2^2 + \frac{\nu^{-4}+1}{4}\|\delta u^n\|_2^2\ .
\end{aligned}$$

Combining all estimates we get

$$\begin{aligned}
&\frac{1}{\tau}\|\delta u^{n+1}\|_2^2 + \frac{1}{4\tau}\left(\|\delta u^{n+1}\|_2^2 - \|\delta u^n\|_2^2 + \|\delta^2 u^{n+1}\|_2^2\right) \\
&+\frac{\nu}{2}\left(\|\nabla u^{n+1}\|_2^2 - \|\nabla u^n\|_2^2 + \|\delta\nabla u^{n+1}\|_2^2\right) \\
&+A\tau\|\delta u^{n+1}\|_2^2 \\
&\leq -\int_{\mathbb{T}} F(u^{n+1})\ dx + \int_{\mathbb{T}} F(u^n)\ dx - \frac{1}{2}\|\delta u^{n+1}\|_2^2 \\
&+\frac{3}{2}\left(\|u^n\|_\infty^2 + \|u^{n+1}\|_\infty^2\right) \cdot \|\delta u^{n+1}\|_2^2 \\
&+\frac{\left(1 + 3\|u^n\|_\infty^2 + 3\|u^{n-1}\|_\infty^2\right)^2}{\nu^{-4}+1} \cdot \|\delta u^{n+1}\|_2^2 + \frac{\nu^{-4}+1}{4}\|\delta u^n\|_2^2\ .
\end{aligned}$$

After simplification we obtain that

$$\begin{aligned}
&\left(\frac{1}{\tau} + A\tau - \frac{\nu^{-4}+1}{4} + \frac{1}{2}\right) \cdot \|\delta u^{n+1}\|_2^2 + \frac{\nu}{2}\|\delta\nabla u^{n+1}\|_2^2 + \tilde{E}(u^{n+1}) \\
&\leq \left\{\frac{3}{2}(\|u^n\|_\infty^2 + \|u^{n+1}\|_\infty^2) + \frac{\left(1 + 3\|u^n\|_\infty^2 + 3\|u^{n-1}\|_\infty^2\right)^2}{\nu^{-4}+1}\right\} \cdot \|\delta u^{n+1}\|_2^2 + \tilde{E}(u^n)\ .
\end{aligned} \tag{4.14}$$

4.14

Clearly from (4.14) in order to show $\tilde{E}(u^{n+1}) \le \tilde{E}(u^n)$, it suffices for us to prove

$$\begin{aligned}&\frac{1}{\tau} + A\tau - \frac{\nu^{-4}+1}{4} + \frac{1}{2} \ge \\ &\frac{3}{2}(\|u^n\|_\infty^2 + \|u^{n+1}\|_\infty^2) + \frac{\left(1+3\|u^n\|_\infty^2 + 3\|u^{n-1}\|_\infty^2\right)^2}{\nu^{-4}+1}\ .\end{aligned} \tag{4.15}$$ 2nd_condtionI

Now we prove this sufficient condition inductively. Set

$$B = \max\left\{\tilde{E}(u^1)\ ,\ E(u^0)\right\}\ . \tag{4.16}$$ {?}

It then follows by Lemma 4.1 that $B \lesssim 1$. We will prove for every $m \ge 2$,

$$\begin{cases}\tilde{E}(u^m) \le B\ ,\ \tilde{E}(u^m) \le \tilde{E}(u^{m-1})\ , \\ \|u^m\|_\infty \le \alpha_B \cdot \left\{\left(\nu^{-\frac{1}{2}} + \sqrt{\frac{\tau}{\nu}}(1+\nu^{-\frac{3}{2}})\right)^{\frac{1}{2}} \cdot \left(\nu^{-1}\tau^{-\frac{1}{2}} + \sqrt{A}\nu^{-1}\tau^{\frac{1}{2}} + \nu^{-\frac{5}{2}} + \nu^{-1}\right)^{\frac{1}{2}} + \tau + 1\right\}\ ,\end{cases} \tag{4.17}$$?4.17?

where $\alpha_B > 0$ is the same constant in Lemma 4.4. To start with, we first check the base case when $m = 2$. Note that $E(u^1) \le \tilde{E}(u^1) \le B$ and $E(u^0) \le B$, then Lemma 4.4 immediately leads to

$$\|u^2\|_\infty \le \alpha_B \cdot \left\{\left(\nu^{-\frac{1}{2}} + \sqrt{\frac{\tau}{\nu}}(1+\nu^{-\frac{3}{2}})\right)^{\frac{1}{2}} \cdot \left(\nu^{-1}\tau^{-\frac{1}{2}} + \sqrt{A}\nu^{-1}\tau^{\frac{1}{2}} + \nu^{-\frac{5}{2}} + \nu^{-1}\right)^{\frac{1}{2}} + \tau + 1\right\}\ .$$

