On the Stability of a Semi-Implicit Scheme of Cahn-Hilliard Type Equations

by

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Abstract

It is well known that Allen-Cahn equation and Cahn-Hilliard equation are essential to study the phase separation phenomenon of a two-phase or a multiple-phase mixture. An important property of the solutions to those two equations is that the energy functional, which is defined in this thesis, decreases in time. To study these solutions, researchers developed different numerical schemes to give accurate approximations, since analytic solutions are only available in a very few simple cases. However, not all schemes satisfy the energy-decay property, which is an important standard to determine whether the scheme is stable. In recent work, Li, Qiao and Tang developed a semi-implicit scheme for the Cahn-Hilliard equation and proved the energy-decay property. In this thesis, we extend the semi-implicit scheme to the Allen-Cahn equation and fractional Cahn-Hilliard equation with a proof of the energy-decay property. Moreover, this semi-implicit scheme is practical and could be applied to more general diffusion equations while preserving the energy-decay stability.

Lay Summary

This thesis extends a numerical scheme from previous literature for the Cahn-Hilliard equation to the Allen-Cahn equation and fractional Cahn-Hilliard equation, which are more general partial differential equations. These equations describe physical phenomena of interest in material science. We proved the stability of such scheme by showing the energy is decreasing. Based on our result, schemes with similar stability properties can be analyzed for more general equations.

Preface

The topic of this thesis is based on the previous work of the author's supervisor, Dr. Dong Li in [11], [10] and [9].

The content of Chapter 3 and 4 is based on [11]. However, the author provides unique variations of original ideas. Therefore, the content of Chapter 3 and 4 is independent of [11] and hence original work by the author.

The content of Chapter 5 is original work by the author with help of unpublished ideas by the author's supervisors, Dr. Dong Li and Dr. Brian Wetton.

The content of Chapter 6 is based on [10] and the content of Chapter 7 is based on [9] but the author provides original variations of these ideas. Therefore, the content of Chapter 6 and 7 is produced by the author independently and originally.

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Secondly, I would like to express my thanks to my colleagues and office-mates for their warmness and caring, that made me feel more enjoyable doing research.

Dedication

This thesis is dedicated to my firmest supporters, my parents, Mrs. Xiaodong Huang and Mr. Chun Cheng.

Chapter 1

Introduction

Partial differential equations (PDE) often describe mathematical models of physical phenomena. For example, wave equations describe the properties of waves including sound waves, light waves and other waves, which help us to study sound including noise and music, electromagnetics and fluid dynamics.

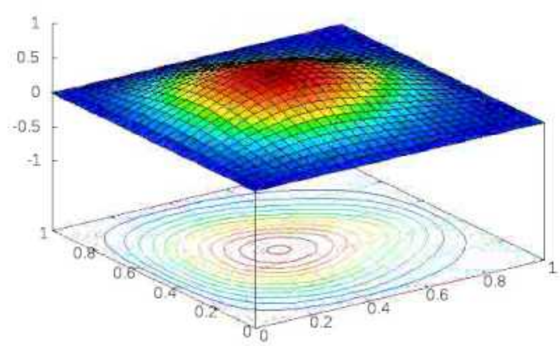

Figure 1.1: Computational Simulation of 2D Waves [20]

To study PDE, we are interested in the solutions to a certain equation in some domain under specific initial conditions and boundary conditions. More information about the solution can help the physical model to be better understood. In mathematics, usually these studies focus on the existence, uniqueness, regularity and some long-time behaviors of the solution.

Although sometimes it is possible to find explicit solutions of certain simple PDE, usually there are no explicit solutions. Thus, it is necessary to compute approximate solutions using computer simulations. As a result, throughout the area of partial differential equations, it is necessary to develop well behaved numerical schemes that are guaranteed to approximate PDE to an expected accuracy.

In this thesis, we consider modified versions of the Cahn-Hilliard equation. These equations were developed in [2] to describe the separation of different metals in a binary alloy. They have been recognized as a generic model that arises in many applications. Hence they have been well studied by mathematicians, physicists and other scientists. The Cahn-Hilliard equation for $u(x,t)$ is:

$$\begin{cases} \partial_t u = \Delta(-\nu\Delta u + f(u)), & (x,t) \in \Omega \times (0,\infty) \\ u(x,0) = u_0 \end{cases}, \tag{1.1}$$

where the vector position x is in the spatial domain Ω, which is taken to be two dimensional periodic domain in this work, and t is time. The values of u generally lie in the range $[-1,1]$, with -1 representing the pure state of one phase and $+1$ representing the pure state of the other phase. Values of u in $(-1,1)$ represent a mixture of the two phases. Here ν is a small parameter, $\sqrt{\nu}$ represents an average distance over which phases mix. The energy term

$f(u)$ is defined by

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

The Cahn-Hilliard equation (1.1) describes the evolution of the phase fractions under a competition between diffusion (which tends to mix phases) and the preference of the phases to separate.

In this thesis, we consider the spatial domain Ω to be the 2π-periodic torus $\mathbb{T}^2 = \mathbb{R}/2\pi\mathbb{Z} \times \mathbb{R}/2\pi\mathbb{Z}$. Often, the Cahn-Hilliard equation and related equations we consider in this thesis, describe the micro structure of macroscopic material. Thus, considering a periodic domain is not a serious simplification: we are modelling a representative piece of the micro structure. Considering the periodic domain allows the use of efficient and accurate Fourier-spectral numerical methods, which will be introduced later in the thesis.

It is not possible to find analytic solutions to the Cahn-Hilliard equation. As a result, it is necessary to develop numerical methods to approximate the solutions. Many approaches have been developed, [4] as an example. Another example computational result is shown in Figure 1.2 [19]. Such numerical approximations should give accurate results to the values and qualitative features of the solution. In the literature, a key feature is energy decay, discussed in detail below. In [11], Li, Qiao and Tang propose a numerical scheme for Cahn-Hilliard equation and hence prove that it preserves energy decay with no a-priori assumptions. In this thesis, we extend their result to other related models.

By standard arguments, the mass of the smooth solution of Cahn-Hilliard equation is conserved, i.e. $\frac{d}{dt}M(t) \equiv 0$, $M(t) = \int_\Omega u(x,t)\,dx$. This represents the conservation of the two phases in the mixture. In particular, $M(t) \equiv 0$ if $M(0) = 0$ and hence oftentimes zero-mean initial data would be considered as a simpler but representative case. The associated energy functional is given by

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

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

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

which implies energy decay: $\frac{d}{dt}E(u(t)) \leq 0$, and hence contributes to the existence of global solutions to Cahn-Hilliard equation as it provides a priori H^1-norm bound. On the other hand, the energy decay property is an impor-

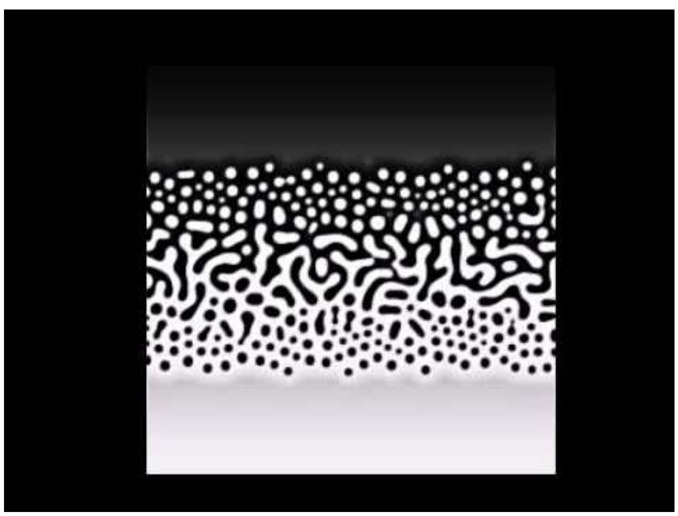

Figure 1.2: Spectral Simulation of the Cahn Hilliard Equation in a 2D Domain [19]

tant index for whether a numerical scheme is "stable" or not.

Previous works by others [8, 14, 17, 18] 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. To improve that, Li, Qiao and Tang proved an unconditional stability theory on a large time-stepping semi-implicit Fourier-spectral scheme.

The scheme has the form:

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

As usual τ is the time step, A is a large coefficient for the $O(\tau)$ stabilizing term. Here $O(\tau)$ is defined as the well-known "big O" notation, i.e. $|O(\tau)| \leq |c\tau|$ for a non-zero constant c, or in other words at most linear function of τ. As a result of their work, the energy decay could still be satisfied with a well-chosen large number A, with at least a size of $O(1/\nu|\log(\nu)|^2)$, or $c/\nu|\log(\nu)|^2$ for some positive constant c that depends on the initial conditions.

Our work extends their semi-implicit scheme to the related Allen-Cahn equation and fractional Cahn-Hilliard equation. The Allen-Cahn equation is defined as:

$$\begin{cases} \partial_t u = \nu\Delta u - f(u) \\ u(x,0) = u_0\ ; \end{cases} \tag{1.3}$$

while the zero-mass projected Allen-Cahn equation is defined as:

$$\begin{cases} \partial_t u = \Pi_0(\nu\Delta u - f(u)) \\ u(x,0) = u_0 \ , \end{cases} \tag{1.4}$$

where Π_0 is the zero mass projector, i.e. $\Pi_0(f) = \frac{1}{(2\pi)^d}\sum_{|k|\geq 1}\widehat{f}(k)e^{ik\cdot x}$. The difference between the Allen-Cahn equation and zero-mass projected Allen-Cahn equation results from the fact that the mass functional is not preserved in Allen-Cahn equation.

The fractional Cahn-Hilliard equation is defined as the following:

$$\begin{cases} \partial_t u = \nu\Delta\left((-\Delta)^{\alpha} u + (-\Delta)^{\alpha-1} f(u)\right) \ , \ 0 < \alpha \leq 1 \\ u(x,0) = u_0 \end{cases} . \tag{1.5}$$

As $\alpha \to 0$, (1.3) becomes the zero-mass projected Allen-Cahn equation and for $\alpha = 1$, it coincides the original Cahn-Hilliard equation. Roughly speaking, the fractional Cahn-Hilliard equation is an interpolation of the Allen-Cahn and Cahn-Hilliard equations.

Remark 1. *More general cases could be discussed. Roughly speaking we could define a general "gradient" operator $\mathscr{G}$ and rewrite the equation as :*

$$\begin{cases} \partial_t u = \mathscr{G}(\nu\Delta u - f(u)) \\ u(x,0) = u_0 \end{cases} . \tag{1.6}$$

When $\mathscr{G} = id$, the identity map, (1.4) becomes the Allen-Cahn equation; when $\mathscr{G} = (-\Delta)^{\alpha}$, (1.4) becomes the fractional Cahn-Hilliard equation as discussed *above. And the corresponding semi-implicit scheme is*

$$\begin{cases} \dfrac{u^{n+1}-u^n}{\tau} = \mathcal{G}\left(\nu\Delta u^{n+1} - f(u^n)\right) - A\mathcal{G}(u^{n+1}-u^n)\ ,\ n \geq 0 \\ u^0 = u_0 \end{cases} . \tag{1.7}$$

The main result of this thesis states that for any fixed time step τ, we can always define a large constant A independent of τ in (1.5), such that the numerical solution would be stable in the sense of satisfying the energy-decay condition for "gradient" cases of A-C and fractional C-H. The analysis of other gradients is left to future work.

For completeness, preliminaries would be given and the main lemma would be proved in chapter 2; stability of first order semi-implicit schemes for Allen-Cahn equation and fractional Cahn-Hilliard would be proved in chapter 3 and 5 respectively. Moreover, we extend the results to the 3D case in chapter 6. On the other hand, main results of error estimate and convergence are given in chapter 4. Finally, we introduce two second order semi-implicit schemes in chapter 7 while proving stability results and error estimates.

Chapter 2

Preliminaries and the Main Lemma

2.1 Definitions and Useful Theorems

2.1.1 L^p Space

Throughout this paper we will denote the domain $\Omega = \mathbb{T}^2$. If $1 \le p < \infty$, the space $L^p(\Omega)$ consists of all complex-valued measurable functions that satisfy

$$\int_\Omega |f(x)|^p \, dx < \infty \, .$$

For $f \in L^p(\Omega)$ we define the L^p norm of f by

$$||f||_{L^p(\Omega)} = \left(\int_\Omega |f(x)|^p \, dx \right)^{1/p} \, .$$

2.1.2 Weak Derivatives and Sobolev Space

We use the notation below:

$$\begin{aligned} x &= (x_1, x_2, ..., x_n) \in \mathbb{R}^n \\ \alpha &= (\alpha_1, \alpha_2, ..., \alpha_n) \in \mathbb{Z}_+^n \\ \partial^\alpha f &= \frac{\partial^{\alpha_1 + ... + \alpha_n} f}{\partial_{x_1}^{\alpha_1} \partial_{x_2}^{\alpha_2} ... \partial_{x_n}^{\alpha_n}} \quad . \end{aligned} \tag{2.1}$$

We define 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

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

then v is defined to be the weak partial derivative of u, denoted by $\partial^\alpha u$. If u is "smooth" enough, its weak derivative coincides with its derivative and the equation above is basically integration by parts.

Suppose $u \in L^p(\Omega)$ and all weak derivatives $\partial^\alpha u$ exist for $|\alpha| = \alpha_1 + ... + \alpha_n \le k$, such that $\partial^\alpha u \in L^p(\Omega)$ for $|\alpha| \le k$, then we say $u \in W^{k,p}(\Omega)$, and such space is called Sobolev space. The norm in $W^{k,p}(\Omega)$ is defined as :

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

Throughout this paper, for $p = 2$ case, we use the convention $H^k(\Omega)$ denote the space $W^{k,2}(\Omega)$. For more details, we refer to chapter 5, [6].

2.1.3 Fourier Transform

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

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

By taking advantage of Fourier expansion, we use the equivalent H^s-norm and $\dot{H}^s$-norm of function f by

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

The equivalence of two norms are well known, we refer to Appendix A in [16].

2.1.4 Convergence of Fourier Series in Periodic Domains

Given f being a $L^p(\mathbb{T}^d)$ periodic function for $p > 1$, and denote the Dirichlet partial sum $D_N f := \frac{1}{(2\pi)^d} \sum_{|k|\le N} \widehat{f}(k) e^{ik\cdot x}$, then

$$||D_N f - f||_{L^p(\mathbb{T}^d))} \to 0 \ , \ and \ D_N f \to f \text{ pointwise almost everywhere} \ . \tag{2.2}$$

This was originally proved by Carleson in [3].

2.1.5 Uniform Boundedness Principle

Let X be a Banach space and Y be a normed vector space. Suppose that F is a collection of continuous linear operator from X to Y. If for all x in X one has

$$\sup_{T\in F} ||T(x)||_Y < \infty \ ,$$

Then

$$\sup_{T\in F} ||T|| < \infty \text{ where } ||T|| \text{ is the operator norm.}$$

We refer to a simple proof in [15].

2.1.6 Fixed-point Theorem

Given a Banach space $(X, ||.||)$ and a contraction map $T : X \to X$ s.t $||T(x) - T(y)|| \leq \beta ||x - y||$ with $0 < \beta < 1$, then there exists a fix-point x, s.t $T(x) = x$. We refer to [1] for details.

2.1.7 Duhamel's Formula

Consider a linear inhomogeneous evolution equation for a function $u(x,t) : \Omega \times (0,\infty) \to \mathbb{R}$, with a spatial domain $\Omega \subset \mathbb{R}^d$, of the form

$$\begin{cases} u_t(x,t) - Lu(x,t) = f(x,t)\ ,\ (x,t) \in \Omega \times (0,\infty) \\ u|_{\partial\Omega} = 0 \\ u(x,0) = u_0(x)\ ,\ x \in \Omega\ , \end{cases} \tag{2.3}$$

where L is a linear differential operator that involves no time derivatives and the boundary condition could be replaced by periodic boundary condition. Then formally, the solution to this equation system is:

$$u(x,t) = e^{Lt}u_0 + \int_0^t e^{L(t-s)} f\ ds \tag{2.4}$$

where e^{Lt} is the homogeneous solution operator, or $e^{Lt}u_0$ solves the homogeneous equation with initial data u_0. In fact $e^{Lt}u_0$ is often given as a convolution between a well-defined kernel and the initial data u_0. For more details, we refer to [6].

2.2 Several Important Inequalities

2.2.1 Hölder's Inequality

Given $f \in L^p(\Omega)$ and $g \in L^q(\Omega)$, such that $\frac{1}{p} + \frac{1}{q} = 1$ then

$$||fg||_{L^1(\Omega)} \leq ||f||_{L^p(\Omega)}||g||_{L^q(\Omega)}.$$

2.2.2 Young's Inequality

Given a, b, p, q positive real numbers, such that $\frac{1}{p} + \frac{1}{q} = 1$, then

$$ab \leq \frac{a^p}{p} + \frac{b^q}{q}.$$

2.2.3 Sobolev Inequality on $\mathbb{T}^d$

Note that the this Sobolev inequality is slightly different from the standard version. Let $0 < s < d$ and $f \in L^q(\mathbb{T}^d)$ for any $\frac{d}{d-s} < p < \infty$, then

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

Here $\langle \nabla \rangle^{-s}$ denotes $(1-\Delta)^{-\frac{s}{2}}$, or on the Fourier side $(1+|k|^2)^{-\frac{s}{2}}$ and $A \lesssim_{s,p,d} B$ is defined as $A \leq C_{s,p,d}\, B$ where $C_{s,p,d}$ is a constant dependent on s, p and d. See [11] for the details.