It then suffices to show $\tilde{E}(u^2) \le \tilde{E}(u^1)$. By the sufficient condition (4.15), we only need to check the inequality

$$\frac{1}{\tau} + A\tau - \frac{\nu^{-4}+1}{4} + \frac{1}{2} \ge \frac{3}{2}(\|u^1\|_\infty^2 + \|u^2\|_\infty^2) + \frac{\left(1+3\|u^1\|_\infty^2 + 3\|u^0\|_\infty^2\right)^2}{\nu^{-4}+1}\ .$$

By Lemma 4.1, $\|u^0\|_\infty\ ,\ \|u^1\|_\infty \lesssim 1$, it suffices to choose A such that

$$\begin{aligned}\frac{1}{\tau} + A\tau - \frac{\nu^{-4}+1}{4} + \frac{1}{2} \ge & C\left(\nu^{-\frac{1}{2}} + \sqrt{\frac{\tau}{\nu}}(1+\nu^{-\frac{3}{2}})\right) \cdot \left(\nu^{-1}\tau^{-\frac{1}{2}} + \sqrt{A}\nu^{-1}\tau^{\frac{1}{2}} + \nu^{-\frac{5}{2}} + \nu^{-1}\right) \\ & + C\frac{\nu^4}{1+\nu^4} + C + C\tau^2\ .\end{aligned} \tag{4.18}$$ 4.18

The left-hand-side of (4.18) can be bounded below by

$$\text{LHS} = \frac{1}{\tau} + A\tau - \frac{\nu^{-4}+1}{4} + \frac{1}{2} \ge C(A^{\frac{1}{2}} + A\tau + A^{\frac{1}{4}}\tau^{-\frac{1}{2}} + A^{\frac{3}{4}}\tau^{\frac{1}{2}}) + \frac{1}{4} - \frac{\nu^{-4}}{4}. \tag{4.19}$$ {?}

Then the condition (4.18) can be modified to the following:

$$\begin{aligned}&A^{\frac{1}{2}} + A\tau + A^{\frac{1}{4}}\tau^{-\frac{1}{2}} + A^{\frac{3}{4}}\tau^{\frac{1}{2}} + C_1(\frac{1}{4} - \frac{\nu^{-4}}{4}) \\ \ge & C_2\left(\nu^{-\frac{1}{2}} + \sqrt{\frac{\tau}{\nu}}(1+\nu^{-\frac{3}{2}})\right) \cdot \left(\nu^{-1}\tau^{-\frac{1}{2}} + \sqrt{A}\nu^{-1}\tau^{\frac{1}{2}} + \nu^{-\frac{5}{2}} + \nu^{-1}\right) \\ & + C_2\frac{\nu^4}{1+\nu^4} + C_2 + C_2\tau^2.\end{aligned} \tag{4.20}$$ 4.20

We therefore discuss two cases.

`Case 1:` $0 < \nu \le 1$. In this case the requirement (4.20) is of the following form:

$$\begin{aligned}&A^{\frac{1}{2}} + A\tau + A^{\frac{1}{4}}\tau^{-\frac{1}{2}} + A^{\frac{3}{4}}\tau^{\frac{1}{2}} + C_1(\frac{1}{4} - \frac{\nu^{-4}}{4}) \\ \ge & C_2(\nu^{-\frac{1}{2}} + \tau^{\frac{1}{2}}\nu^{-2}) \cdot (\nu^{-1}\tau^{-\frac{1}{2}} + A^{\frac{1}{2}}\nu^{-1}\tau^{\frac{1}{2}} + \nu^{-\frac{5}{2}}) + C_2\frac{\nu^4}{1+\nu^4} + C_2\tau^2\ .\end{aligned}$$

It then suffices to choose

$$A \gg \nu^{-8}\ .$$

`Case 2:` $\nu > 1$. Then we need (4.20) to be

$$\begin{aligned}&A^{\frac{1}{2}} + A\tau + A^{\frac{1}{4}}\tau^{-\frac{1}{2}} + A^{\frac{3}{4}}\tau^{\frac{1}{2}} + C_1(\frac{1}{4} - \frac{\nu^{-4}}{4})\\ \geq & C_2(\nu^{-\frac{1}{2}} + \tau^{\frac{1}{2}}\nu^{-\frac{1}{2}}) \cdot (\nu^{-1}\tau^{-\frac{1}{2}} + A^{\frac{1}{2}}\nu^{-1}\tau^{\frac{1}{2}} + \nu^{-1}) + C_2 + C_2\tau^2 \ .\end{aligned}$$