2.2.4 Morrey's Inequality on $H^2(\mathbb{T}^d)$

Assume $d \leq 3$ and $f \in H^2(\mathbb{T}^d)$ then

$$||f||_{\infty(\mathbb{T}^d)} \lesssim ||f||_{H^2(\mathbb{T}^d)} \ .$$

In fact stronger argument could be made with the help of Hölder space arguments, but in this paper only the infinity norm is needed. More detailed information is in chapter 5, [6].

2.2.5 Gagliardo–Nirenberg Interpolation Inequality

For functions $u : \Omega \to \mathbb{R}$ defined on a bounded Lipschitz domain $\Omega \subset \mathbb{R}^d$, fix $1 \leq q,\ r \leq \infty$ and a natural number m. Suppose also that a real number α and a natural number j are such that

$$\frac{1}{p} = \frac{j}{d} + \left(\frac{1}{r} - \frac{m}{d}\right)\alpha + \frac{1-\alpha}{q}$$

and

$$\frac{j}{m} \leq \alpha \leq 1 \ .$$

Then

$$||D^j u||_{L^p} \leq C_1(\Omega)||D^m u||^{\alpha}_{L^r}||u||^{1-\alpha}_{L^q} + C_2(\Omega)||u||_{L^s}$$

where $s > 0$ is arbitrary.

2.2.6 Grönwall's Inequality

On the interval $I = [a,b]$ where $a < b$ and b could be ∞. Let β and u be real-valued continuous functions defined on I. If u is differentiable in (a,b) and satisfies

$$u'(t) \le \beta(t)u(t)\ ,\ t \in (a,b)\ ,$$

then

$$u(t) \le u(a)\exp\left(\int_a^t \beta(s)\ ds\right)\ ,\ t \in [a,b]\ .$$

We refer to [7] for details.

2.2.7 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 $m \ge 1$, we have

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

The proof is given in [11].

2.3 the Main Lemma

For all $f \in H^s(\mathbb{T}^2)$, $s > 1$, then

$$||f||_\infty \le C_s \cdot \left(||f||_{\dot{H}^1}\sqrt{\log(||f||_{\dot{H}^s} + 3)} + |\widehat{f}(0)| + 1\right)\ . \tag{2.5}$$

Here C_s is a constant which only depends on s.

Proof. To prove the lemma, we write $f(x) = \frac{1}{(2\pi)^2}\sum_{k\in\mathbb{Z}^2}\widehat{f}(k)\ e^{ik\cdot x}$, i.e. the Fourier series of f, which is convergent pointwisely to f. So,

$$\begin{aligned}
||f||_\infty &\leq \frac{1}{(2\pi)^2}\sum_{k\in\mathbb{Z}^2}|\widehat{f}(k)| \\
&\leq \frac{1}{(2\pi)^2}\left(|\widehat{f}(0)| + \sum_{0<|k|\leq N}|\widehat{f}(k)| + \sum_{|k|>N}|\widehat{f}(k)|\right) \\
&\lesssim |\widehat{f}(0)| + \sum_{0<|k|\leq N}(|\widehat{f}(k)||k|\cdot|k|^{-1}) + \sum_{|k|>N}(|\widehat{f}(k)||k|^{s}\cdot|k|^{-s}) \\
&\lesssim |\widehat{f}(0)| + \left(\sum_{0<|k|\leq N}|\widehat{f}(k)|^2|k|^2\right)^{\frac{1}{2}}\cdot\left(\sum_{0<|k|\leq N}|k|^{-2}\right)^{\frac{1}{2}} + \left(\sum_{|k|>N}|\widehat{f}(k)|^2|k|^{2s}\right)^{\frac{1}{2}}\cdot(\sum_{|k|>N}|k|^{-2s})^{\frac{1}{2}} \\
&\lesssim |\widehat{f}(0)| + \frac{1}{N^{s-1}}\left(\sum_{|k|>N}|\widehat{f}(k)|^2|k|^{2s}\right)^{\frac{1}{2}} + \left(\sum_{0<|k|\leq N}|\widehat{f}(k)|^2|k|^2\right)^{\frac{1}{2}}\cdot\sqrt{\log(N+3)} \\
&\lesssim |\widehat{f}(0)| + \frac{1}{N^{s-1}}||f||_{\dot{H}^s} + \sqrt{\log(N+3)}||f||_{\dot{H}^1}\ .
\end{aligned} \tag{2.6}$$

In the previous step, we use Hölder's inequality for counting measure and integral approximation of $\sum_{0<|k|\leq N}|k|^{-2}$ and $\sum_{|k|>N}|k|^{-2s}$ in $\mathbb{Z}^2$. To be more clear,

$$\begin{aligned}
\sum_{0<|k|\leq N}|k|^{-2} &\lesssim \int_1^N \frac{1}{r^2}\cdot 2\pi r\ dr \\
&\lesssim \int_1^N \frac{1}{r}\ dr \\
&\lesssim \log(N+3)\ ,
\end{aligned} \tag{2.7}$$

$$\begin{aligned}
\sum_{|k|>N}|k|^{-2s} &\lesssim \int_N^\infty \frac{1}{r^{2s}}\cdot 2\pi r\ dr \\
&\lesssim \int_N^\infty \frac{1}{r^{2s-1}}\ dr \\
&\lesssim \frac{1}{N^{2s-2}}\ .
\end{aligned} \tag{2.8}$$

If $||f||_{\dot{H}^s} \leq 3$, we could simply take $N = 1$; otherwise take N^{s-1} close to $||f||_{\dot{H}^s}$. For a similar lemma and proof, we refer to [12] and [11]. □

Chapter 3

Stability of a First Order Semi-implicit Scheme on 2D Allen-Cahn Equation

$Allen-Cahn$ equation is a Δ^1 version of $Cahn-Hilliard$ equation with bilaplacian:

$$\begin{cases} \partial_t u = \nu \Delta u - f(u) \\ u(x,0) = u_0 \end{cases}.$$

Here $f(u) = u^3 - u$, and the spatial domain Ω is often taken to be the $2\pi-$periodic torus $\mathbb{T}^2$. Also we sometimes use ε^2 instead of ν as ν is a small parameter. The corresponding energy is defined by $E(u) = \int_\Omega (\frac{\nu}{2}|\nabla u|^2 + F(u))\, dx$, where $F(u) = \frac{1}{4}(u^2-1)^2$, the anti-derivative of $f(u)$.

As is well known, the energy satisfies $E(u(t)) \le E(u(s))$,$\forall\ t \ge s$, which gives a priori bound. Now we consider a stabilized semi-implicit scheme introduced in [11]. The form is the following:

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

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

$$X_N = \text{span}\left\{\cos(k\cdot x)\,,\sin(k\cdot x):\ \ k=(k_1,k_2)\in\mathbb{Z}^2\ ,\ |k|_\infty = \max\{|k_1|,|k_2|\}\leq N\right\}\ .$$

So define the L^2 projection operator $\Pi_N: L^2(\Omega)\to X_N$ by $(\Pi_N u - u,\phi) = 0\ \ \forall\phi\in X_N$, where $(\cdot,\cdot)$ denotes the L^2 inner product on Ω. In other words, the projection operator Π_N is just the truncation of Fourier modes $|k|_\infty \leq N$. $\Pi_N u_0 \in X_N$ and by induction, we have $u^n \in X_N\ ,\forall n\geq 0$.

3.1 Stability Theorem for Allen-Cahn Equation

Theorem 3.1.1. *(unconditional energy stability for AC). Consider (3.1) with $\nu > 0$ and assume $u_0 \in H^2(\mathbb{T}^2)$. Then there exists a constant β_0 depending only on the initial energy $E_0 = E(u_0)$ such that if*

$$A \geq \beta\cdot\left(||u_0||_{H^2}^2 + \nu^{-1}|\log\nu| + 1\right)\ ,\ \beta\geq\beta_0 \tag{3.2}$$

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

Remark 2. *Similar to [11], the stability result is valid for any time step τ. Our choice of A is independent of τ as long as it has size of $O(1/\nu|\log(\nu)|)$ at least. Note that the choice of A may not be optimal and further work could be done.*

Remark 3. *The condition $u_0 \in H^2(\mathbb{T}^2)$ results from the classic Sobolev embedding* $\sup_N \|\Pi_N u_0\|_\infty \lesssim \|u_0\|_{H^2(\mathbb{T}^2)}$. *No mean zero assumption is needed for u_0 .*

To prove this we need a log-type interpolation inequality, which is the main lemma.

3.2 Proof of the Stability Theorem

The proof uses an induction argument. To start with, let's recall the numerical scheme (3.1)

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

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

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

Because u^n is periodic, (as $u^n \in X_N$), hence by integration by parts, we have

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

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

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

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

$$(\frac{1}{\tau}+A)\int_{\mathbb{T}^2}|u^{n+1}-u^n|^2+\frac{\nu}{2}\int_{\mathbb{T}^2}|\nabla u^{n+1}|^2-|\nabla u^n|^2+|\nabla(u^{n+1}-u^n)|^2=-\left(f(u^n),u^{n+1}-u^n\right). \tag{3.3}$$

Now, by fundamental theorem of calculus and integration by parts,

$$\begin{aligned}F(u^{n+1})-F(u^n)&=f(u^n)(u^{n+1}-u^n)+\int_{u^n}^{u^{n+1}}f'(s)(u^{n+1}-s)\,ds\\&=f(u^n)(u^{n+1}-u^n)+\int_{u^n}^{u^{n+1}}(3s^2-1)(u^{n+1}-s)\,ds\\&=f(u^n)(u^{n+1}-u^n)+\frac{1}{4}(u^{n+1}-u^n)^2\left(3(u^n)^2+(u^{n+1})^2+2u^nu^{n+1}-2\right).\end{aligned} \tag{3.4}$$

Combine previous two equations, and denote $E(u^n)$ by E^n we have

$$\begin{aligned}&(\frac{1}{\tau}+A)||u^{n+1}-u^n||_{L^2}^2+\frac{\nu}{2}||\nabla(u^{n+1}-u^n)||_{L^2}^2+\frac{\nu}{2}||\nabla u^{n+1}||_{L^2}^2-\frac{\nu}{2}||\nabla u^n||_{L^2}^2\\&+\int_{\mathbb{T}^2}F(u^{n+1})-F(u^n)=\frac{1}{4}\left((u^{n+1}-u^n)^2,3(u^n)^2+(u^{n+1})^2+2u^nu^{n+1}-2\right)\\&\text{Note }\frac{\nu}{2}||\nabla u^{n+1}||_{L^2}^2+\int_{\mathbb{T}^2}F(u^{n+1})=E(u^{n+1})=E^{n+1}\\&\Longrightarrow(\frac{1}{\tau}+A+\frac{1}{2})||u^{n+1}-u^n||_{L^2}^2+\frac{\nu}{2}||\nabla(u^{n+1}-u^n)||_{L^2}^2+E^{n+1}-E^n\\&=\frac{1}{4}\left((u^{n+1}-u^n)^2,3(u^n)^2+(u^{n+1})^2+2u^nu^{n+1}\right)\\&\le||u^{n+1}-u^n||_{L^2}^2\left(||u^n||_\infty^2+\frac{1}{2}||u^{n+1}||_\infty^2\right).\end{aligned} \tag{3.5}$$

To show $E^{n+1}\le E^n$, clearly it suffices to show

$$\frac{1}{\tau}+A+\frac{1}{2}\ge\frac{3}{2}\max\left\{||u^n||_\infty^2\ ,\ ||u^{n+1}||_\infty^2\right\}. \tag{3.6}$$

Note that $E^0 = E(\Pi_N u_0)$ while $E_0 = E(u_0)$. In general $E_0 \neq E^0$. In effect, we claim that

Proposition 1.

$$\sup_N E(\Pi_N u_0) \lesssim 1 + E_0, where\ u_0 \in H^1(\mathbb{T}^2)\ . \tag{3.7}$$

Proof. First, we write $\Pi_N u_0$ as $\frac{1}{(2\pi)^2}\sum_{|k|\le N}\widehat{u_0}(k)e^{ik\cdot x}$, namely the Dirichlet partial sum of u_0.

$$||\nabla(\Pi_N u_0)||^2_{L^2(\mathbb{T}^2)} = \frac{1}{(2\pi)^2}\sum_{|k|\le N}|k|^2|\widehat{u_0}(k)|^2 \le \frac{1}{(2\pi)^2}\sum_{|k|\in\mathbb{Z}^2}|k|^2|\widehat{u_0}(k)|^2 = ||\nabla(u_0)||^2_{L^2(\mathbb{T}^2)}\ . \tag{3.8}$$

The first equality above is because the operator Π_N is just a truncation of Fourier modes.

On the potential energy part, by standard Sobolev inequality, $||u_0||_{L^4(\mathbb{T}^2)} \lesssim ||u_0||_{H^1(\mathbb{T}^2)}$, this shows $u_0 \in L^4(\mathbb{T}^2)$ and hence the Dirichlet partial sum $\Pi_N u_0$ converges to u_0 in $L^4(\mathbb{T}^2)$. Then, $||\Pi_N u_0||_{L^4(\mathbb{T}^2)} \to ||u_0||_{L^4(\mathbb{T}^2)}$, which leads to $\sup_N ||\Pi_N u_0||_{L^4(\mathbb{T}^2)} < \infty$. By Uniform Boundedness Principle, we derive $\sup_N ||\Pi_N|| < \infty$, i.e. $\sup_N ||\Pi_N u_0||_{L^4(\mathbb{T}^2)} \le c||u_0||_{L^4(\mathbb{T}^2)}$ for an absolute constant c. Combine two estimates above we conclude the proof for the claim.

For an alternate proof, see [10], and this claim holds for 3D case as well with a similar proof. □

We rewrite the numerical scheme (3.1) as following:

$$u^{n+1} = \frac{1+A\tau}{1+A\tau-\nu\tau\Delta}u^n - \frac{\tau}{1+A\tau-\nu\tau\Delta}\Pi_N[f(u^n)]\ . \tag{3.9}$$

By the lemma, to control $||u^{n+1}||_\infty$ and $||u^n||_\infty$, we may consider $\dot{H}^1$-norm and $\dot{H}^{\frac{3}{2}}$-norm together with $0th$-mode $|\widehat{u}^{n+1}(0)|$.

To start with,

$$\begin{aligned}
|\widehat{u}^{n+1}(0)| &\leq |\widehat{u}^n(0)| + \frac{\tau}{1+A\tau}|\widehat{f}(u^n)(0)| \\
&\leq |\widehat{u}^n(0)| + \frac{1}{A}|\widehat{f}(u^n)(0)| \\
&\leq |\int_{\mathbb{T}^2} u^n \; dx| + |\int_{\mathbb{T}^2} u^n - (u^n)^3 \; dx| \qquad (3.10) \\
&\lesssim 1 + |\int_{\mathbb{T}^2} (u^n)^2 \; dx|^{\frac{1}{2}} + |\int_{\mathbb{T}^2} (1-(u^n)^2)^2 \; dx|^{\frac{1}{2}} \\
&\lesssim 1 + \sqrt{E^n} \; ,
\end{aligned}$$

where the last 2 inequalities are by Cauchy-Schwarz inequalities and Hölder's inequalities.

Lemma 3.2.1. *There is an absolute constant $c_1 > 0$ such that for any $n \geq 0$*

$$\begin{cases}
||u^{n+1}||_{\dot{H}^{\frac{3}{2}}(\mathbb{T}^2)} \leq c_1 \cdot \left(\dfrac{A+1}{\nu} + \dfrac{1}{\nu\tau}\right) \cdot (E^n + 1) \\
||u^{n+1}||_{\dot{H}^1(\mathbb{T}^2)} \leq \left(1 + \dfrac{1}{A} + \dfrac{3}{A}||u^n||_\infty^2\right) \cdot ||u^n||_{\dot{H}^1(\mathbb{T}^2)} \; .
\end{cases} \qquad (3.11)$$

Proof. As $0th$-mode will not contribute to $\dot{H}^1$ norm and $\dot{H}^{\frac{3}{2}}$ norm, we could just consider Fourier modes $|k| \geq 1$ from the Fourier side. Use the symbol $f \lesssim g$ to denote $f \leq c \cdot g$ with c being a constant.

$$\begin{cases}
\dfrac{(1+A\tau)|k|^{\frac{3}{2}}}{1+A\tau+\nu\tau|k|^2} \lesssim \dfrac{1+A\tau}{\nu\tau} \\
\dfrac{\tau|k|^{\frac{3}{2}}}{1+A\tau+\nu\tau|k|^2} \lesssim \dfrac{\tau}{\tau\nu}|k|^{-\frac{1}{2}} = \dfrac{1}{\nu}|k|^{-\frac{1}{2}} \; .
\end{cases} \qquad (3.12)$$

Hence

$$||u^{n+1}||_{\dot{H}^{\frac{3}{2}}(\mathbb{T}^2)} \lesssim \left(\frac{1+A\tau}{\nu\tau}\right)||u^n||_{L^2(\mathbb{T}^2)} + \frac{1}{\nu}||\langle\nabla\rangle^{-\frac{1}{2}} f(u^n)||_{L^2(\mathbb{T}^2)}. \tag{3.13}$$

Here the notaion $\langle\nabla\rangle^s = (1-\Delta)^{\frac{s}{2}}$, corresponds to the Fourier side $(1+|k|^2)^{s/2}$. Note $||u^n||_{L^2(\mathbb{T}^2)} \lesssim \int_{\mathbb{T}^2} \frac{1}{4}(u^4 - 2u^2 + 1)\ dx + 1 \lesssim E^n + 1$ by Cauchy-Schwarz inequality. By Sobolev inequality $||\langle\nabla\rangle^{-\frac{1}{2}} f(u^n)||_{L^2(\mathbb{T}^2)} \lesssim ||f(u^n)||_{L^{\frac{4}{3}}(\mathbb{T}^2)} = ||(u^n)^3 - u^n||_{L^{\frac{4}{3}}(\mathbb{T}^2)} = \left(\int_{\mathbb{T}^2}((u^n)^3 - u^n)^{\frac{4}{3}}\ dx\right)^{\frac{3}{4}} \lesssim \left(\int_{\mathbb{T}^2}(u^n)^4\ dx\right)^{\frac{3}{4}} \lesssim E^n + 1$. Hence (3.13) becomes

$$||u^{n+1}||_{\dot{H}^{\frac{3}{2}}(\mathbb{T}^2)} \lesssim \left(\frac{1+A\tau}{\nu\tau} + \frac{1}{\nu}\right)(E^n + 1). \tag{3.14}$$

Similarly,

$$\begin{cases} \dfrac{(1+A\tau)|k|}{1+A\tau+\nu\tau|k|^2} \lesssim |k| \\ \dfrac{\tau|k|}{1+A\tau+\nu\tau|k|^2} \lesssim \dfrac{\tau}{\tau A}|k| = \dfrac{1}{A}|k|\ . \end{cases} \tag{3.15}$$

This implies

$$\begin{aligned} ||u^{n+1}||_{\dot{H}^1(\mathbb{T}^2)} &\lesssim ||u^n||_{\dot{H}^1(\mathbb{T}^2)} + \frac{1}{A}||f(u^n)||_{\dot{H}^1(\mathbb{T}^2)} \\ &\lesssim ||u^n||_{\dot{H}^1(\mathbb{T}^2)} + \frac{1}{A}||\nabla(f(u^n))||_{L^2(\mathbb{T}^2)} \\ &\lesssim ||u^n||_{\dot{H}^1(\mathbb{T}^2)} + \frac{1}{A}||(3(u^n)^2 - 1)\cdot(\nabla u^n)||_{L^2(\mathbb{T}^2)} \\ &\lesssim ||u^n||_{\dot{H}^1(\mathbb{T}^2)} + (\frac{1}{A} + \frac{3||u||_\infty^2}{A})||u^n||_{\dot{H}^1(\mathbb{T}^2)} \\ &\lesssim \left(1 + \frac{1}{A} + \frac{3||u||_\infty^2}{A}\right)||u^n||_{\dot{H}^1(\mathbb{T}^2)}\ . \end{aligned} \tag{3.16}$$

□

Now we prove by induction.

Step 1: The induction $n \implies n+1$ step. Assume $E^n \leq E^{n-1} \leq \cdots \leq E^0$ and $E^n \leq \sup_N E(\Pi_N u_0)$, we would show $E^{n+1} \leq E^n$. This implies $||u^n||_{\dot{H}^1}^2 = ||\nabla u^n||_{L^2}^2 \leq \frac{2E^n}{\nu} \leq \frac{2E^0}{\nu}$.

So by the main lemma, use the notation $f \lesssim_{E^0} g$ to denote there exists a constant $C(E^0)$ depends only on E^0 such that $f \leq C(E^0) \cdot g$, we have

$$\begin{aligned}
||u^n||_\infty^2 &\lesssim ||u^n||_{\dot{H}^1}^2 \left(\sqrt{\log(3 + c_1 \left(\frac{1}{\nu\tau} + \frac{A+1}{\nu} \right)(E^n + 1))} \right)^2 + E^n + 1 \\
&\lesssim \frac{2E^0}{\nu} \left(1 + \log(A) + \log(\frac{1}{\nu}) + (\log(1 + \frac{1}{\tau})) \right) + E^0 + 1 \\
&\lesssim_{E^0} \nu^{-1} \left(1 + \log(A) + \log(\frac{1}{\nu}) \right) + \nu^{-1} |\log(\tau)| + 1 \, .
\end{aligned} \tag{3.17}$$

Define $m_0 := \nu^{-1}(1 + \log(A) + |\log(\nu)|)$, and note that $E^0 \leq \sup_N E(\Pi_N u_0) \lesssim E_0 + 1$, the inequality above is

$$||u^n||_\infty^2 \lesssim_{E_0} m_0 + \nu^{-1} |\log(\tau)| + 1. \tag{3.18}$$

On the other hand,

$$
\begin{aligned}
||u^{n+1}||_\infty^2 &\lesssim \left(1+||u^{n+1}||_{\dot{H}^1}\sqrt{\log(3+||u^{n+1}||_{\dot{H}^{\frac{3}{2}}})}\right)^2 \\
&\lesssim \left(1+(\frac{1+||u^n||_\infty^2}{A})||u^n||_{\dot{H}^1}\sqrt{\log(3+||u^{n+1}||_{\dot{H}^{\frac{3}{2}}})}\right)^2 \\
&\lesssim_{E_0} \left(1+(1+\frac{m_0+\nu^{-1}|\log(\tau)|}{A})(\sqrt{\frac{1}{\nu}}\sqrt{\log(3+||u^{n+1}||_{\dot{H}^{\frac{3}{2}}})}\right)^2 \\
&\lesssim_{E_0} \left(1+(1+\frac{m_0+\nu^{-1}|\log(\tau)|}{A})(\sqrt{m_0+\nu^{-1}|\log(\tau)|})\right)^2 \\
&\lesssim_{E_0} \left(1+\sqrt{m_0+\nu^{-1}|\log(\tau)|}+\frac{(\sqrt{m_0+\nu^{-1}|\log(\tau)|})^3}{A}\right)^2 \\
&\lesssim_{E_0} 1+\frac{m_0^3}{A^2}+m_0+\nu^{-3}|\log(\tau)|^3 \ .
\end{aligned}
\tag{3.19}
$$

Hence sufficient condition (3.6) becomes

$$
\begin{cases}
A+\frac{1}{2}+\frac{1}{\tau} \geq C(E_0)\left(m_0+1+\frac{m_0^3}{A^2}+\nu^{-3}|\log(\tau)|^3\right) \\
m_0=\nu^{-1}(1+\log(A)+|\log(\nu)|) \ .
\end{cases}
\tag{3.20}
$$

We discuss two cases.

Case 1:$\frac{1}{\tau} \geq C(E_0)\nu^{-3}|\log(\tau)|^3$. In this case, we need to choose A such that

$$A \gg_{E_0} m_0=\nu^{-1}(1+\log(A)+|\log(\nu)|) \ .$$

In fact, for $\nu \gtrsim 1$, we could take $A \gg_{E_0} 1$; if $0<\nu \ll 1$, we would choose $A = C_{E_0}\cdot \nu^{-1}|\log\nu|$, where C_{E_0} is a large constant depending only on E_0. Therefore in both cases it suffices to choose

$$A = C_{E_0}\cdot \max\left\{\nu^{-1}|\log(\nu)| \ , \ 1\right\}. \tag{3.21}$$

Case 2:$\frac{1}{\tau} \le C(E_0)\nu^{-3}|\log(\tau)|^3$. This implies $|\log(\tau)| \lesssim_{E_0} 1 + |\log(\nu)|$. Now we go back to equations (3.17), we have

$$||u^n||_\infty^2 \lesssim_{E_0} m_0, \tag{3.22}$$

as $\nu^{-1}|\log(\tau)|$ would be absorbed by m_0, recall $m_0 = \nu^{-1}(1+\log(A)+|\log(\nu)|)$. Hence substitute this new bound to (3.19), we would get

$$\begin{aligned} ||u^{n+1}||_\infty^2 &\lesssim \left(1+(\frac{1+||u^n||_\infty^2}{A})||u^n||_{\dot H^1}\sqrt{\log(3+||u^{n+1}||_{\dot H^{\frac{3}{2}}})}\right)^2 \\ &\lesssim_{E_0} \left(1+(1+\frac{m_0}{A})\sqrt{\frac{1}{\nu}}\sqrt{\log(3+||u^{n+1}||_{\dot H^{\frac{3}{2}}})}\right)^2 \\ &\lesssim_{E_0} \left(1+(1+\frac{m_0}{A})\sqrt{m_0}\right)^2 \\ &\lesssim_{E_0} 1+\frac{m_0^3}{A^2}+m_0 \ . \end{aligned} \tag{3.23}$$

This shows it suffices to take

$$A \ge C_{E_0} m_0, \tag{3.24}$$

for a large enough constant C_{E_0} depending only on E_0. The same choice of A in Case 1(with a larger C_{E_0} if necessary) would still work.

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

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

By the lemma 3.2.1,

$$\begin{aligned} ||u^1||_{\dot{H}^1} &\le \left(1+\frac{1}{A}+\frac{3}{A}||\Pi_N u_0||_\infty^2\right)\cdot ||u_0||_{\dot{H}^1} \\ &\le \left(1+\frac{1}{A}+\frac{3}{A}||\Pi_N u_0||_\infty^2\right)\cdot \sqrt{\frac{2E^0}{\nu}}\ . \end{aligned} \tag{3.25}$$

As a result,

$$\begin{aligned} ||u^1||_\infty^2 &\lesssim \left(1+|\widehat{u}^1(0)|+||u^1||_{\dot{H}^1}\sqrt{\log(3+||u^1||_{\dot{H}^{\frac{3}{2}}})}\right)^2 \\ &\lesssim \left(1+\sqrt{E^0}+\left(1+\frac{1}{A}+\frac{3}{A}||\Pi_N u_0||_\infty^2\right)\sqrt{\frac{2E^0}{\nu}}\sqrt{\log\left(3+c_1\left(\frac{A+1}{\nu}+\frac{1}{\nu\tau}\right)(E_0+1)\right)}\right)^2 \\ &\lesssim_{E^0} \left(1+\left(1+\frac{1}{A}+\frac{3}{A}||\Pi_N u_0||_\infty^2\right)\cdot \nu^{-\frac{1}{2}}\cdot\sqrt{1+\log(A)+|\log(\nu)|+|\log(\tau)|}\right)^2 \\ &\lesssim_{E_0} \left(1+\frac{1}{A}+\frac{3}{A}||\Pi_N u_0||_\infty^2\right)^2\cdot \nu^{-1}\cdot(1+\log(A)+|\log(\nu)|+|\log(\tau)|)\ . \end{aligned} \tag{3.26}$$

Thus we need to choose A such that

$$\begin{aligned} A+\frac{1}{2}+\frac{1}{\tau} \ge ||\Pi_N u_0||_\infty^2 + C_{E_0}\cdot\left(1+\frac{1}{A}+\frac{3}{A}||\Pi_N u_0||_\infty^2\right)^2\cdot\nu^{-1} \\ \cdot(1+\log(A)+|\log(\nu)|+|\log(\tau)|)\ , \end{aligned} \tag{3.27}$$

where C_{E_0} is a large constant depending only on E_0. Note that by Morrey's inequality for 2D domains,

$$||\Pi_N u_0||_{L^\infty(\mathbb{T}^2)} \lesssim ||\Pi_N u_0||_{H^2(\mathbb{T}^2)} \lesssim ||u_0||_{H^2(\mathbb{T}^2)}.$$

Then it suffices to take A s.t.

$$A \gg_{E_0} ||u_0||_{H^2}^2 + \nu^{-1}|\log(\nu)| + 1\ . \tag{3.28}$$

This completes the induction and hence the theorem.

Chapter 4

L^2 Error Estimate of the First Order Scheme on 2D Allen-Cahn Equation

In this chapter, we would like to study the L^2 error between the semi-implicit numerical solution and the exact PDE solution in the domain $\mathbb{T}^2$. To start with, we consider the auxiliary L^2 error estimate for near solutions.

4.1 Auxiliary L^2 Error Estimate for Near Solutions

Consider the following system:

$$\begin{cases} \dfrac{u^{n+1}-u^n}{\tau} = \nu\Delta u^{n+1} - \Pi_N f(u^n) - A(u^{n+1}-u^n) + G_n^1 \\ \dfrac{v^{n+1}-v^n}{\tau} = \nu\Delta v^{n+1} - \Pi_N f(v^n) - A(v^{n+1}-v^n) + G_n^2 \\ u^0 = u_0 \ , \ v^0 = v_0 \end{cases} \tag{4.1}$$

where we would denote $G_n = G_n^1 - G_n^2$.

We state the proposition here.

Proposition 2. *For solutions of (4.1), assume for some $N_1 > 0$,*

$$\sup_{n\geq 0} ||u^n||_\infty + \sup_{n\geq 0} ||v^n||_\infty \leq N_1 \ . \tag{4.2}$$

Then for any $m \geq 1$,

$$\begin{aligned} &||u^m - v^m||_{L^2}^2 = ||e^m||_{L^2}^2 \\ &\leq \exp\left(m\tau \cdot \left\{ C\left(\frac{(1+N_1^2)N_1}{\nu} + N_1^2 + \nu(1+N_1^2)N_1 \right) + \frac{B}{\nu} \right\} \right) \\ &\cdot \left((1+A\tau)||u_0 - v_0||_{L^2}^2 + B\tau\nu \sum_{n=0}^{m-1} ||G_n||_{L^2}^2 \right) \end{aligned} \tag{4.3}$$

where B , $C > 0$ are two absolute constants.

Proof. Write $e^n = u^n - v^n$. Then

$$\frac{e^{n+1} - e^n}{\tau} = \nu\Delta e^{n+1} - A(e^{n+1} - e^n) - \Pi_N \left(f(u^n) - f(v^n) \right) + G_n \ . \tag{4.4}$$

Take the L^2 inner product with e^{n+1} on both sides and recall similar computations in chapter 3, one has

$$\begin{aligned} &\frac{1}{2\tau}\left(||e^{n+1}||_{L^2}^2 - ||e^n||_{L^2}^2 + ||e^{n+1} - e^n||_{L^2}^2 \right) + \nu||\nabla e^{n+1}||_{L^2}^2 + \frac{A}{2}(||e^{n+1}||_{L^2}^2 - ||e^n||_{L^2}^2 + \\ &||e^{n+1} - e^n||_{L^2}^2) = \left(G_n,\ e^{n+1} \right) + \left(f(u^n) - f(v^n),\ \Pi_N e^{n+1} \right) \end{aligned} \tag{4.5}$$

where (. , .) denotes the L^2 inner product and the last term is because Π_N is a self-adjoint operator $(\Pi_N f,\ g) = (f,\ \Pi_N g)$, since it is just an N-th Fourier mode truncation.