It then suffices to choose

$$A \gg 1 \ .$$

In conclusion, it suffices for us to take for sufficiently large constant $C > 0$ such that

$$A \geq C \cdot (1 + \nu^{-8}). \tag{4.21}$$ {?}

We hereby check the induction step. Assume the induction hypothesis hold for $2 \leq m \leq n$, then for $m = n + 1$,

$$\|u^{n+1}\|_\infty \leq \alpha_B \cdot \left\{ \left(\nu^{-\frac{1}{2}} + \sqrt{\frac{\tau}{\nu}}(1 + \nu^{-\frac{3}{2}}) \right)^{\frac{1}{2}} \cdot \left(\nu^{-1}\tau^{-\frac{1}{2}} + \sqrt{A}\nu^{-1}\tau^{\frac{1}{2}} + \nu^{-\frac{5}{2}} + \nu^{-1} \right)^{\frac{1}{2}} + \tau + 1 \right\},$$

by Lemma 4.4. It remains to show $\tilde{E}(u^{n+1}) \leq \tilde{E}(u^n)$. It suffices to choose A such that

$$\begin{aligned}&A^{\frac{1}{2}} + A\tau + A^{\frac{1}{4}}\tau^{-\frac{1}{2}} + A^{\frac{3}{4}}\tau^{\frac{1}{2}} + C_1(\frac{1}{4} - \frac{\nu^{-4}}{4})\\ \geq & C_2 \left(\nu^{-\frac{1}{2}} + \sqrt{\frac{\tau}{\nu}}(1 + \nu^{-\frac{3}{2}}) \right) \cdot \left(\nu^{-1}\tau^{-\frac{1}{2}} + \sqrt{A}\nu^{-1}\tau^{\frac{1}{2}} + \nu^{-\frac{5}{2}} + \nu^{-1} \right)\\ &+ C_2\frac{\nu^4}{1+\nu^4} \left(\nu^{-\frac{1}{2}} + \sqrt{\frac{\tau}{\nu}}(1 + \nu^{-\frac{3}{2}}) \right)^2 \cdot \left(\nu^{-1}\tau^{-\frac{1}{2}} + \sqrt{A}\nu^{-1}\tau^{\frac{1}{2}} + \nu^{-\frac{5}{2}} + \nu^{-1} \right)^2 + C_2\frac{\nu^4}{1+\nu^4}(\tau^4 + 1) + C_2 + C_2\tau^2.\end{aligned} \tag{4.22}$$?4.21?

As in the base case, we again discuss two cases.

`Case 1:` $0 < \nu \leq 1$. Then it suffices to choose

$$A \gg \nu^{-8}.$$

`Case 2:` $\nu > 1$. Then again we need

$$A \gg 1.$$

To conclude these two cases, we require that for sufficiently large constant $C > 0$ that

$$A \geq C \cdot (1 + \nu^{-8}) \ . \tag{4.23}$$ 4.23

This completes the induction. Then $\tilde{E}(u^{n+1}) \leq \tilde{E}(u^n)$, for $n \geq 1$ by the choice of A in (4.23).

4.2. L^2 error estimate of the second order scheme

subsection:error2nd⟩? It remains to estimate the L^2 error of this second order scheme.

Theorem 4.5 (L^2 error estimate)**.** Let $\nu > 0$ and $u_0 \in H^s$, $s \geq 8$. Let $0 < \tau \leq M$ for some $M > 0$. Let $u(t)$ be the continuous solution to the 3D Allen-Cahn equation with initial data u_0. Let u^1 be defined according to (1.6) with initial data $u^0 = \Pi_N u_0$. Let u^m, $m \geq 2$ be defined in (1.5) with initial data u^0 and u^1. Assume A satisfies the same condition in Theorem 1.4. Define $t_0 = 0$, $t_1 = \tau_1$ and $t_m = \tau_1 + (m-1)\tau$ for $m \geq 2$. Then for any $m \geq 1$,

$$\|u(t_m) - u^m\|_2 \leq C_1 \cdot e^{C_2 t_m} \cdot (N^{-s} + \tau^2) \ ,$$

where C_1 , $C_2 > 0$ are constants depending only on $(u_0,\ \nu,\ s,\ A,\ M)$.

Similar to [8], we will study the auxiliary error estimate behavior and time discretization behavior of Allen-Cahn equation before proving the theorem.

4.2.1. **Auxiliary L^2 error estimate for near solutions**

Consider for $n \geq 1$,

$$\begin{cases} \dfrac{3u^{n+1} - 4u^n + u^{n-1}}{2\tau} = \nu\Delta u^{n+1} - A\tau(u^{n+1} - u^n) - \Pi_N\left(2f(u^n) - f(u^{n-1})\right) + G^n \\ \dfrac{3v^{n+1} - 4v^n + v^{n-1}}{2\tau} = \nu\Delta v^{n+1} - A\tau(v^{n+1} - v^n) - \Pi_N\left(2f(v^n) - f(v^{n-1})\right) \quad , \end{cases} \tag{4.24}$$ 2nd_I_aux

where $(u^1,\ u^0,\ v^1,\ v^0)$ are given.

⟨2ndpropI⟩ **Proposition 4.6.** For solutions to (4.24), assume for some $N_1 > 0$,

$$\sup_{n\geq 0}\|u^n\|_\infty + \sup_{n\geq 0}\|v^n\|_\infty \leq N_1 \ ,$$

Then for any $m \geq 2$,

$$\begin{aligned} \|u^m - v^m\|_2^2 &\leq C \cdot \exp\left((m-1)\tau \cdot \frac{C(1+N_1^4)}{\eta}\right) \\ &\cdot \left((1+A\tau^2)\|u^1 - v^1\|_2^2 + \|u^0 - v^0\|_2^2 + \frac{\tau}{\eta}\sum_{n=1}^{m-1}\|G^n\|_2^2\right) \ , \end{aligned}$$

where $C > 0$ is a absolute constant that can be computed and $0 < \eta < \frac{1}{100M}$ is a constant depending only on M, that is the upper bound for τ.