Now by Hölder's inequality

$$|\left(G_n,\ e^{n+1}\right)| \leq ||e^{n+1}||_{L^2}||G_n||_{L^1} \leq B||e^{n+1}||_{L^2}||G_n||_{L^2} \leq 2B\left(\nu||G_n||^2_{L^2} + \frac{||e^{n+1}||^2_{L^2}}{\nu}\right) \tag{4.6}$$

Next, by fundamental theorem of calculus, we compute

$$\begin{aligned} f(u^n) - f(v^n) &= \int_0^1 f'(v^n + se^n)ds\ e^n \\ &= (a_1 + a_2(v^n)^2)e^n + a_3 v^n (e^n)^2 + a_4(e^n)^3\ , \end{aligned} \tag{4.7}$$

where a_i are constants could be computed. Now we shall denote by C an absolute constant whose value may vary in different lines. Now,

$$\begin{aligned} |\left((a_1 + a_2(v^n)^2)e^n\ ,\ e^{n+1}\right)| &\leq C(1 + ||v^n||^2_\infty)||e^{n+1}||_{L^2}||e^n||_{L^2} \\ &\leq C(1+N_1^2)N_1(\frac{||e^{n+1}||^2_{L^2}}{\nu} + \nu||e^n||^2_{L^2}) \\ &\leq \frac{C(1+N_1^2)N_1}{\nu}||e^{n+1}||^2_{L^2} + \nu \cdot C(1+N_1^2)N_1||e^n||^2_{L^2}\ , \end{aligned} \tag{4.8}$$

also,

$$\begin{aligned} |\left(a_3 v^n (e^n)^2\ ,\ e^{n+1}\right)| &\leq C||v^n||_\infty ||e^{n+1}||_\infty ||e^n||^2_{L^2} \\ &\leq CN_1^2||e^n||^2_{L^2}\ , \end{aligned} \tag{4.9}$$

$$\begin{aligned} |\left(a_4(e^n)^3\ ,\ e^{n+1}\right)| &\leq C||e^{n+1}||_\infty ||e^n||_\infty ||e^n||^2_{L^2} \\ &\leq CN_1^2||e^n||^2_{L^2}\ . \end{aligned} \tag{4.10}$$

To simplify the formula, we would use the notation $||u||_2$ to denote the L^2 norm. Collecting all estimates, we get

$$\frac{||e^{n+1}||_2^2-||e^n||_2^2}{\tau}+A(||e^{n+1}||_2^2-||e^n||_2^2)\leq B\nu||G_n||_2^2+\frac{B}{\nu}||e^{n+1}||_2^2$$
$$C\left(\nu(1+N_1^2)N_1+N_1^2\right)||e^n||_2^2+\frac{C(1+N_1^2)N_1}{\nu}||e^{n+1}||_2^2 \tag{4.11}$$

where B and C are two absolute constants that could be computed exactly. Hence for ν small, recall A is chosen large than $O(\nu^{-1}|\log\nu|)$, we derive

$$\frac{||e^{n+1}||_2^2-||e^n||_2^2}{\tau}+\left(A-\frac{C(1+N_1^2)N_1}{\nu}-\frac{B}{\nu}\right)(||e^{n+1}||_2^2-||e^n||_2^2)\leq B\nu||G_n||_2^2+$$
$$\left\{C\left(\frac{(1+N_1^2)N_1}{\nu}+N_1^2+\nu(1+N_1^2)N_1\right)+\frac{B}{\nu}\right\}||e^n||_2^2 \tag{4.12}$$

Define

$$y_n=\left(1+\left(A-\frac{C(1+N_1^2)N_1}{\nu}-\frac{B}{\nu}\right)\tau\right)||e^n||_2^2\ ,$$
$$\alpha=C\left(\frac{(1+N_1^2)N_1}{\nu}+N_1^2+\nu(1+N_1^2)N_1\right)+\frac{B}{\nu}\ , \tag{4.13}$$
$$\beta_n=B\nu||G_n||_2^2\ .$$

This shows for ν small,

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

Applying discrete Gronwall's inequality, we have

$$
\begin{aligned}
||u^m - v^m||_2^2 = ||e^m||_2^2 \le y_m \le \exp\left(m\tau \cdot \left\{ C\left(\frac{(1+N_1^2)N_1}{\nu} + N_1^2 + \nu(1+N_1^2)N_1\right) + \frac{B}{\nu}\right\}\right) \\
\cdot \left(\left(1 + \left(A - \frac{C(1+N_1^2)N_1}{\nu} - \frac{B}{\nu}\right)\tau\right)||u_0 - v_0||_2^2 + B\tau\nu \sum_{n=0}^{m-1} ||G_n||_2^2\right) \\
\le \exp\left(m\tau \cdot \left\{ C\left(\frac{(1+N_1^2)N_1}{\nu} + N_1^2 + \nu(1+N_1^2)N_1\right) + \frac{B}{\nu}\right\}\right) \\
\cdot \left((1 + A\tau)||u_0 - v_0||_2^2 + B\tau\nu \sum_{n=0}^{m-1} ||G_n||_2^2\right) .
\end{aligned}
\tag{4.14}
$$

□

4.2 L^2 Error Estimate of 2D Allen-Cahn Equation

In this section, to simplify the notation, we would write $x \lesssim y$ if $x \le C(\nu\ ,\ u_0)\ y$ for a constant C depending on ν and u_0. We consider the system

$$
\begin{cases}
\dfrac{u^{n+1} - u^n}{\tau} = \nu\Delta u^{n+1} - \Pi_N f(u^n) - A(u^{n+1} - u^n) \\
\partial_t u = \nu\Delta u - f(u) \\
u^0 = \Pi_N u_0\ ,\ u(0) = u_0\ .
\end{cases}
\tag{4.15}
$$

Theorem 4.2.1. *Let $\nu > 0$. Let $u_0 \in H^s$, $s \ge 4$ 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 $t_m = m\tau$, $m \ge 1$. Then*

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

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

In order to prove this theorem, it is clear that we shall estimate G_n in previous proposition. Note that for a one-variable function $h(t)$, one has the formula:

$$\begin{cases} \dfrac{1}{\tau}\displaystyle\int_{t_n}^{t_{n+1}} h(t) = h(t_n) + \dfrac{1}{\tau}\int_{t_n}^{t_{n+1}} h'(t)\cdot(t_{n+1}-t)\, dt \\ \dfrac{1}{\tau}\displaystyle\int_{t_n}^{t_{n+1}} h(t) = h(t_{n+1}) + \dfrac{1}{\tau}\int_{t_n}^{t_{n+1}} h'(t)\cdot(t_n - t)\, dt\ . \end{cases} \tag{4.16}$$

Using the formula above and integrating Allen-Cahn equation on the time interval $[t_n\ ,\ t_{n+1}]$, we get

$$\begin{aligned} &\frac{u(t_{n+1}) - u(t_n)}{\tau} = \\ &\nu\Delta u(t_{n+1}) - A\left(u(t_{n+1}) - u(t_n)\right) - \Pi_N f(u(t_n)) - \Pi_{>N} f(u(t_n)) + G_n \end{aligned} \tag{4.17}$$

where $\Pi_{>N} = id - \Pi_N$, the large mode truncation and

$$G_n = \frac{\nu}{\tau}\int_{t_n}^{t_{n+1}} \partial_t \Delta u\cdot(t_n - t)\, dt - \frac{1}{\tau}\int_{t_n}^{t_{n+1}} \partial_t(f(u))(t_{n+1}-t)\, dt + A\int_{t_n}^{t_{n+1}} \partial_t u\ dt\ . \tag{4.18}$$

To bound $||G_n||_2$, we introduce some useful lemmas.

4.2.1 Bounds on Allen-Cahn Exact Solution and Numerical Solution

Lemma 4.2.2. *(maximum principle for smooth solutions to Allen-Cahn equation) Let $T > 0$ 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

$$||u(.\ ,\ t)||_\infty \leq \max\{||u_0||_\infty\ ,\ 1\}\ ,\ \forall 0 \leq t \leq T\ . \tag{4.19}$$

Remark 4. *As proved in [5], there exists a global $H_x^4 C_t^1$ solution to Allen-Cahn equation. In fact as pointed out by Li, Qiao and Tang in [12], the regularity would be even higher due to the smoothing effect of heat kernel and the non-linear term. So we would assume a smooth solution here.*

Proof. We define $f(x,t) = u(x,t)^2$ and $f^\epsilon(x,t) = f(x,t) - \epsilon t$. Since f^ϵ is a continuous function on the compact domain $\mathbb{T}^d \times [0,T]$, it achieves maximum at some point (x_*, t_*), i.e.

$$\max_{0\leq t\leq T\ ,\ x\in\mathbb{T}^d} f^\epsilon(x,t) = f^\epsilon(x_*,t_*) := M_\epsilon\ .$$

We discuss several cases.

Case 1. $0 < t_* \leq T$ and $M\epsilon > 1$. This shows $\nabla f^\epsilon(x_*,t_*) = 0\ ,\ \Delta f^\epsilon(x_*,t_*) \leq 0$. Note that

$$\nabla f^\epsilon = 2u\nabla u\ ,\ \Delta f^\epsilon = 2|\nabla u|^2 + 2u\Delta u\ , \tag{4.20}$$

this shows $\nabla u(x_*,t_*) = 0$, $u\Delta u(x_*,t_*) < 0$.

However,

$$
\begin{aligned}
\partial_t f^\epsilon(x_*,t_*) &= 2u(x_*,t_*)\partial_t u(x_*,t_*) - \epsilon \\
&= 2u(x_*,t_*)(\nu\Delta u(x_*,t_*) - u^3(x_*,t_*) + u(x_*,t_*)) - \epsilon \\
&< -2u^4(x_*,t_*) + 2u^2(x_*,t_*) - \epsilon \\
&< -2(u^2(x_*,t_*) - \frac{1}{2})^2 + \frac{1}{2} - \epsilon \\
&< -\epsilon < 0
\end{aligned}
\tag{4.21}
$$

as $u^2(x_*,t_*) > 1$ by assumption. This contradicts the hypothesis that f^ϵ achieves its maximum at (x_*,t_*) and hence Case 1 is impossible.

Case 2. $0 < t_* \le T$ and $M\epsilon \le 1$. In this case we obtain

$$\max_{0\le t\le T\ ,\ x\in\mathbb{T}^d} f(x,t) \le 1 + \epsilon T\ ,$$

letting $\epsilon \to 0$, we obtain $f(x,t) \le 1$.

Case 3. $t_* = 0$, then

$$\max_{0\le t\le T\ ,\ x\in\mathbb{T}^d} f(x,t) \le \max_{x\in\mathbb{T}^d} f(x,0) + \epsilon T\ ,$$

sending ϵ to 0, we obtain $f(x,t) \le f(x,0)$.

This concludes $||u||_\infty \le \max\{||u_0||\infty\ ,\ 1\}$. □

Lemma 4.2.3. *(H^k boundedness of exact solution) Assume $u(x,t)$ is a smooth solution to Allen-Cahn equation in $\mathbb{T}^d$ with $d \le 3$ and the initial data $u_0 \in H^k(\mathbb{T}^d)$ for $k \ge 2$. Then,*

$$\sup_{t\ge 0} ||u(t)||_{H^k(\mathbb{T}^d)} \lesssim_k 1 \tag{4.22}$$

where we omits the dependence on ν and u_0.

Proof. By the Duhamel formula, we write

$$u(t) = e^{\nu t\Delta}u_0 + \int_0^t e^{\nu(t-s)\Delta}(u-u^3)\ ds\ . \tag{4.23}$$

We would prove this argument inductively. By previous lemma, we have $||u||_2 \lesssim 1$ as $||u||_\infty \lesssim 1$ and we would show $||u||_{H^1} \lesssim 1$ for any $t \geq 1$. Then by taking spatial derivative and L^2 norm in the formula above, we derive

$$||Du||_2 \leq ||De^{\nu t\Delta}u_0||_2 + \int_0^t ||De^{\nu(t-s)\Delta}(u-u^3)||_2\ ds \tag{4.24}$$

where Du denotes any differential operator $D^\alpha u$ for any $|\alpha| = 1$, for example D^2 denotes $\partial^2_{x_i x_j} u$ for $1 \leq i\ , j \leq d$.

First, we consider the nonlinear part.

$$||De^{\nu(t-s)\Delta}(u-u^3)||_2 \lesssim ||De^{\nu(t-s)\Delta}(u-u^3)||_\infty \lesssim |K_1 * (u-u^3)|\ , \tag{4.25}$$

where K_1 is the kernel corresponding to $De^{\nu(t-s)\Delta}$.

$$\begin{aligned} |K_1 * (u-u^3)| &\leq ||K_1||_2 \cdot ||u-u^3||_2 \\ &\lesssim ||K_1||_2 \cdot ||u||_2 \end{aligned} \tag{4.26}$$

by the boundedness of $||u||_\infty$. Note that

$$\begin{aligned} ||K_1||_2 &\lesssim \left(\sum_{k\in\mathbb{Z}^d} |k|^2 e^{-2\nu(t-s)|k|^2}\right)^{\frac{1}{2}} \\ &= \left(\sum_{|k|\geq 1} |k|^2 e^{-2\nu(t-s)|k|^2}\right)^{\frac{1}{2}} \\ &\lesssim \left(\int_1^\infty e^{-2\nu(t-s)r^2} r^{d+1}\, dr\right)^{\frac{1}{2}} . \end{aligned} \tag{4.27}$$

The estimate for even dimensional case and odd dimensional case is a bit different. Now we would assume $t \geq 1$, as the other case $t < 1$ is much easier.

1. **Case 1**, $d = 1$. $\int_1^\infty e^{-2\nu(t-s)r^2} r^2\, dr \lesssim \frac{e^{-2\nu(t-s)}}{t-s} + \frac{\text{erfc}(\sqrt{2\nu(t-s)})}{(t-s)^{3/2}}$, where $\text{erfc}(x) := \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-t^2}\, dt$, the complementary error function. Letting $\gamma = t - s$,

   $$\int_0^t ||De^{\nu(t-s)\Delta} u||_2\, ds \lesssim \left(\int_0^t \frac{e^{-\nu\gamma}}{\gamma^{1/2}} + \frac{(\text{erfc}(\sqrt{\nu\gamma}))^{1/2}}{\gamma^{3/4}}\, d\gamma\right) \cdot ||u||_2 . \tag{4.28}$$

   For γ close to 0, $\frac{(\text{erfc}(\sqrt{\nu\gamma}))^{1/2}}{\gamma^{3/4}}$ will dominate the estimate and for γ away from 0, $\frac{e^{-\nu\gamma}}{\gamma^{1/2}}$ shall dominate the estimate. Then we split the integral as following (recall $t \geq 1$):

   $$\begin{aligned} \int_0^t \frac{e^{-\nu\gamma}}{\gamma^{1/2}} + \frac{(\text{erfc}(\sqrt{\nu\gamma}))^{1/2}}{\gamma^{3/4}}\, d\gamma &\lesssim \int_0^1 \frac{1}{\gamma^{3/4}}\, d\gamma + \int_1^t \frac{e^{-\nu\gamma}}{\gamma^{1/2}}\, d\gamma \\ &\lesssim 1 + \int_0^\infty \frac{e^{-\nu\gamma}}{\gamma^{1/2}}\, d\gamma \\ &\lesssim 1 . \end{aligned} \tag{4.29}$$

2. **Case 2**, $d = 2$. $\int_1^\infty e^{-2\nu(t-s)r^2} r^3\, dr \lesssim \frac{e^{-2\nu(t-s)}}{(t-s)^2} + \frac{e^{-2\nu(t-s)}}{t-s}$. Similar to case 1,

we would split the integral as well. Letting $\gamma = t - s$, we have

$$\begin{aligned}\int_1^t \frac{e^{-\nu\gamma}}{\gamma} + \frac{e^{-\nu\gamma}}{\gamma^{1/2}}\, d\gamma &\lesssim \int_1^t \frac{e^{-\nu\gamma}}{\gamma^{1/2}}\, d\gamma \\ &\lesssim \int_0^\infty \frac{e^{-\nu\gamma}}{\gamma^{1/2}}\, d\gamma \\ &\lesssim 1\,.\end{aligned} \tag{4.30}$$

However, it does not work for $\gamma \le 1$. Now we use another estimate for $||K_1 * (u - u^3)||_{L^2(\mathbb{T}^d)}$. We compute from Fourier side:

$$\begin{aligned}||K_1 * (u-u^3)||^2_{L^2(\mathbb{T}^d)} &= \sum_{|k|\ge 1} |k|^2 e^{-2\nu(t-s)|k|^2} |\widehat{u-u^3}(k)|^2 \\ &\le \max_{|k|\ge 1}\left\{|k|^2 e^{-2\nu(t-s)|k|^2}\right\} \cdot \sum_{|k|\ge 1} |\widehat{u-u^3}(k)|^2 \\ &\lesssim \max_{|k|\ge 1}\left\{|k|^2 e^{-2\nu(t-s)|k|^2}\right\} \cdot ||u||^2_{L^2(\mathbb{T}^d)}\,.\end{aligned} \tag{4.31}$$

Define $g(x) = x^2 e^{-2\nu\gamma x^2}$, where $x \ge 0$. Then,

$$g'(x) = 2x e^{-2\nu\gamma x^2}\left(1 - 2\nu\gamma x^2\right)\,, \tag{4.32}$$

this shows the maximum achieves at $x = \frac{1}{\sqrt{2\nu\gamma}}$ and hence

$$g(x) \le g(\frac{1}{\sqrt{2\nu\gamma}}) \lesssim \frac{1}{\gamma} \tag{4.33}$$

and hence

$$||De^{\nu(t-s)\Delta}(u-u^3)||_{L^2(\mathbb{T}^d)} \lesssim \frac{1}{\sqrt{t-s}}||u||_{L^2(\mathbb{T}^d)}\,, \tag{4.34}$$

note that this proof works for any dimension.

As a result,

$$\int_0^1 ||De^{\nu\gamma\Delta}u||_2 \, d\gamma \lesssim \int_0^1 \frac{1}{\sqrt{\gamma}} \, d\gamma \cdot ||u||_2 \lesssim 1 \, . \tag{4.35}$$

This shows $\int_0^t ||De^{\nu(t-s)\Delta}u||_2 \, ds \lesssim 1$.

3. **Case 3**, $d = 3$. As proved in previous case, we would only need to check the case $\gamma \geq 1$. $\int_1^\infty e^{-2\nu\gamma r^2} r^4 \, dr \lesssim \frac{e^{-2\nu\gamma}}{\gamma}$ for $\gamma \geq 1$. Hence,

$$\begin{aligned} \int_1^t \frac{e^{-\nu\gamma}}{\gamma^{1/2}} \, d\gamma &\lesssim \int_0^\infty \frac{e^{-\nu\gamma}}{\gamma^{1/2}} \, d\gamma \\ &\lesssim 1 \, . \end{aligned} \tag{4.36}$$

For $t \leq 1$ case, it is easier because we do not need to split the integral and all integrals from 0 to t could be bounded by the integral from 0 to 1.

Now for the linear part, by Duhamel's Principle, $e^{\nu t\Delta}u_0$ denotes the solution to the system:

$$\begin{cases} \partial_t u = \nu\Delta u \\ u(x,0) = u_0 \, . \end{cases} \tag{4.37}$$

As is well known, every spatial derivative of the solution $e^{\nu t\Delta}u_0$ solves same PDE, hence by the energy decay property, we have $||e^{\nu t\Delta}u_0||_{H^m} \lesssim ||u_0||_{H^m}$ for any $1 \leq m \leq k$. Combine the nonlinear part and linear part, we derive $||u||_{H^1} \lesssim 1$ independent of $t \geq 0$ and hence $\sup_{t\geq 0} ||u||_{H^1} \lesssim 1$.

Now if we already obtain $\sup_{t\geq 0} ||u||_{H^{m-1}} \lesssim 1$, we just need to consider

$$\begin{aligned}
||D(D^{m-1}u)||_2 &\leq ||De^{\nu t\Delta}D^{m-1}u_0||_2 + \int_0^t ||De^{\nu(t-s)\Delta}D^{m-1}u||_2 \, ds \\
&\lesssim ||u_0||_{H^m} + \int_0^1 ||De^{\nu\gamma\Delta}D^{m-1}u||_2 \, d\gamma + \int_1^t ||De^{\nu\gamma\Delta}D^{m-1}u||_2 \\
&\lesssim 1 + \int_0^1 \frac{1}{\sqrt{\gamma}} \, d\gamma \cdot ||D^{m-1}u||_2 + \int_0^\infty \frac{e^{-\nu\gamma}}{\sqrt{\gamma}} \, d\gamma \cdot ||D^{m-1}u||_2 \\
&\lesssim 1 \,,
\end{aligned} \tag{4.38}$$

by repeating the process above. In the end we would achieve

$$\sup_{t\geq 0} ||u||_{H^k(\mathbb{T}^d)} \lesssim_k 1 \,. \tag{4.39}$$

□

Lemma 4.2.4. *(Discrete version H^k boundedness) Suppose $u_0 \in H^k(\mathbb{T}^d)$ with $d \leq 3$ and $k \geq 2$. Then, suppose u^n is the numerical solution that satisfies*

$$\begin{cases} \dfrac{u^{n+1}-u^n}{\tau} = \nu\Delta u^{n+1} - A(u^{n+1}-u^n) - \Pi_N f(u^n) \\ u^0 = \Pi_N u_0 \,, \end{cases} \tag{4.40}$$

then

$$\sup_{n\geq 0} ||u^n||_{H^k(\mathbb{T}^d)} \lesssim_{A,k} 1 \,. \tag{4.41}$$

Remark 5. *The bound on u^n is independent of time step τ and truncation number N.*

Remark 6. *The proof is involved with energy decay property of the numerical scheme, so we would assume this property for now, as the proof for energy* *decay in 3D case would be given in chapter 6.*

Proof. To simplify the notation, we would use "$\lesssim$" instead of "$\lesssim_{\nu,u_0,A,k}$" only in this lemma. We would like to use a similar method provided in [10].

Write

$$\begin{aligned} u^{n+1} &= \underbrace{\frac{1+A\tau}{1+A\tau-\nu\tau\Delta}}_{:=L_1} u^n + \underbrace{\frac{-\tau\Pi_N}{1+A\tau-\nu\tau\Delta}}_{:=L_2} f(u^n) \\ &= L_1\left(L_1 u^{n-1} + L_2 f(u^{n-1})\right) + L_2 f(u^n) \\ &= L_1^{m_0+1} u^{n-m_0} + \sum_{l=0}^{m_0} L_1^l L_2 f(u^{n-1}) , \end{aligned} \tag{4.42}$$

where m_0 would be chosen later.

Similar to continuous version, we prove inductively. First, we show

$$\sup_{n\geq 0} ||u^n||_{H^2(\mathbb{T}^d)} \lesssim 1 . \tag{4.43}$$

Recall $\sup_{n\geq 0}||u^n||_2 \lesssim 1$ and $\sup_{n\geq 0}||f(u^n)||_2 \lesssim 1$ by energy decay property, then we just need to consider $\dot{H}^2$ semi norm.

We discuss 3 cases:

1. **Case 1**: $\tau \geq \frac{1}{10}$. Then for each $0 \neq k \in \mathbb{Z}^d$,

$$\begin{aligned} \left|\widehat{L_1}(k)\right| &= \frac{1+A\tau}{1+A\tau+\nu\tau|k|^2} \\ &\leq \frac{1}{A\tau+\nu\tau|k|^2} + \frac{A}{A+\nu|k|^2} \\ &\lesssim \frac{1}{1+|k|^2} ; \end{aligned} \tag{4.44}$$

$$\left|\widehat{L_2}(k)\right| \leq \frac{\tau}{A\tau+\nu\tau|k|^2} \lesssim \frac{1}{1+|k|^2} . \tag{4.45}$$

As a result,

$$\begin{aligned}||u^{n+1}||_{\dot{H}^2} &\le ||L_1 u^n||_{\dot{H}^2} + ||L_2 f(u^n)||_{\dot{H}^2} \\ &\lesssim ||u^n||_2 + ||f(u^n)||_2 \\ &\lesssim 1\,.\end{aligned} \tag{4.46}$$

2. **Case 2**: $\tau < \frac{1}{10}$ and $A\tau \ge \frac{1}{10}$. Then for $0 \ne k \in \mathbb{Z}^d$:

$$\begin{aligned}\left|\widehat{L_1}(k)\right| &= \frac{1 + A\tau}{1 + A\tau + \nu\tau|k|^2} \\ &\le \frac{11A\tau}{A\tau + \nu\tau|k|^2} \\ &\lesssim \frac{1}{1+|k|^2}\,,\end{aligned} \tag{4.47}$$

and

$$\left|\widehat{L_2}(k)\right| = \frac{\tau}{1 + A\tau + \nu\tau|k|^2} \lesssim \frac{1}{1+|k|^2}\,. \tag{4.48}$$

Then similar to Case 1,

$$\begin{aligned}||u^{n+1}||_{\dot{H}^2} &\le ||L_1 u^n||_{\dot{H}^2} + ||L_2 f(u^n)||_{\dot{H}^2} \\ &\lesssim ||u^n||_2 + ||f(u^n)||_2 \\ &\lesssim 1\,.\end{aligned} \tag{4.49}$$

3. **Case 3**: $\tau < \frac{1}{10}$ but $A\tau < \frac{1}{10}$. Take m_0 to be one integer such that $\frac{1}{2} \le$

$m_0\tau < 1$ and thus $m_0 \geq 5$.

$$\begin{aligned}\left|\widehat{L_1^{m_0+1}}(k)\right| &\leq \left(\frac{1+A\tau}{1+A\tau+\nu\tau|k|^2}\right)^{m_0+1} \\ &\leq \left(\frac{1+A\tau}{1+A\tau+\nu\tau|k|^2}\right)^{m_0} \\ &= \left(1+\frac{\nu\tau|k|^2}{1+A\tau}\right)^{-m_0} .\end{aligned} \tag{4.50}$$

Recall $A\tau < \frac{1}{10} < 1$, then

$$\left(1+\frac{\nu\tau|k|^2}{1+A\tau}\right)^{-m_0} \leq \left(1+\frac{\nu\tau|k|^2}{2}\right)^{-m_0} , \tag{4.51}$$

define $t_0 := m_0\tau$ and we derive

$$\left|\widehat{L_1^{m_0+1}}(k)\right| \leq \left(1+\frac{1}{2}\nu|k|^2\frac{t_0}{m_0}\right)^{-m_0} . \tag{4.52}$$

For any $a > 0$, we consider the function $h(x) = -x\log\left(1+\frac{a}{x}\right)$, $x > 0$. Then

$$\begin{aligned}h'(x) &= -\log\left(1+\frac{a}{x}\right)+\frac{a}{a+x} \\ h''(x) &= \frac{a}{x+a}\left(\frac{1}{x}-\frac{1}{x+a}\right) > 0 .\end{aligned} \tag{4.53}$$

By direct computation, $h(x)$ decreases on $(0,\infty)$. Therefore, recalling $m_0 \geq 5$,

$$\left|\widehat{L_1^{m_0+1}}(k)\right| \leq \left(1+\frac{1}{2}\nu|k|^2\frac{t_0}{m_0}\right)^{-m_0} \leq \left(1+\frac{1}{2}\nu|k|^2\cdot\frac{t_0}{5}\right)^{-5} . \tag{4.54}$$

Now,

$$\begin{aligned}\left|\widehat{L_2}(k)\right|\cdot\sum_{l=0}^{m_0}\left|\widehat{L_1}(k)\right|^l &\le \left|\widehat{L_2}(k)\right|\cdot\frac{1}{1-\left|\widehat{L_1}(k)\right|}\\ &=\frac{\tau}{1+A\tau+\nu\tau|k|^2}\cdot\frac{1}{1-\frac{1+A\tau}{1+A\tau+\nu\tau|k|^2}}\\ &=\frac{1}{\nu|k|^2}\\ &\lesssim\frac{1}{|k|^2}\ .\end{aligned}\tag{4.55}$$

Therefore for $n \ge m_0$,

$$\|u^{n+1}\|_{\dot{H}^2} \lesssim \|u^{n-m_0}\|_2 + \sup_{0\le l\le m_0}\|f(u^{n-l})\|_2 \lesssim 1\ .\tag{4.56}$$

For $1 \le n \le m_0+1$, then we apply

$$u^n = L_1^n u^0 + \sum_{l=0}^{n-1} L_1^l L_2 f(u^{n-1-l})\ .\tag{4.57}$$

Hence

$$\|u^n\|_{\dot{H}^2} \lesssim \|u^0\|_{\dot{H}^2} + \sup_{0\le l\le n-1}\|f(u^{n-l-1})\|_2 \lesssim 1\ .\tag{4.58}$$

This concludes

$$\sup_{n\ge 0}\|u^n\|_{H^2(\mathbb{T}^d)} \lesssim 1\ .\tag{4.59}$$

Inductively,

$$\begin{cases} \|u^{n+1}\|_{\dot{H}^m} \lesssim \|u^n\|_{\dot{H}^{m-2}} + \|f(u^n)\|_{\dot{H}^{m-2}} \ , \ \tau \geq \frac{1}{10} \\ \|u^{n+1}\|_{\dot{H}^m} \lesssim \|u^n\|_{\dot{H}^{m-2}} + \|f(u^n)\|_{\dot{H}^{m-2}} \ , \ \tau < \frac{1}{10} \ , \ A\tau \geq \frac{1}{10} \\ \|u^{n+1}\|_{\dot{H}^m} \lesssim \|u^{n-m_0}\|_{\dot{H}^{m-2}} + \sup\limits_{0\leq l\leq m_0} \|f(u^{n-l})\|_{\dot{H}^{m-2}} \ , \ \tau < \frac{1}{10} \ , \ A\tau < \frac{1}{10} \ , \ n \geq m_0 \\ \|u^n\|_{\dot{H}^m} \lesssim \|u^0\|_{\dot{H}^m} + \sup\limits_{0\leq l\leq n-1} \|f(u^{n-l-1})\|_{\dot{H}^{m-2}} \ , \ \tau < \frac{1}{10} \ , \ A\tau < \frac{1}{10} \ , \ n \leq m_0 + 1 \end{cases} \tag{4.60}$$

thus prove

$$\sup_{n\geq 0} \|u^n\|_{H^k(\mathbb{T}^d)} \lesssim 1 \ . \tag{4.61}$$

□

Remark 7. *The proof for exact solution and numerical solution is similar in the sense that we develop bootstrap process and split the time interval.*

4.2.2 Proof of L^2 Error Estimate of 2D Allen-Cahn Equation

Proof. By the previous high Sobolev bound lemma, $\sup_{n\geq 0}\|u^n\|_\infty \lesssim 1$ using Morrey's inequality. Thus the assumptions of proposition 2 (auxiliary L^2 error estimate proposition) are satisfied.

Recall that

$$G_n = \frac{\nu}{\tau}\int_{t_n}^{t_{n+1}} \partial_t \Delta u \cdot (t_n - t)\ dt - \frac{1}{\tau}\int_{t_n}^{t_{n+1}} \partial_t (f(u))(t_{n+1} - t)\ dt + A\int_{t_n}^{t_{n+1}} \partial_t u\ dt \ . \tag{4.62}$$

Then

$$\begin{aligned} ||G_n||_2 &\lesssim \int_{t_n}^{t_{n+1}} ||\partial_t \Delta u||_2 \, dt + \int_{t_n}^{t_{n+1}} ||\partial_t (f(u))||_2 \, dt + A \int_{t_n}^{t_{n+1}} ||\partial_t u||_2 \, dt \\ &\lesssim \underbrace{\int_{t_n}^{t_{n+1}} ||\partial_t \Delta u||_2 \, dt}_{I_1} + \underbrace{\int_{t_n}^{t_{n+1}} ||\partial_t u||_2 \, dt \cdot \left(A + ||f'(u)||_{L_t^\infty L_x^\infty}\right)}_{I_2} \, . \end{aligned} \tag{4.63}$$

Note that $\partial_t u = \nu \Delta u - u + u^3$ and hence by high Sobolev bound lemma,

$$||\partial_t u||_2 \lesssim 1 \, , \quad ||f'(u)||_\infty \lesssim 1 \, . \tag{4.64}$$

Recall the energy decay property,

$$\begin{aligned} \frac{dE}{dt} &= \frac{d}{dt}\left(\int \frac{\nu |\nabla u|^2}{2} + F(u) \, dx\right) \\ &= \int \nu \nabla u \cdot \nabla \partial_t u + f(u) \cdot \partial_t u \, dx \\ &= \int (-\nu \Delta u + f(u)) \partial_t u \, dx \\ &= -||\partial_t u||_2^2 \, . \end{aligned} \tag{4.65}$$

This shows

$$\int_0^\infty ||\partial_t u||_2^2 \, dt \lesssim 1 \, . \tag{4.66}$$

Note that by Gagliardo–Nirenberg interpolation inequality,

$$||\partial_t \Delta u||_2 \lesssim ||\langle \nabla \rangle^3 \partial_t u||_2^{\frac{2}{3}} \cdot ||\partial_t u||_2^{\frac{1}{3}} \lesssim ||\partial_t u||_2^{\frac{1}{3}} \, . \tag{4.67}$$

Here the notaion $\langle \nabla \rangle^s = (1-\Delta)^{\frac{s}{2}}$, corresponds to the Fourier side $(1+|k|^2)^{s/2}$.

This implies

$$\begin{aligned}
&\int_0^\infty ||\partial_t \Delta u||_2^6 \, dt \lesssim 1 \, , \\
\Longrightarrow &\int_0^T ||\partial_t \Delta u||_2^2 \, dt \lesssim \left(\int_0^T ||\partial_t \Delta u||_2^6 \, dt \right)^{\frac{1}{3}} \cdot \left(\int_0^T 1 \, dt \right)^{\frac{2}{3}} \lesssim 1 + T^{\frac{2}{3}} \, .
\end{aligned} \tag{4.68}$$

Moreover,

$$I_1 = \int_{t_n}^{t_{n+1}} ||\partial_t \Delta u||_2 \, dt \lesssim \left(\int_{t_n}^{t_{n+1}} ||\partial_t \Delta u||_2^2 \, dt \right)^{\frac{1}{2}} \cdot \sqrt{\tau} \, . \tag{4.69}$$

Similarly,

$$I_2 \lesssim (1+A) \cdot \int_{t_n}^{t_{n+1}} ||\partial_t u||_2 \, dt \lesssim (1+A) \cdot \left(\int_{t_n}^{t_{n+1}} ||\partial_t u||_2^2 \, dt \right)^{\frac{1}{2}} \cdot \sqrt{\tau} \, . \tag{4.70}$$

Hence for $t_m \geq 1$,

$$\begin{aligned}
\sum_{n=0}^{m-1} ||G_n||_2^2 &\lesssim \sum_{n=0}^{m-1} \left((I_1)^2 + (I_2)^2 \right) \\
&\lesssim \sum_{n=0}^{m-1} \left(\tau \int_{t_n}^{t_{n+1}} ||\partial_t \Delta u||_2^2 \, dt + (1+A)^2 \tau \int_{t_n}^{t_{n+1}} ||\partial_t u||_2^2 \, dt \right) \\
&\lesssim \tau \int_0^{t_m} ||\partial_t \Delta u||_2^2 \, dt + (1+A)^2 \tau \int_0^{t_m} ||\partial_t u||_2^2 \, dt \\
&\lesssim \tau (1 + t_m) + (1+A)^2 \tau \\
&\lesssim (1+A)^2 \tau \cdot (1 + t_m) \, .
\end{aligned} \tag{4.71}$$

On the other hand, by the high Sobolev bound lemma $\sup_{t \geq 0} ||u(t)||_{H^s} \lesssim_s 1$, we have $\sup_{n \geq 0} ||f(u(t_n))||_{H^s} \lesssim_s 1$.

$$
\begin{aligned}
||\Pi_{>N} f(u(t_n))||_2^2 &= \sum_{|k|>N} \left|\widehat{f(u(t_n))}(k)\right|^2 \\
&\leq \sum_{|k|>N} |k|^{2s} \left|\widehat{f(u(t_n))}(k)\right|^2 \cdot |k|^{-2s} \\
&\lesssim N^{-2s} \cdot \sum_{|k|>N} |k|^{2s} \left|\widehat{f(u(t_n))}(k)\right|^2 \\
&\lesssim N^{-2s} \cdot ||f(u(t_n))||_{H^s}^2 \\
&\lesssim N^{-2s} \ ,
\end{aligned}
\tag{4.72}
$$

thus

$$
\sum_{n=0}^{m-1} ||\Pi_{>N} f(u(t_n))||_2^2 \lesssim_s m \cdot N^{-2s} \lesssim \frac{t_m N^{-2s}}{\tau} \ . \tag{4.73}
$$

Therefore,

$$
\tau \sum_{n=0}^{m-1} \left(||G_n||_2^2 + ||\Pi_{>N} f(u(t_n))||_2^2\right) \lesssim_s (1+t_m)(\tau^2 + N^{-2s})(1+A)^2 \ . \tag{4.74}
$$

Also for the same reason

$$
||u^0 - u(0)||_2^2 = ||\Pi_N u_0 - u_0||_2^2 \lesssim N^{-2s} \ . \tag{4.75}
$$

Applying the auxiliary solutions proposition and note that $t_m = m\tau$,

$$
||u^m - u(t_m)||_2^2 \lesssim_s (1+A)^2 e^{Ct_m} \left(N^{-2s} + \tau \cdot N^{-2s} + (1+t_m)(\tau^2 + N^{-2s})\right) \ . \tag{4.76}
$$

Note that

$$
\begin{cases}
\tau \cdot N^{-2s} \lesssim \tau^2 + N^{-4s} \lesssim \tau^2 + N^{-2s} \\
1 + t_m \lesssim e^{C' t_m} \ ,
\end{cases}
\tag{4.77}
$$

this leads to

$$||u^m - u(t_m)||_2^2 \lesssim_s (1+A)^2 e^{Ct_m} \left(N^{-2s} + \tau^2\right) . \tag{4.78}$$

Thus

$$||u^m - u(t_m)||_2 \le (1+A) \cdot C_2 \cdot e^{C_1 t_m} \left(N^{-s} + \tau\right) , \tag{4.79}$$

where $C_1 > 0$ is a constant depending on ν , u_0; $C_2 > 0$ is a constant depending on s , ν and u_0.