Proof. We still denote the constant by C whose value may vary in different lines. Denote $e^n = u^n - v^n$, then

$$\begin{aligned} &\frac{3e^{n+1} - 4e^n + e^{n-1}}{2\tau} - \nu\Delta e^{n+1} + A\tau(e^{n+1} - e^n) \\ = &-\Pi_N\left(2f(u^n) - 2f(v^n)\right) + \Pi_N\left(f(u^{n-1}) - f(v^{n-1})\right) + G^n \end{aligned} \tag{4.25}$$ 4.25

Taking the L^2 inner product with e^{n+1} on both sides of (4.25), we derive that

$$\begin{aligned} &\frac{1}{2\tau}(3e^{n+1} - 4e^n + e^{n-1}, e^{n+1}) + \nu\|\nabla e^{n+1}\|_2^2 + \frac{A\tau}{2}\left(\|e^{n+1}\|_2^2 - \|e^n\|_2^2 + \|e^{n+1} - e^n\|_2^2\right) \\ &= -2(f(u^n) - f(v^n),\ e^{n+1}) + (f(u^{n-1}) - f(v^{n-1}),\ e^{n+1}) + (G^n,\ e^{n+1}) \ . \end{aligned} \tag{4.26}$$ 2nd_I_Ineq1

To estimate the right hand side of (4.26), first we observe that

$$|(f(u^n) - f(v^n), e^{n+1})| \leq \|f(u^n) - f(v^n)\|_2\|e^{n+1}\|_2 \leq \frac{\|f(u^n) - f(v^n)\|_2^2}{\eta} + \eta\|e^{n+1}\|_2^2,$$

where $\eta < \frac{1}{100M}$ is a small number only depending on M. Moreover, as computed below we have

$$\begin{aligned} f(u^n) - f(v^n) &= f(u^n) - f(u^n - e^n) \\ &= (u^n)^3 - (u^n - e^n)^3 - e^n \\ &= -(e^n)^3 - e^n - 3u^n(e^n)^2 + 3(u^n)^2e^n \ . \end{aligned}$$

By assumption we then have

$$\begin{aligned} \|f(u^n) - f(v^n)\|_2^2 \lesssim &\|e^n\|_\infty^4\|e^n\|_2^2 + \|e^n\|_2^2 + \|u^n\|_\infty^2\|e^n\|_2^2 + \|u^n\|_\infty^4\|e^n\|_2^2 \\ \lesssim &(1+N_1^4)\|e^n\|_2^2 \ . \end{aligned}$$

Similarly, we have

$$\|f(u^{n-1}) - f(v^{n-1})\|_2^2 \lesssim (1+N_1^4)\|e^{n-1}\|_2^2 \ .$$

As a result, we obtain that

$$\text{RHS of (4.26)} \leq \frac{C(1+N_1^4)}{\eta}\left(\|e^n\|_2^2 + \|e^{n-1}\|_2^2\right) + \frac{1}{\eta}\|G^n\|_2^2 + \eta\|e^{n+1}\|_2^2 \ .$$

On the other hand, we have

$$(3e^{n+1}-4e^n+e^{n-1}, e^{n+1}-e^n) = (2\delta e^{n+1}+\delta^2 e^{n+1},\ \delta e^{n+1})$$
$$= 2\|\delta e^{n+1}\|_2^2 + \frac{1}{2}\left(\|\delta e^{n+1}\|_2^2 - \|\delta e^n\|_2^2 + \|\delta^2 e^{n+1}\|_2^2\right)\ .$$

We also have that

$$(3e^{n+1}-4e^n+e^{n-1},\ e^n) = 3(\delta e^{n+1},\ e^n) - (\delta e^n,\ e^n)$$
$$=\frac{3}{2}\left(\|e^{n+1}\|_2^2 - \|e^n\|_2^2 - \|e^{n+1}-e^n\|_2^2\right) - \frac{1}{2}\left(\|e^n\|_2^2 - \|e^{n-1}\|_2^2 + \|e^n - e^{n-1}\|_2^2\right)\ .$$

These two equations give that

$$\begin{aligned}&(3e^{n+1}-4e^n+e^{n-1},\ e^{n+1})\\ =&\frac{3}{2}(\|e^{n+1}\|_2^2 - \|e^n\|_2^2) - \frac{1}{2}(\|e^n\|_2^2 - \|e^{n-1}\|_2^2) + \|\delta e^{n+1}\|_2^2 - \|\delta e^n\|_2^2\\ &+\frac{1}{2}\|\delta^2 e^{n+1}\|_2^2\ .\end{aligned}$$