This completes the proof of L^2 error estimate.

□

Chapter 5

Stability of a First Order Semi-implicit Scheme on 2D Fractional Cahn-Hilliard Equation

As mentioned in the introduction, the fractional Cahn-Hilliard equation are "interpolation" between Allen-Cahn equation and original Cahn-Hilliard equation.

$$\begin{cases} \partial_t u = \nu\Delta\left((-\Delta)^\alpha u + (-\Delta)^{\alpha-1} f(u)\right) \ , \ 0 < \alpha \le 1 \\ u(x,0) = u_0 \end{cases} .$$

As before, we consider the region as 2π-periodic torus $\mathbb{T}^2 = \mathbb{R}^2/2\pi\mathbb{Z}^2$. $f(u) = u^3 - u$ and hence the energy $E(u) = \int_{\mathbb{T}^2} \left(\frac{\nu}{2}|\nabla u|^2 + F(u)\right) \, dx$, with $F(u) = \frac{1}{4}(u^2 - 1)^2$. Similarly, the semi-implicit scheme is given by the following:

$$\begin{cases} \dfrac{u^{n+1} - u^n}{\tau} = -\nu(-\Delta)^{\alpha+1} u^{n+1} - (-\Delta)^\alpha A(u^{n+1} - u^n) - (-\Delta)^\alpha \Pi_N f(u^n) \\ u^0 = \Pi_N u_0 \end{cases} . \quad (5.1)$$

Theorem 5.0.1. *(unconditional energy stability for fractional CH). Consider (5.1) with $\nu > 0$ and assume $u_0 \in H^2(\mathbb{T}^2)$ and has zero-mean condition. Then there exists a constant β_0 depending only on the initial energy $E_0 = E(u_0)$ such that if*

$$A \geq \beta \cdot \left(||u_0||_{H^2}^2 + \nu^{-1} |\log \nu| + 1 \right) , \; \beta \geq \beta_0 \tag{5.2}$$

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

Remark 8. *Here we require zero-mean assumption on u_0 hence that implies u^n all have mean zero because zero-mean assumption would guarantee that negative fractional Laplacian is well defined. Here we use the notation $|\nabla|^{-\alpha} = (-\Delta)^{-\frac{\alpha}{2}}$ to denote the fractional Laplacian.*

Proof. The proof is involved with similar computation given in previous chapter. We recall the scheme (5.1):

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

Now we multiply the equation by $(-\Delta)^{-\alpha}(u^{n+1} - u^n)$ and apply Fundamental Theorem of Calculus and integration by parts as in Chapter 3, we obtain

$$\begin{aligned} &\frac{1}{\tau} \left|\left| |\nabla|^{-\alpha} (u^{n+1} - u^n) \right|\right|_{L^2}^2 + \frac{\nu}{2} \left(\left|\left| \nabla (u^{n+1} - u^n) \right|\right|_{L^2}^2 + \left|\left| \nabla u^{n+1} \right|\right|_{L^2}^2 - \left|\left| \nabla u^n \right|\right|_{L^2}^2 \right) \\ &+ A \left|\left| u^{n+1} - u^n \right|\right|_{L^2}^2 = -\left(f(u^n), u^{n+1} - u^n \right) \; . \end{aligned} \tag{5.3}$$

This thus implies:

$$\frac{1}{\tau}\left|\left||\nabla|^{-\alpha}(u^{n+1}-u^n)\right|\right|_{L^2}^2+\frac{\nu}{2}\left|\left|\nabla(u^{n+1}-u^n)\right|\right|_{L^2}^2+\left(A+\frac{1}{2}\right)\left|\left|u^{n+1}-u^n\right|\right|_{L^2}^2+E^{n+1}-E^n$$
$$\leq \left|\left|u^{n+1}-u^n\right|\right|_{L^2}^2\left(||u^n||_\infty^2+\frac{1}{2}||u^{n+1}||_\infty^2\right). \tag{5.4}$$

It is clear that the first two norms $\frac{1}{\tau}\left|\left||\nabla|^{-\alpha}(u^{n+1}-u^n)\right|\right|_{L^2}^2$ and $\frac{\nu}{2}\left|\left|\nabla(u^{n+1}-u^n)\right|\right|_{L^2}^2$ would be problematic as we would expect more help from $||u^{n+1}-u^n||_{L^2}^2$.

Lemma 5.0.2.

$$\frac{1}{\tau}\left|\left||\nabla|^{-\alpha}(u^{n+1}-u^n)\right|\right|_{L^2(\mathbb{T}^2)}^2+\frac{\nu}{2}\left|\left|\nabla(u^{n+1}-u^n)\right|\right|_{L^2(\mathbb{T}^2)}^2\geq C_{\alpha\nu\tau}||u^{n+1}-u^n||_{L^2(\mathbb{T}^2)}^2 \tag{5.5}$$

with $C_{\alpha\nu\tau}$ is determined by α, ν and τ.

Proof. It is natural to examine the above norms $\frac{1}{\tau}\left|\left||\nabla|^{-\alpha}(u^{n+1}-u^n)\right|\right|_{L^2(\mathbb{T}^2)}^2$ and
$\frac{\nu}{2}\left|\left|\nabla(u^{n+1}-u^n)\right|\right|_{L^2(\mathbb{T}^2)}^2$ on the Fourier side. Then we obtain that

$$\begin{aligned}\frac{1}{\tau}\sum_{k\neq 0}|k|^{-2\alpha}|\widehat{u}^{n+1}(k)-\widehat{u}^n(k)|^2+\frac{\nu}{2}\sum_{k\neq 0}|\widehat{u}^{n+1}(k)-\widehat{u}^n(k)|^2\\ =\sum_{k\neq 0}|\widehat{u}^{n+1}(k)-\widehat{u}^n(k)|^2\cdot\left(\frac{|k|^{-2\alpha}}{\tau}+\frac{\nu|k|^2}{2}\right).\end{aligned} \tag{5.6}$$

Note we expect $\sum_{k\neq 0}|\widehat{u}^{n+1}(k)-\widehat{u}^n(k)|^2$, it is clear we could apply standard Young's inequality for product : $ab\leq\frac{a^\gamma}{\gamma}+\frac{b^\beta}{\beta}$, with $\frac{1}{\gamma}+\frac{1}{\beta}=1$.
As expected, $ab=|k|^0$, hence we could take $a=|k|^p$, $b=|k|^q$, thus $p+q=0$.
This implies

$$\begin{cases}a^\gamma=|k|^{p\gamma}=|k|^{-2\alpha}\\ b^\beta=|k|^{q\beta}=|k|^2\end{cases}. \tag{5.7}$$

As a result,

$$\begin{cases} -2\alpha = p\gamma \\ 2 = q\beta \end{cases} \Longrightarrow \begin{cases} p = \dfrac{-2\alpha}{\alpha+1} \\ q = \dfrac{2\alpha}{\alpha+1} \\ \gamma = \alpha+1 \\ \beta = \dfrac{\alpha+1}{\alpha}\ . \end{cases} \tag{5.8}$$

So,

$$\begin{aligned} &\sum_{k\neq 0} |\widehat{u}^{n+1}(k)-\widehat{u}^{n}(k)|^2 \cdot \left(\frac{|k|^{-2\alpha}}{\tau}+\frac{\nu|k|^2}{2}\right) \\ =&\sum_{k\neq 0} |\widehat{u}^{n+1}(k)-\widehat{u}^{n}(k)|^2 \cdot \left[\frac{\alpha+1}{\tau}\cdot\left(\frac{|k|^{-2\alpha}}{\alpha+1}\right)+\frac{\nu(\alpha+1)}{2\alpha}\cdot\left(\frac{|k|^2}{\frac{\alpha+1}{\alpha}}\right)\right] \\ \geq&\sum_{k\neq 0} |\widehat{u}^{n+1}(k)-\widehat{u}^{n}(k)|^2 \cdot \left(\frac{\alpha+1}{\tau}\right)^{\frac{1}{\alpha+1}}\cdot\left(\frac{\nu(\alpha+1)}{2\alpha}\right)^{\frac{\alpha+1}{\alpha}}\ . \end{aligned} \tag{5.9}$$

So it is plain to take $C_{\alpha\tau\nu} = \left(\frac{\alpha+1}{\tau}\right)^{\frac{1}{\alpha+1}}\cdot\left(\frac{\nu(\alpha+1)}{2\alpha}\right)^{\frac{\alpha+1}{\alpha}}$. □

Remark 9. *In the proof above, $C_{\alpha\tau\nu}\to\infty$ as $\alpha\to 0$. Hence it would not work for $\alpha=0$ case, but we could refer to chapter 3.*

Back to the proof of Theorem 5.0.1, (5.4) leads to

$$(A+\frac{1}{2}+C_{\alpha\tau\nu})\left|\left|u^{n+1}-u^{n}\right|\right|_{L^2}^2+E^{n+1}-E^{n} \leq \left|\left|u^{n+1}-u^{n}\right|\right|_{L^2}^2\left(||u^n||_\infty^2+\frac{1}{2}||u^{n+1}||_\infty^2\right)\ . \tag{5.10}$$

To prove $E^{n+1}\leq E^n$, it suffices to show $A+\frac{1}{2}+C_{\alpha\tau\nu}\geq\frac{3}{2}\max\left\{||u^{n+1}||_\infty^2\ ,\ ||u^n||_\infty^2\right\}$. As in chapter 3, we rewrite the scheme (5.1) as

$$u^{n+1} = \frac{1+A\tau(-\Delta)^\alpha}{1+\tau\nu(-\Delta)^{\alpha+1}+A\tau(-\Delta)^\alpha}u^n - \frac{\tau(-\Delta)^\alpha}{1+\tau\nu(-\Delta)^{\alpha+1}+A\tau(-\Delta)^\alpha}\Pi_N[f(u^n)]\ . \tag{5.11}$$

Similarly, we could still apply the main lemma under the assumption u_0 satisfies zero-mean condition. Recall that

$$||u^{n+1}||_\infty \lesssim ||u^{n+1}||_{\dot{H}^1}\sqrt{\log(||u^{n+1}||_{\dot{H}^{\frac{3}{2}}}+3)}\,. \tag{5.12}$$

We would like to estimate $||u^{n+1}||_{\dot{H}^1}$ and $||u^{n+1}||_{\dot{H}^{\frac{3}{2}}}$. As we did in chapter 3,

$$\begin{cases} \dfrac{1+A\tau|k|^{2\alpha}}{1+A\tau|k|^{2\alpha}+\nu\tau|k|^{2+2\alpha}}\cdot|k| \lesssim |k| \\ \dfrac{\tau|k|^{2\alpha}}{1+A\tau|k|^{2\alpha}+\nu\tau|k|^{2+2\alpha}}\cdot|k| \lesssim \dfrac{\tau}{\tau A}|k| = \dfrac{1}{A}|k| \end{cases}. \tag{5.13}$$

Hence we derive

$$||u^{n+1}||_{\dot{H}^1(\mathbb{T}^2)} \lesssim \left(1+\frac{1}{A}+\frac{3||u||_\infty^2}{A}\right)||u^n||_{\dot{H}^1(\mathbb{T}^2)}\,, \tag{5.14}$$

which is the same argument as in chapter 3.

Similarly, we could derive

$$||u^{n+1}||_{\dot{H}^{\frac{3}{2}}(\mathbb{T}^2)} \lesssim \left(\frac{1+A\tau}{\nu\tau}+\frac{1}{\nu}\right)(E^n+1)\,, \tag{5.15}$$

So prove by induction again,

Step 1 : The induction $n \implies n+1$ 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 would show $E^{n+1} \le E^n$. This implies $||u^n||_{\dot{H}^1}^2 = ||\nabla u^n||_{L^2}^2 \le \frac{2E^n}{\nu} \le \frac{2E^0}{\nu}$. By applying the main lemma carefully and $E^0 \lesssim E_0+1$,

$$||u^n||_\infty^2 \lesssim_{E_0} \nu^{-1}(1+\log(A)+|\log(\nu)|)+\nu^{-1}|\log(\tau)|+1 \quad . \tag{5.16}$$

Define $m_0 := \nu^{-1}(1+\log(A)+|\log(\nu)|)$ again, then the inequality above is

$$||u^n||_\infty^2 \lesssim_{E_0} m_0 + \nu^{-1}|\log(\tau)| + 1\ . \tag{5.17}$$

Similarly,

$$||u^{n+1}||_\infty^2 \lesssim_{E_0} 1 + \frac{m_0^3}{A^2} + m_0 + \nu^{-3}|\log(\tau)|^3. \tag{5.18}$$

So we need the following condition holds:

$$\begin{cases} A + \frac{1}{2} + (\frac{\alpha+1}{\tau})^{\frac{1}{\alpha+1}} \cdot (\frac{\nu(\alpha+1)}{2\alpha})^{\frac{\alpha+1}{\alpha}} \geq C(E_0)\left(m_0 + 1 + \frac{m_0^3}{A^2} + \nu^{-3}|\log(\tau)|^3\right) \\ m_0 = \nu^{-1}(1+\log(A)+|\log(\nu)|)\ . \end{cases} \tag{5.19}$$

Now we discuss 2 cases again:

Case 1: $(\frac{\alpha+1}{\tau})^{\frac{1}{\alpha+1}} \cdot (\frac{\nu(\alpha+1)}{2\alpha})^{\frac{\alpha+1}{\alpha}} \geq C(E_0)\nu^{-3}|\log(\tau)|^3$. In this case, it suffices to choose A such that

$$A \gg_{E_0} m_0 = \nu^{-1}(1+\log(A)+|\log(\nu)|)\ .$$

In fact, for $\nu \gtrsim 1$, we could take $A \gg_{E_0} 1$; if $0 < \nu \ll 1$, we would choose $A = C_{E_0} \cdot \nu^{-1}|\log \nu|$, where C_{E_0} is a large constant depending only on E_0. Therefore in both cases it suffices to choose

$$A = C_{E_0} \cdot \max\{\nu^{-1}|\log(\nu)|\ ,\ 1\}. \tag{5.20}$$

Case 2:$(\frac{\alpha+1}{\tau})^{\frac{1}{\alpha+1}} \cdot (\frac{\nu(\alpha+1)}{2\alpha})^{\frac{\alpha+1}{\alpha}} \leq C(E_0)\nu^{-3}|\log(\tau)|^3$. This still implies $(\frac{1}{\tau})^{\frac{1}{\alpha+1}} \lesssim$