Collecting all the estimates above, we notice that the following inequality holds from (4.26):

$$\begin{aligned}&\frac{1}{2\tau}\left(\frac{3}{2}\|e^{n+1}\|_2^2 - \frac{1}{2}\|e^n\|_2^2 + \|e^{n+1}-e^n\|_2^2\right) + \frac{A\tau}{2}\|e^{n+1}\|_2^2\\ \le&\frac{1}{2\tau}\left(\frac{3}{2}\|e^n\|_2^2 - \frac{1}{2}\|e^{n-1}\|_2^2 + \|e^n-e^{n-1}\|_2^2\right) + \frac{A\tau}{2}\|e^n\|_2^2\\ &+\frac{C(1+N_1^4)}{\eta}\left(\|e^n\|_2^2 + \|e^{n-1}\|_2^2\right) + \frac{1}{\eta}\|G^n\|_2^2 + \eta\|e^{n+1}\|_2^2\ .\end{aligned} \tag{4.27}$$

2nd_I_Ineq2

Define $X^{n+1} := \frac{3}{2}\|e^{n+1}\|_2^2 - \frac{1}{2}\|e^n\|_2^2 + \|e^{n+1}-e^n\|_2^2$. We observe that X^{n+1} can be written into two different ways:

$$X^{n+1} = \begin{cases}\frac{1}{2}\|e^{n+1}\|_2^2 + \frac{1}{2}\|2e^{n+1}-e^n\|_2^2\\ \frac{1}{10}\|e^n\|_2^2 + \frac{5}{2}\|e^{n+1} - \frac{2}{5}e^n\|_2^2\ .\end{cases} \tag{4.28}$$

4.28

This shows

$$X^{n+1} \ge \frac{1}{10}\max\left\{\|e^{n+1}\|_2^2,\ \|e^n\|_2^2\right\}\ . \tag{4.29}$$

?4.29?

Making use of (4.28), (4.27) becomes

$$\begin{aligned}&\frac{\left(X^{n+1} + A\tau^2\|e^{n+1}\|_2^2\right) - \left(X^n + A\tau^2\|e^n\|_2^2\right)}{2\tau}\\ \le&\frac{C(1+N_1^4)}{\eta}\left(\|e^n\|_2^2 + \|e^{n-1}\|_2^2\right) + \frac{1}{\eta}\|G^n\|_2^2 + \eta\|e^{n+1}\|_2^2\ .\end{aligned}$$

This leads to

$$\begin{aligned}&\frac{\left(X^{n+1} - 2\eta\tau\|e^{n+1}\|_2^2 + A\tau^2\|e^{n+1}\|_2^2\right) - \left(X^n - 2\eta\tau\|e^n\|_2^2 + A\tau^2\|e^n\|_2^2\right)}{2\tau}\\ \le&\frac{C(1+N_1^4)}{\eta}\left(\|e^n\|_2^2 + \|e^{n-1}\|_2^2\right) + \frac{1}{\eta}\|G^n\|_2^2 + \eta\|e^n\|_2^2\\ \le&\left(\frac{C(1+N_1^4)}{\eta} + C\eta\right)\cdot\left(X^n - 2\eta\tau\|e^n\|_2^2\right) + \frac{1}{\eta}\|G^n\|_2^2\ .\end{aligned}$$

Define that

$$\begin{aligned}y_n &= X^n - 2\eta\tau\|e^n\|_2^2 + A\tau^2\|e^n\|_2^2\ ,\\ \alpha &= \frac{C(1+N_1^4)}{\eta} + C\eta\ ,\\ \beta_n &= \frac{\|G_n\|_2^2}{\eta}\ .\end{aligned}$$

Then for ν small, we get

$$\frac{y_{n+1}-y_n}{\tau} \leq \alpha y_n + \beta_n \ .$$

Applying the discrete Gronwall's inequality (Lemma 2.3), we have for $m \geq 2$,

$$\|e^m\|_2^2 \leq C\left(X^m - 2\eta\tau\|e^m\|_2^2\right) \leq Ce^{(m-1)\tau\cdot\frac{C(1+N_1^4)}{\eta}}\left(X^1 + A\tau^2\|e^1\|_2^2 + \frac{\tau}{\eta}\sum_{n=1}^{m-1}\|G^n\|_2^2\right),$$

which gives

$$\begin{aligned}
&\|u^m - v^m\|_2^2 \\
\leq& C\cdot\exp\left((m-1)\tau\cdot\frac{C(1+N_1^4)}{\eta}\right)\cdot\left(\frac{3}{2}\|e^1\|_2^2 - \frac{1}{2}\|e^0\|_2^2 + \|e^1-e^0\|_2^2\right. \\
&\left. + A\tau^2\|e^1\|_2^2 + \frac{\tau}{\eta}\sum_{n=1}^{m-1}\|G^n\|_2^2\right) \\
\leq& C\cdot\exp\left((m-1)\tau\cdot\frac{C(1+N_1^4)}{\eta}\right)\cdot\left((1+A\tau^2)\|u^1-v^1\|_2^2 + \|u^0-v^0\|_2^2\right. \\
&\left. + \frac{\tau}{\eta}\sum_{n=1}^{m-1}\|G^n\|_2^2\right) \ .
\end{aligned}$$

□

4.2.2. **Time discretization of the Allen-Cahn equation**

We first rewrite the AC equation in terms of the second order scheme.

⟨2ndSchemem_I_lem4⟩ **Lemma 4.7** (Time discrete Allen-Cahn equation)**.** Let $u(t)$ be the exact solution to Allen-Cahn equation with initial data $u_0 \in H^s$, $s \geq 8$. Define $t_0 = 0$, $t_1 = \tau_1$ and $t_m = \tau_1 + (m-1)\tau$ for $m \geq 2$. Then for any $n \geq 1$,

$$\begin{aligned}
&\frac{3u(t_{n+1}) - 4u(t_n) + u(t_{n-1})}{2\tau} \\
&= \nu\Delta u(t_{n+1}) - A\tau\left(u(t_{n+1}) - u(t_n)\right) - \Pi_N\left[2f(u(t_n)) - f(u(t_{n-1}))\right] + G^n \ .
\end{aligned}$$

For any $m \geq 2$,

$$\tau\sum_{n=1}^{m-1}\|G^n\|_2^2 \lesssim (1+t_m)\cdot(\tau^4 + N^{-2s}) \ .$$

Proof. The proof will be proceeded in several steps and we write $\lesssim$ instead of $\lesssim_{A,\ \nu,\ u_0}$ for simplicity.

Step 1: We write the PDE in the discrete form in time. Recall that

$$\partial_t u = \nu\Delta u - f(u) \ .$$

For a one variable function $h(t)$, the following equation holds:

$$h(t) = h(t_0) + h'(t_0)(t-t_0) + \frac{1}{2}h''(t_0)(t-t_0)^2 + \frac{1}{2}\int_{t_0}^{t} h'''(s)(s-t)^2 \ ds \ .$$

We then apply this to AC and obtain that

$$\begin{cases}
u(t_n) = u(t_{n+1}) - \partial_t u(t_{n+1})\cdot\tau + \frac{1}{2}\partial_{tt}u(t_{n+1})\tau^2 + \frac{1}{2}\int_{t_{n+1}}^{t_n}\partial_{ttt}u(s)(s-t_n)^2 \ ds \\
u(t_{n-1}) = u(t_{n+1}) - \partial_t u(t_{n+1})\cdot 2\tau + 2\partial_{tt}u(t_{n+1})\tau^2 + \frac{1}{2}\int_{t_{n+1}}^{t_{n-1}}\partial_{ttt}u(s)(s-t_{n-1})^2 \ ds.
\end{cases} \tag{4.30}$$ 4.30

The second equation in (4.30) minus 4 times the first equation in (4.30) leads to the following equation:

$$
\begin{aligned}
&\frac{3u(t_{n+1})-4u(t_n)+u(t_{n-1})}{2\tau}\\
&=\frac{1}{2\tau}\left(2\tau\cdot\partial_t u(t_{n+1})-2\int_{t_{n+1}}^{t_n}\partial_{ttt}u(s)(s-t_n)^2\,ds\right.\\
&\left.+\frac{1}{2}\int_{t_{n+1}}^{t_{n-1}}\partial_{ttt}u(s)(s-t_{n-1})^2\,ds\right)\\
&=\partial_t u(t_{n+1})+\frac{1}{\tau}\int_{t_n}^{t_{n+1}}\partial_{ttt}u(s)(s-t_n)^2\,ds-\frac{1}{4\tau}\int_{t_{n-1}}^{t_{n+1}}\partial_{ttt}u(s)(s-t_{n-1})^2\,ds\\
&=\nu\Delta u(t_{n+1})-A\tau\left(u(t_{n+1})-u(t_n)\right)-\Pi_N\left[2f(u(t_n))-f(u(t_{n-1}))\right]\\
&+A\tau\left(u(t_{n+1})-u(t_n)\right)-\Pi_{>N}\left[2f(u(t_n))-f(u(t_{n-1}))\right]\\
&+2f(u(t_n))-f(u(t_{n-1}))-f(u(t_{n+1})\\
&+\frac{1}{\tau}\int_{t_n}^{t_{n+1}}\partial_{ttt}u(s)(s-t_n)^2\,ds-\frac{1}{4\tau}\int_{t_{n-1}}^{t_{n+1}}\partial_{ttt}u(s)(s-t_{n-1})^2\,ds\ .
\end{aligned}
\tag{4.31}
$$

Clearly to write (4.31) as the discrete form in (4.24) we have

$$
\begin{aligned}
G^n=&A\tau\left(u(t_{n+1})-u(t_n)\right)-\Pi_{>N}\left[2f(u(t_n))-f(u(t_{n-1}))\right]\\
&+2f(u(t_n))-f(u(t_{n-1}))-f(u(t_{n+1}))\\
&+\frac{1}{\tau}\int_{t_n}^{t_{n+1}}\partial_{ttt}u(s)(s-t_n)^2\,ds-\frac{1}{4\tau}\int_{t_{n-1}}^{t_{n+1}}\partial_{ttt}u(s)(s-t_{n-1})^2\,ds\\
:=&I_1+I_2+I_3+I_4+I_5.
\end{aligned}
\tag{4.32}
$$

Step 2: We will control $\|G^n\|_2$ in (4.32) by estimating $\|I_1\|_2\sim\|I_5\|_2$.