$(\frac{1}{\nu})^{-4-\frac{1}{\alpha}}$, hence $|\log(\tau)| \lesssim_{E_0} 1+|\log(\nu)|$ for fixed $0<\alpha\le 1$. Now we go back to equations (4.17), we have

$$||u^n||_\infty^2 \lesssim_{E_0} m_0 \tag{5.21}$$

as $\nu^{-1}|\log(\tau)|$ would be absorbed by m_0, recall $m_0 = \nu^{-1}(1+\log(A)+|\log(\nu)|)$. Hence substitute this new bound to (4.18), we would derive

$$\begin{aligned} ||u^{n+1}||_\infty^2 &\lesssim \left(1+(\frac{1+||u^n||_\infty^2}{A})||u^n||_{\dot{H}^1}\sqrt{\log(3+||u^{n+1}||_{\dot{H}^{\frac{3}{2}}})}\right)^2 \\ &\lesssim_{E_0} \left(1+(1+\frac{m_0}{A})(\sqrt{\frac{1}{\nu}}\sqrt{\log(3+||u^{n+1}||_{\dot{H}^{\frac{3}{2}}})}\right)^2 \\ &\lesssim_{E_0} \left(1+(1+\frac{m_0}{A})\sqrt{m_0}\right)^2 \\ &\lesssim_{E_0} 1+\frac{m_0^3}{A^2}+m_0 \ . \end{aligned} \tag{5.22}$$

Thus it still suffices to take

$$A \ge C_{E_0} m_0 \ . \tag{5.23}$$

For the induction base $Step$ 2, the proof is exactly the same as in chapter 3 and this shows stability of the semi-implicit scheme in fractional Laplacian case. □

Chapter 6

Stability of a First Order Semi-implicit Scheme on 3D Allen-Cahn Equation

In this chapter, we would like to explore a bit more in three dimension case. What makes the difference is that the main lemma proved in chapter 2 should not hold. To clarify, the $\dot{H}^1$-norm should be replaced by $\dot{H}^{\frac{3}{2}}$-norm in the log-type inequality proved in chapter 2, as a result of scaling invariance. However, $\dot{H}^{\frac{3}{2}}$-norm would not help to prove 3D theorem as there is no a-priori energy bound for $\dot{H}^{\frac{3}{2}}$-norm. To solve this issue, we would 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 chapter as other Cahn-Hilliard type equations could be handled similarly. To begin with, we recall the numerical scheme (3.1) for Allen-Cahn equation.

$$\begin{cases} \dfrac{u^{n+1}-u^n}{\tau} = \nu\Delta u^{n+1} - A(u^{n+1}-u^n) - \Pi_N f(u^n) \\ u^0 = \Pi_N u_0 \end{cases} . \tag{6.1}$$

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

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

Theorem 6.0.1. *(3D energy stability for AC) Consider (6.1) 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*

$$A \geq \beta\cdot\left(||u_0||_{H^2}^2 + \nu^{-3} + 1\right)\,,\;\beta\geq\beta_0 \tag{6.2}$$

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

Remark 10. *Unlike in chapter 3, 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.*

Before proving Theorem 6.0.1, we would prove a new main lemma here.

6.1 the Main Lemma

For all $f \in H^2(\mathbb{T}^3)$, one has

$$||f||_\infty \lesssim ||f||_{\dot{H}^1}^{\frac{1}{2}}||f||_{\dot{H}^2}^{\frac{1}{2}} + |\widehat{f}(0)|\,. \tag{6.3}$$

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

So,

$$\begin{aligned}
||f||_\infty &\le \frac{1}{(2\pi)^3}\sum_{k\in\mathbb{Z}^3}|\hat{f}(k)| \\
&\le \frac{1}{(2\pi)^3}|\hat{f}(0)| + \frac{1}{(2\pi)^3}\left(\sum_{0<|k|\le N}|\hat{f}(k)| + \sum_{|k|>N}|\hat{f}(k)|\right) \\
&\lesssim |\hat{f}(0)| + \sum_{0<|k|\le N}(|\hat{f}(k)||k|\cdot|k|^{-1}) + \sum_{|k|>N}(|\hat{f}(k)||k|^2\cdot|k|^{-2}) \\
&\lesssim |\hat{f}(0)| + \left(\sum_{0<|k|\le N}|\hat{f}(k)|^2|k|^2\right)^{\frac{1}{2}}\cdot\left(\sum_{0<|k|\le N}|k|^{-2}\right)^{\frac{1}{2}} + \left(\sum_{|k|>N}|\hat{f}(k)|^2|k|^4\right)^{\frac{1}{2}}\cdot(\sum_{|k|>N}|k|^{-4})^{\frac{1}{2}} \\
&\lesssim |\hat{f}(0)| + \left(\sum_{|k|>N}|\hat{f}(k)|^2|k|^4\right)^{\frac{1}{2}}\cdot\left(\int_N^\infty \frac{\pi r^2}{r^4}\,dr\right)^{\frac{1}{2}} + \left(\sum_{0<|k|\le N}|\hat{f}(k)|^2|k|^2\right)^{\frac{1}{2}}\cdot\left(\int_1^N \frac{\pi r^2}{r^2}\,dr\right)^{\frac{1}{2}} \\
&\lesssim |\hat{f}(0)| + ||f||_{\dot{H}^2}\cdot N^{-\frac{1}{2}} + ||f||_{\dot{H}^1}\cdot N^{\frac{1}{2}}\ .
\end{aligned} \tag{6.4}$$

We optimize N and hence derive

$$||f||_\infty \lesssim |\hat{f}(0)| + ||f||_{\dot{H}^1}^{\frac{1}{2}}||f||_{\dot{H}^2}^{\frac{1}{2}}\ . \tag{6.5}$$

□

6.2 Proof of 3D Stability Theorem

By the same argument in chapter 3 with notation $E^n = E(u^n)$,

$$\begin{aligned}
&(\frac{1}{\tau} + A + \frac{1}{2})||u^{n+1} - u^n||_{L^2}^2 + \frac{\nu}{2}||\nabla(u^{n+1} - u^n)||_{L^2}^2 + E^{n+1} - E^n \\
&\le ||u^{n+1} - u^n||_{L^2}^2\left(||u^n||_\infty^2 + \frac{1}{2}||u^{n+1}||_\infty^2\right)\ .
\end{aligned} \tag{6.6}$$

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

$$\frac{1}{\tau} + A + \frac{1}{2} \ge \frac{3}{2} \max\left\{ ||u^n||_\infty^2 \ , \ ||u^{n+1}||_\infty^2 \right\} . \tag{6.7}$$

Now we rewrite the scheme (5.1) as the following:

$$u^{n+1} = \frac{1 + A\tau}{1 + A\tau - \nu\tau\Delta} u^n - \frac{\tau}{1 + A\tau - \nu\tau\Delta} \Pi_N[f(u^n)]. \tag{6.8}$$

Recall that

$$||u^{n+1}||_\infty \lesssim |\widehat{u}^{n+1}(0)| + ||u^{n+1}||_{\dot{H}^1}^{\frac{1}{2}} ||u^{n+1}||_{\dot{H}^2}^{\frac{1}{2}} . \tag{6.9}$$

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 in chapter 3,

$$|\widehat{u}^{n+1}(0)| \lesssim 1 + \sqrt{E^n} . \tag{6.10}$$

Note that

$$\begin{cases} \dfrac{(1 + A\tau)|k|}{1 + A\tau + \nu\tau|k|^2} \le |k| \\ \dfrac{\tau|k|}{1 + A\tau + \nu\tau|k|^2} \le \dfrac{\tau|k|}{2\tau\sqrt{A\nu}|k|} \lesssim \dfrac{1}{\sqrt{A\nu}} \end{cases} . \tag{6.11}$$

Hence

$$\begin{aligned} ||u^{n+1}||_{\dot{H}^1} &\lesssim ||u^n||_{\dot{H}^1} + \frac{1}{\sqrt{A\nu}} ||f(u^n)||_{L^2} \\ &\lesssim ||u^n||_{\dot{H}^1} + \frac{1}{\sqrt{A\nu}} (||(u^n)^3||_{L^2} + 1) . \end{aligned} \tag{6.12}$$

Similarly,

$$\begin{cases} \dfrac{(1 + A\tau)|k|^2}{1 + A\tau + \nu\tau|k|^2} \lesssim \left(\dfrac{1}{\tau\sqrt{A\nu}} + \sqrt{\dfrac{A}{\nu}} \right) |k| \\ \dfrac{\tau|k|^2}{1 + A\tau + \nu\tau|k|^2} \le \dfrac{1}{\nu} \end{cases} . \tag{6.13}$$

This implies

$$\begin{aligned}||u^{n+1}||_{\dot{H}^2} &\lesssim \left(\frac{1}{\tau\sqrt{A\nu}}+\sqrt{\frac{A}{\nu}}\right)||u^n||_{\dot{H}^1}+\frac{1}{\nu}||f(u^n)||_{L^2} \\ &\lesssim \left(\frac{1}{\tau\sqrt{A\nu}}+\sqrt{\frac{A}{\nu}}\right)||u^n||_{\dot{H}^1}+\frac{1}{\nu}\left(||(u^n)^3||_{L^2}+1\right)\ .\end{aligned} \tag{6.14}$$

Note that by standard Sobolev inequality,

$$||(u^n)^3||_{L^2}=||u^n||^3_{L^6}\lesssim ||u^n||^3_{H^1}\lesssim ||\nabla u^n||^3_{L^2}+||u^n||^3_{L^2}\lesssim ||u^n||^3_{\dot{H}^1}+1+(E^n)^{\frac{3}{2}}\ . \tag{6.15}$$

As a result,

$$\begin{cases}||u^{n+1}||_{\dot{H}^1}\lesssim ||u^n||_{\dot{H}^1}+\dfrac{1}{\sqrt{A\nu}}\left(||(u^n)||^3_{\dot{H}^1}+1+(E^n)^{\frac{3}{2}}\right) \\ ||u^{n+1}||_{\dot{H}^2}\lesssim \left(\dfrac{1}{\tau\sqrt{A\nu}}+\sqrt{\dfrac{A}{\nu}}\right)||u^n||_{\dot{H}^1}+\dfrac{1}{\nu}\left(||(u^n)||^3_{\dot{H}^1}+1+(E^n)^{\frac{3}{2}}\right)\end{cases}. \tag{6.16}$$

We would prove the 3D stability theorem inductively as in chapter 3.

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

$$\begin{cases}||u^{n+1}||_{\dot{H}^1}\lesssim_{E_0} \nu^{-\frac{1}{2}}+A^{-\frac{1}{2}}\nu^{-\frac{1}{2}}\left(\nu^{-\frac{3}{2}}+1\right)\lesssim_{E_0} \nu^{-\frac{1}{2}}+A^{-\frac{1}{2}}\nu^{-2} \\ ||u^{n+1}||_{\dot{H}^2}\lesssim_{E_0} A^{\frac{1}{2}}\nu^{-1}+\nu^{-\frac{5}{2}}+\tau^{-1}A^{-\frac{1}{2}}\nu^{-1}\end{cases}. \tag{6.17}$$

Applying the new main lemma,

$$\begin{aligned}||u^{n+1}||_\infty^2 &\lesssim_{E_0} \left(\nu^{-\frac{1}{2}} + A^{-\frac{1}{2}}\nu^{-2}\right)\cdot\left(A^{\frac{1}{2}}\nu^{-1} + \nu^{-\frac{5}{2}} + \tau^{-1}A^{-\frac{1}{2}}\nu^{-1}\right) + 1 \\ &\lesssim_{E_0} A^{\frac{1}{2}}\nu^{-\frac{3}{2}} + \nu^{-3} + A^{-\frac{1}{2}}\nu^{-\frac{9}{2}} + \tau^{-1}A^{-\frac{1}{2}}\nu^{-\frac{3}{2}} + \tau^{-1}A^{-1}\nu^{-3} + 1\,.\end{aligned} \tag{6.18}$$

To satisfy the sufficient condition (6.7)

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

it suffices to take

$$A \geq C_{E_0}\nu^{-3}\,, \tag{6.19}$$

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

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

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

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

$$||\Pi_N u_0||_\infty^2 \lesssim ||\Pi_N u_0||_{H^2}^2 \lesssim ||u_0||_{H^2}^2\,. \tag{6.20}$$

On the other hand, by the main lemma it suffices to take

$$A + \frac{1}{\tau} \geq c_1||u_0||_{H^2}^2 + \alpha_{E_0}\left(A^{\frac{1}{2}}\nu^{-\frac{3}{2}} + \nu^{-3} + A^{-\frac{1}{2}}\nu^{-\frac{9}{2}} + \tau^{-1}A^{-\frac{1}{2}}\nu^{-\frac{3}{2}} + \tau^{-1}A^{-1}\nu^{-3}\right)\,, \tag{6.21}$$

where c_1 is an absolute constant and α_{E_0} is a constant only depending on E_0.

Hence it suffices to take

$$A \geq C_{E_0}\left(||u_0||_{H^2}^2 + \nu^{-3} + 1\right) , \tag{6.22}$$

for a large constant C_{E_0} only depending on E_0. This completes the proof. By using this new main lemma, the 3D fractional Cahn-Hilliard could be handled similarly.

6.3 L^2 Error Estimate of 3D Allen-Cahn Equation

Theorem 6.3.1. *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. Recall

$$\begin{cases} \dfrac{u^{n+1} - u^n}{\tau} = \nu\Delta u^{n+1} - \Pi_N f(u^n) - A(u^{n+1} - u^n) \\ \partial_t u = \nu\Delta u - f(u) \\ u^0 = \Pi_N u_0 \ , \ u(0) = u_0 \ . \end{cases} \tag{6.23}$$

As we proved in chapter 4, the auxiliary L^2 estimate lemma and all boundedness lemma work for 3D case. The only difference is the estimate for $||\partial_t \Delta u||_2$

using Gagliardo–Nirenberg interpolation inequality,

$$||\partial_t \Delta u||_2 \lesssim ||\langle \nabla \rangle^3 \partial_t u||_2^{\frac{2}{3}} \cdot ||\partial_t u||_2^{\frac{1}{3}} \lesssim ||\partial_t u||_2^{\frac{1}{3}} \,, \tag{6.24}$$

which works as well for the same power. This leads to the conclusion of Theorem 6.3.1 by exactly same argument in chapter 4.

□

Chapter 7

Second Order Semi-Implicit Schemes

In previous chapters we introduce first order semi-implicit schemes for Allen-Cahn equation and fractional Cahn-Hilliard equation in both two dimensional periodic domain and three dimensional periodic domain. For the completeness, we would like to study some second order schemes. As a representative case, we only consider 2D Allen-Cahn equation here. The analysis of other cases would be similar. We introduce two second order schemes and prove the unconditional stability for Scheme I and conditional stability for Scheme II.

7.1 Introduction of Scheme I:

As introduced in [9], the second order semi-implicit Fourier spectral scheme I is given by:

$$\frac{3u^{n+1}-4u^n+u^{n-1}}{2\tau} = \nu\Delta u^{n+1} - A\tau(u^{n+1}-u^n) - \Pi_N\left(2f(u^n)-f(u^{n-1})\right) \quad , \; n \geq 1 \; , \tag{7.1}$$

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.

To start the iteration, we need to derive u^1 according to the following first order scheme:

$$\begin{cases} \dfrac{u^1 - u^0}{\tau_1} = \nu \Delta u^1 - \Pi_N f(u^0) \ , \\ u^0 = \Pi_N u_0 \ , \end{cases} \tag{7.2}$$

where $\tau_1 = \min\{\tau^{\frac{4}{3}} \ , \ 1\}$. The choice of τ is because of the error analysis which will be proved 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 for the second order scheme, we require that $\tau_1^{\frac{3}{2}} \lesssim \tau^2$ hence $\tau_1 \lesssim \tau^{\frac{4}{3}}$.

7.2 Estimate of the First Order Scheme (7.2)

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

Lemma 7.2.1. *Consider the scheme (7.2). Assume $u_0 \in H^2(\mathbb{T}^2)$, then*

$$||u^1||_\infty + \frac{||u^1 - u^0||_2^2}{\tau_1} + \frac{\nu}{2}||\nabla u^1||_2^2 \lesssim_{E(u_0)\ ,\ ||u_0||_{H^2}} 1 \ . \tag{7.3}$$

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

$$u^1 = \frac{1}{1-\tau_1 \nu \Delta} u^0 - \frac{\tau_1 \Pi_N}{1-\tau_1 \nu \Delta} f(u^0) \,. \tag{7.4}$$

Note that

$$\frac{1}{1+\tau_1 \nu |k|^2} \leq 1 \;,\; \tau_1 \leq 1 \;, \tag{7.5}$$

thus

$$\begin{aligned} ||u^1||_\infty \lesssim ||u^1||_{H^2} &\lesssim ||u^0||_{H^2} + ||f(u^0)||_{H^2} \\ &\lesssim ||u^0||_{H^2} + ||(u^0)^3||_{H^2} \\ &\lesssim_{||u_0||_{H^2}} 1 \;, \end{aligned} \tag{7.6}$$

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

Second, we take the L^2 inner product with $u^1 - u^0$ on both sides of (7.2).

$$\begin{aligned} &\frac{||u^1-u^0||_2^2}{\tau_1} + \frac{\nu}{2}\left(||\nabla u^1||_2^2 - ||\nabla u^0||_2^2 + ||\nabla (u^1-u^0)||_2^2\right) \\ &= -(f(u^0) \,,\; u^1 - u^0) \\ &\leq ||f(u^0)||_{\frac{4}{3}} ||u^1-u^0||_4 \\ &\lesssim_{E(u^0)} 1 \;, \end{aligned} \tag{7.7}$$

by $||u_0||_\infty \;,\; ||u_1||_\infty \lesssim 1$.