I_1: Apply the fundamental theorem of calculus, we have

$$
\begin{aligned}
\|I_1\|_2^2=&\|A\tau\left(u(t_{n+1})-u(t_n)\right)\|_2^2\\
\lesssim&\tau^2\|u(t_{n+1})-u(t_n)\|_2^2\\
\lesssim&\tau^2\|\int_{t_n}^{t_{n+1}}\partial_t u(s)\,ds\|_2^2\\
\lesssim&\tau^2\int_{\mathbb{T}}\left(\int_{t_n}^{t_{n+1}}\partial_t u(s)\,ds\right)^2\\
\lesssim&\tau^2\int_{\mathbb{T}}\left((\int_{t_n}^{t_{n+1}}|\partial_t u(s)|^2\,ds)^{1/2}\cdot\sqrt{\tau}\right)^2\\
\lesssim&\tau^2\cdot\tau\cdot\int_{t_n}^{t_{n+1}}\|\partial_t u(s)\|_2^2\,ds\\
\lesssim&\tau^3\int_{t_n}^{t_{n+1}}\|\partial_t u(s)\|_2^2\,ds\ .
\end{aligned}
$$

I_2: By the maximum principle Lemma 2.4 and $u\in L_t^\infty H_x^s$,

$$
\begin{aligned}
\|I_2\|_2\lesssim&N^{-s}\cdot\left(\|f(u(t_n))\|_{H^s}+\|f(u(t_{n-1}))\|_{H^s}\right)\\
\lesssim&N^{-s}\ .
\end{aligned}
$$

I_3: To bound $\|I_3\|_2$, we recall that for a one-variable function $h(t)$,

$$
h(t)=h(t_0)+h'(t_0)(t-t_0)-\int_{t_0}^{t}h''(s)\cdot(s-t)\,ds\ .
$$

Then we apply to $f(u(t_n))$ and derive the following:

$$\begin{cases} f(u(t_n)) = f(u(t_{n+1})) - \partial_t(f(u))(t_{n+1}) \cdot \tau + \displaystyle\int_{t_n}^{t_{n+1}} \partial_{tt}(f(u)) \cdot (s - t_n)\ ds \\ f(u(t_{n-1})) = f(u(t_{n+1})) - \partial_t(f(u))(t_{n+1}) \cdot 2\tau + \displaystyle\int_{t_{n-1}}^{t_{n+1}} \partial_{tt}(f(u)) \cdot (s - t_{n-1})\ ds\ . \end{cases}$$

Then we subtract the second equation above by 2 times the first equation and derive:

$$\begin{aligned} &f(u(t_{n+1})) - 2f(u(t_n)) + f(u(t_{n-1})) \\ =& - 2\int_{t_n}^{t_{n+1}} \partial_{tt}(f(u)) \cdot (s - t_n)\ ds + \int_{t_{n-1}}^{t_{n+1}} \partial_{tt}(f(u)) \cdot (s - t_{n-1})\ ds\ . \end{aligned}$$

It then follows that

$$\begin{aligned} \|I_3\|_2^2 =& \|f(u(t_{n+1})) - 2f(u(t_n)) + f(u(t_{n-1}))\|_2^2 \\ \lesssim& \| \int_{t_n}^{t_{n+1}} \partial_{tt}(f(u)) \cdot (s - t_n)\ ds\|_2^2 + \| \int_{t_{n-1}}^{t_{n+1}} \partial_{tt}(f(u)) \cdot (s - t_{n-1})\ ds\|_2^2 \\ \lesssim& \tau^2 \cdot \| \int_{t_n}^{t_{n+1}} \partial_{tt}(f(u))\ ds\|_2^2 + \tau^2 \cdot \| \int_{t_{n-1}}^{t_{n+1}} \partial_{tt}(f(u))\ ds\|_2^2 \\ \lesssim& \tau^3 \int_{t_{n-1}}^{t_{n+1}} \|\partial_{tt}(f(u))\|_2^2\ ds\ , \end{aligned}$$

by a similar estimate in I_1.

$I_4 \& I_5$. We compute I_4 and I_5 as follows:

$$\begin{aligned} &\|I_4\|_2^2 + \|I_5\|_2^2 \\ \lesssim& \left\| \frac{1}{\tau} \int_{t_n}^{t_{n+1}} \partial_{ttt}u(s)(s - t_n)^2\ ds \right\|_2^2 + \left\| \frac{1}{\tau} \int_{t_{n-1}}^{t_{n+1}} \partial_{ttt}u(s)(s - t_{n-1})^2\ ds \right\|_2^2 \\ \lesssim& \left\| \frac{1}{\tau} \int_{t_{n-1}}^{t_{n+1}} \partial_{ttt}u(s) \cdot \tau^2\ ds \right\|_2^2 \\ \lesssim& \tau^2 \cdot \left\| \int_{t_{n-1}}^{t_{n+1}} \partial_{ttt}u(s)\ ds \right\|_2^2 \\ \lesssim& \tau^3 \int_{t_{n-1}}^{t_{n+1}} \|\partial_{ttt}u(s)\|_2^2\ ds\ . \end{aligned}$$

Step 3: Estimate $\tau \cdot \sum_{n=1}^{m-1} \|G^n\|_2^2$.

Collecting estimates above, we have

$$\begin{aligned} \tau \cdot \sum_{n=1}^{m-1} \|G^n\|_2^2 =& \tau \cdot \sum_{n=1}^{m-1} (\|I_1\|_2^2 + \|I_2\|_2^2 + \|I_3\|_2^2 + \|I_4\|_2^2 + \|I_5\|_2^2) \\ &\lesssim m\tau \cdot N^{-2s} + \tau^4 \cdot \int_0^{t_m} \|\partial_t u\|_2^2 + \|\partial_{tt}(f(u))\|_2^2 + \|\partial_{ttt}u\|_2^2\ d\tilde{s}\ . \end{aligned}$$

Note that by differentiating the original AC equation in time, we indeed have

$$\begin{cases} \partial_{tt}u = \nu\partial_t\Delta u - \partial_t(f(u)) \\ \partial_{ttt}u = \nu\partial_{tt}\Delta u - \partial_{tt}(f(u)) \\ \partial_t(f(u)) = f'(u)\partial_t u \\ \partial_{tt}(f(u)) = f'(u)\partial_{tt}u + f''(u)(\partial_t u)^2\ , \end{cases}$$

hence together with maximum principle Lemma 2.4 and higher Sobolev bounds Lemma 2.5, one has

$$
\begin{aligned}
\tau \cdot \sum_{n=1}^{m-1} \|G^n\|_2^2 &\lesssim m\tau \cdot N^{-2s} + \tau^4 \cdot \int_0^{t_m} \|\partial_t u\|_2^2 + \|\partial_{tt}(f(u))\|_2^2 + \|\partial_{ttt} u\|_2^2 \, d\tilde{s} \\
&\lesssim t_m \cdot N^{-2s} + \tau^4 \cdot \int_0^{t_m} \|u\|_{H^s}^2 \, d\tilde{s} \\
&\lesssim t_m \cdot N^{-2s} + \tau^4 \cdot (1 + t_m) \\
&\lesssim (1 + t_m) \cdot (\tau^4 + N^{-2s}) \, .
\end{aligned}
$$

This completes the proof of Lemma 4.7. □

4.2.3. **Proof of L^2 error estimate of the second order scheme (1.5)**

Note that the assumptions in Proposition 4.6 are satisfied by the unconditional energy stability Theorem 1.4 and the maximum principle of the Allen-Cahn equation. Thus we apply the auxiliary estimate Proposition 4.6. Then

$$
\|u(t_m) - u^m\|_2^2 \lesssim e^{Cm\tau} \cdot \left((1 + A\tau^2)\|u^1 - v^1\|_2^2 + \|u^0 - v^0\|_2^2 + \tau \sum_{n=1}^{m-1} \|G^n\|_2^2 \right) \, .
$$

By Lemma 4.2 and Lemma 4.7,

$$
\begin{aligned}
\|u(t_m) - u^m\|_2^2 &\lesssim e^{Cm\tau} \cdot \left((1 + A\tau^2)\|u^1 - v^1\|_2^2 + \|u^0 - v^0\|_2^2 + \tau \sum_{n=1}^{m-1} \|G^n\|_2^2 \right) \\
&\lesssim e^{Ct_m} \cdot \big((1 + A\tau^2)(N^{-2s} + \tau^4) + N^{-2s} + (1 + t_m) \cdot (\tau^4 + N^{-2s}) \big) \\
&\lesssim e^{Ct_m} \cdot (N^{-2s} + \tau^4) \, .
\end{aligned}
$$

Thus for $m \geq 2$,

$$
\|u(t_m) - u^m\|_2 \lesssim e^{Ct_m} \cdot (N^{-s} + \tau^2) \, .
$$

Remark 4.8. For the error estimate, we actually do not need high regularity of the initial data because of a smoothing effect of Allen-Cahn equation.

5. Concluding remark

Throughout this paper, we discussed certain first order and second order semi-implicit Fourier spectral methods on the Allen-Cahn equation in a three dimensional torus. We proved the unconditional stability (energy decay) of these numerical schemes by adding stabilizing terms with a large constant A. Note that this stability is preserved independent of time step τ. We also proved a L^2 error estimate between numerical solutions from the semi-implicit scheme and exact solutions. In the future work, more cases can be discussed on other gradient cases (as mentioned in Remark 1.8) such as general nonlocal Allen-Cahn and Cahn-Hilliard equations, MBE equations, phase field crystal model and other equations describing phenomena of interest in material sciences. Higher order schemes and more nonlinear numerical framework including operator splitting schemes will be discussed.

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