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

□

Lemma 7.2.2. *(Error estimate for u^1) Consider*

$$\begin{cases} \dfrac{u^1 - u^0}{\tau_1} = \nu \Delta u^1 - \Pi_N f(u^0) \\ \partial_t u = \nu \Delta u - f(u) \\ u^0 = \Pi_N u_0 \ , \ u(0) = u_0 \ . \end{cases} \tag{7.8}$$

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

Proof. We start the proof in three steps:

Step 1: Time discretization of the PDE.

Write the PDE in time interval $[0, \tau_1]$. Note that for a one-variable function $h(s)$,

$$\begin{aligned} h(0) &= h(\tau_1) + \int_{\tau_1}^{0} h'(s)\, ds \\ &= h(\tau_1) - h'(\tau_1)\tau_1 + \int_0^{\tau_1} h''(s) \cdot s\, ds \ . \end{aligned} \tag{7.9}$$

By applying this formula, we have

$$\begin{aligned} \frac{u(\tau_1) - u(0)}{\tau_1} &= \partial_t u(\tau_1) - \frac{1}{\tau_1} \int_0^{\tau_1} (\partial_{tt} u) \cdot s\, ds \\ &= \nu \Delta u(\tau_1) - f(u(\tau_1)) - \frac{1}{\tau_1} \int_0^{\tau_1} (\partial_{tt} u) \cdot s\, ds \\ &= \nu \Delta u(\tau_1) - \Pi_N f(u(0)) - \Pi_{>N} f(u(0)) - [f(u(\tau_1) - f(u(0))] \\ &\quad - \frac{1}{\tau_1} \int_0^{\tau_1} (\partial_{tt} u) \cdot s\, ds \ , \end{aligned} \tag{7.10}$$

where $\Pi_{>N} = id - \Pi_N$ as in chapter 4.

Hence

$$\frac{u(\tau_1)-u(0)}{\tau_1} = \nu\Delta u(\tau_1) - \Pi_N f(u(0)) + G^0 \ , \tag{7.11}$$

where

$$\begin{aligned} G^0 &= -\Pi_{>N} f(u(0)) - [f(u(\tau_1) - f(u(0))] - \frac{1}{\tau_1}\int_0^{\tau_1} (\partial_{tt} u)\cdot s \ ds \\ &= -\Pi_{>N} f(u(0)) - [f(u(\tau_1) - f(u(0))] - \frac{1}{\tau_1}\int_0^{\tau_1} (\nu\Delta\partial_t u - f'(u)\partial_t u)\cdot s \ ds \end{aligned} \tag{7.12}$$

Step 2: Estimate of $||u(\tau_1)-u^1||_2$. We consider

$$\begin{cases} \dfrac{u(\tau_1)-u(0)}{\tau_1} = \nu\Delta u(\tau_1) - \Pi_N f(u(0)) + G^0 \\ \dfrac{u^1-u^0}{\tau_1} = \nu\Delta u^1 - \Pi_N f(u^0) \\ u^0 = \Pi_N u_0 \ , \ u(0) = u_0 \ . \end{cases} \tag{7.13}$$

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

$$\frac{e^1 - e^0}{\tau_1} = \nu\Delta e^1 - \Pi_N \left(f(u(0)) - f(u^0) \right) + G^0 \ . \tag{7.14}$$

Take the L^2 inner product with e^1 on both sides, we derive

$$\begin{aligned} &\frac{1}{2\tau_1}\left(||e^1||_2^2 - ||e^0||_2^2 + ||e^1 - e^0||_2^2\right) + \nu||\nabla e^1||_2^2 \\ &\le ||f(u(0)) - f(u^0)||_2 \cdot ||e^1||_2 + ||G^0||_2 \cdot ||e^1||_2 \\ &\lesssim \left(||e^0||_2 + ||G^0||_2\right)||e^1||_2 \\ &\lesssim \left(||e^0||_2^2 + ||G^0||_2^2\right) + \frac{1}{4}||e^1||_2^2 \ . \end{aligned} \tag{7.15}$$

As a result,

$$\left(1-\frac{\tau_1}{2}\right)||e^1||_2^2 \le 2\tau_1\left(||e^0||_2^2+||G^0||_2^2\right)+||e^0||_2^2\ . \tag{7.16}$$

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

$$||e^1||_2^2 \lesssim (1+\tau_1)||e^0||_2^2+\tau_1||G^0||_2^2\ . \tag{7.17}$$

Step 3: Estimate of $||e^0||_2^2$ and $||G^0||_2^2$.

Note that $||e^0||_2^2 = ||u(0)-u^0||_2^2 = ||u_0-\Pi_N u_0||_2^2 = ||\Pi_{>N}u_0||_2^2$. As proved in chapter 4, section 4.2.2,

$$||e^0||_2^2 = ||\Pi_{>N}u_0||_2^2 \lesssim N^{-2s}\ . \tag{7.18}$$

For $||G^0||_2$, note that $||\Pi_{>N}f(u(0))||_2 \lesssim N^{-s}$, by the maximum principle proved in chapter 4, Lemma 4.2.2.

On the other hand, by the mean value theorem,

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

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

$$||f(u(\tau_1))-f(u(0))||_2 \lesssim ||u(\tau_1)-u(0)||_2 \lesssim \tau_1||\partial_t u||_{L_t^\infty L_x^2([0\ ,\ \tau_1]\times\mathbb{T}^2)} \lesssim \tau_1\ , \tag{7.19}$$

using the Sobolev bound of the exact solution proved in chapter 4, Lemma 4.2.3.

Finally,

$$\begin{aligned}
&\left\| \frac{1}{\tau_1}\int_0^{\tau_1} (\nu\Delta\partial_t u - f'(u)\partial_t u)\cdot s\ ds \right\|_2 \\
&\lesssim \left\| \int_0^{\tau_1} \nu\Delta\partial_t u - f'(u)\partial_t u\ ds \right\|_2 \\
&\lesssim \int_0^{\tau_1} ||\nu\Delta\partial_t u||_2\ ds + \int_0^{\tau_1} ||f'(u)\partial_t u||_2\ ds \\
&\lesssim \tau_1\ .
\end{aligned} \tag{7.20}$$

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

$$||e^1||_2^2 \lesssim (1+\tau_1)N^{-2s} + \tau_1(N^{-2s} + \tau_1^2) \lesssim N^{-2s} + \tau_1^3\ . \tag{7.21}$$

As a result,

$$||e^1||_2 \lesssim N^{-s} + \tau_1^{\frac{3}{2}}\ . \tag{7.22}$$

□

7.3 Unconditional Stability of the Second Order Scheme I (7.1) & (7.2)

In this section we will prove a unconditional stability theorem for the second order scheme (7.1) combining (7.2). To get started, we state the theorem first.

Theorem 7.3.1. *(Unconditional Stability) Consider the scheme (7.1)-(7.2) with* $\nu > 0$, $\tau > 0$ *and* $N \geq 2$. *Assume* $u_0 \in H^2(\mathbb{T}^2)$. *The initial energy is denoted by* $E_0 = E(u_0)$. *If there exists a constant* $\beta_c > 0$ *depending only on* E_0 *and* $||u_0||_{H^2}$, *such that*

$$A \geq \beta \cdot (\nu^2 + \nu^{-10} |\log \nu|^4) \ , \ \beta \geq \beta_c \ ,$$

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*

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

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

Lemma 7.3.2. *Consider (7.1) for* $n \geq 1$. *Suppose* $E(u^n) \leq B$ *and* $E(u^{n-1}) \leq B$ *for some* $B > 0$. *Then*

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

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

Proof. For simplicity we write $\lesssim$ instead of $\lesssim_B$. Recall (7.1):

$$\frac{3u^{n+1} - 4u^n + u^{n-1}}{2\tau} = \nu \Delta u^{n+1} - A\tau(u^{n+1} - u^n) - \Pi_N \left(2f(u^n) - f(u^{n-1})\right) \ . \tag{7.23}$$

We rewrite as

$$\begin{aligned} u^{n+1} = & \frac{4 + 2A\tau^2}{3 - 2\nu\tau\Delta + 2A\tau^2} u^n - \frac{1}{3 - 2\nu\tau\Delta + 2A\tau^2} u^{n-1} \\ & - \frac{2\tau \Pi_N}{3 - 2\nu\tau\Delta + 2A\tau^2} \left(2f(u^n) - f(u^{n-1})\right) \ . \end{aligned} \tag{7.24}$$

First, for $k=0$,

$$\begin{cases} \dfrac{4+2A\tau^2}{3+2A\tau^2} \lesssim 1 \\ \dfrac{1}{3+2A\tau^2} \lesssim 1 \\ \dfrac{2}{3+2A\tau^2} \lesssim \tau \, . \end{cases} \tag{7.25}$$

Thus

$$|\widehat{u^{n+1}}(0)| \lesssim \tau + 1 \, . \tag{7.26}$$

Note that for $|k| \geq 1$,

$$\begin{cases} \dfrac{4+2A\tau^2}{3+2\nu\tau|k|^2+2A\tau^2} \lesssim 1 \\ \dfrac{1}{3+2\nu\tau|k|^2+2A\tau^2} \lesssim 1 \\ \dfrac{2\tau|k|}{3+2\nu\tau|k|^2+2A\tau^2} \lesssim \dfrac{\tau|k|}{\nu\tau|k|^2} \lesssim \dfrac{1}{\nu}\cdot|k|^{-1} \, . \end{cases} \tag{7.27}$$

Thus

$$\begin{aligned} ||u^{n+1}||_{\dot{H}^1} &\lesssim ||u^n||_{\dot{H}^1} + ||u^{n-1}||_{\dot{H}^1} + \frac{1}{\nu}||\langle\nabla\rangle^{-1}\big(2f(u^n)-f(u^{n-1})\big)||_2 \\ &\lesssim \nu^{-\frac{1}{2}} + \nu^{-1}(||(u^n)^3||_{4/3} + ||(u^{n-1})^3||_{4/3} + ||u^n||_2 + ||u^{n-1}||_2) \\ &\lesssim \nu^{-\frac{1}{2}} + \nu^{-1} \, , \end{aligned} \tag{7.28}$$

here we apply Sobolev's inequality as introduced in chapter 2 and apply the energy bound as proved in chapter 3.

Similarly,

$$\begin{cases} \dfrac{|k|^2(4+2A\tau^2)}{3+2\nu\tau|k|^2+2A\tau^2} \lesssim \dfrac{|k|^2(1+A\tau^2)}{\nu\tau|k|^2} \lesssim \dfrac{1}{\nu\tau}+\dfrac{A\tau}{\nu} \\ \dfrac{|k|^2}{3+2\nu\tau|k|^2+2A\tau^2} \lesssim \dfrac{1}{\nu\tau} \\ \dfrac{2\tau|k|^2}{3+2\nu\tau|k|^2+2A\tau^2} \lesssim \dfrac{\tau|k|^2}{\nu\tau|k|^2} \lesssim \dfrac{1}{\nu} \, . \end{cases} \tag{7.29}$$

This implies

$$\begin{aligned} ||u^{n+1}||_{\dot{H}^2} &\lesssim \left(\frac{1}{\nu\tau}+\frac{A\tau}{\nu}\right)||u^n||_2 + \frac{1}{\nu\tau}||u^{n-1}||_2 + \frac{1}{\nu}||2f(u^n)-f(u^{n-1})||_2 \\ &\lesssim \frac{1}{\nu\tau}+\frac{A\tau}{\nu}+\frac{1}{\nu}\left(||u^n||_6^3+||u^{n-1}||_6^3+||u^n||_2+||u^{n-1}||_2\right) \\ &\lesssim \frac{1}{\nu\tau}+\frac{A\tau}{\nu}+\frac{1}{\nu}\left(||u^n||_{H^1}^3+||u^{n-1}||_{H^1}^3+1\right) \\ &\lesssim \frac{1}{\nu\tau}+\frac{A\tau}{\nu}+\frac{1}{\nu}(\nu^{-\frac{3}{2}}+1) \, . \end{aligned} \tag{7.30}$$

Finally, by applying the main log-interpolation lemma proved in chapter 2, section 2.3, we can derive

$$\begin{aligned} ||u^{n+1}||_\infty &\lesssim (1+||u^{n+1}||_{\dot{H}^1})\cdot\sqrt{\log(3+||u^{n+1}||_{\dot{H}^2})}+|\widehat{u^{n+1}(0)}| \\ &\lesssim (1+\nu^{-1})\cdot\sqrt{\log(3+\frac{A\tau}{\nu}+\frac{1}{\nu\tau}+\nu^{-\frac{5}{2}}+\nu^{-1})}+\tau+1 \, , \end{aligned} \tag{7.31}$$

where $\nu^{-\frac{1}{2}}$ is bounded by $\nu^{-1}+1$.

□

7.3.1 Proof of Unconditional Stability (Theorem 7.3.1)

Before proving the theorem, we first 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,

$$\begin{cases} 3u^{n+1} - 4u^n + u^{n-1} = 2\delta u^{n+1} + \delta^2 u^{n+1} \\ \delta^2 u^{n+1} - \delta u^{n+1} = -\delta u^n \\ \delta u^n \cdot u^n = (u^n - u^{n-1})u^n = \frac{1}{2}\left(|u^n|^2 - |u^{n-1}|^2 + |\delta u^n|^2\right) . \end{cases} \tag{7.32}$$

As a result,

$$\begin{aligned} &\left(3u^{n+1} - 4u^n + u^{n-1} \ , \ u^{n+1} - u^n\right) \\ &= \left(2\delta u^{n+1} + \delta^2 u^{n+1} \ , \ \delta u^{n+1}\right) \\ &= 2\|\delta u^{n+1}\|_2^2 + \left(\delta u^{n+1} - \delta u^n \ , \ \delta u^{n+1}\right) \\ &= 2\|\delta u^{n+1}\|_2^2 + \frac{1}{2}\left(\|\delta u^{n+1}\|_2^2 - \|\delta u^n\|_2^2 + \|\delta^2 u^{n+1}\|_2^2\right) . \end{aligned} \tag{7.33}$$

Now recall the scheme (7.1)

$$\frac{3u^{n+1} - 4u^n + u^{n-1}}{2\tau} = \nu\Delta u^{n+1} - A\tau(u^{n+1} - u^n) - \Pi_N\left(2f(u^n) - f(u^{n-1})\right) . \tag{7.34}$$

Take the L^2 inner product with $\delta u^{n+1} = u^{n+1} - u^n$ on both sides of (7.1). We have

$$\begin{aligned} &\frac{1}{\tau}\|\delta u^{n+1}\|_2^2 + \frac{1}{4\tau}\left(\|\delta u^{n+1}\|_2^2 - \|\delta u^n\|_2^2 + \|\delta^2 u^{n+1}\|_2^2\right) \\ &\qquad + \frac{\nu}{2}\left(\|\nabla u^{n+1}\|_2^2 - \|\nabla u^n\|_2^2 + \|\delta\nabla u^{n+1}\|_2^2\right) \\ &+ A\tau\|\delta u^{n+1}\|_2^2 = -\left(\Pi_N(2f(u^n) - f(u^{n-1})) \ , \ \delta u^{n+1}\right) . \end{aligned} \tag{7.35}$$

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

$\big(f(u^n) - f(u^{n-1}\big)$.

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

$$\begin{aligned} &F(u^{n+1}) - F(u^n) \\ =&f(u^n)\delta u^{n+1} + \int_0^1 f'(u^n + s\delta u^{n+1})(1-s)\, ds \cdot (\delta u^{n+1})^2 \\ =&f(u^n)\delta u^{n+1} + \int_0^1 \tilde{f}(u^n + s\delta u^{n+1})(1-s)\, ds \cdot (\delta u^{n+1})^2 - \frac{1}{2}(\delta u^{n+1})^2 , \end{aligned} \tag{7.36}$$

where $\tilde{f}(x) = 3x^2$, as $f'(x) = 3x^2 - 1$. And this implies

$$f(u^n)\delta u^{n+1} \geq F(u^{n+1}) - F(u^n) + \frac{1}{2}(\delta u^{n+1})^2 - \frac{3}{2}\left(||u^n||_\infty^2 + ||u^{n+1}||_\infty^2\right) \cdot (\delta u^{n+1})^2 . \tag{7.37}$$

On the other hand,

$$f(u^n) - f(u^{n-1}) = f'(\xi)\delta u^n , \tag{7.38}$$

and hence

$$\begin{aligned} &(f(u^n) - f(u^{n-1})) \cdot \delta u^{n+1} \geq -\left(3||u^n||_\infty^2 + 3||u^{n-1}||_\infty^2 + 1\right) \cdot |\delta u^n| \cdot |\delta u^{n+1}| \\ &\geq -\frac{\left(1 + 3||u^n||_\infty^2 + 3||u^{n-1}||_\infty^2\right)^2}{\nu} \cdot ||\delta u^n||_2^2 - \frac{\nu}{4}||\delta u^{n+1}||_2^2 . \end{aligned} \tag{7.39}$$

Hence the estimate of the nonlinear term is as following:

$$
\begin{aligned}
&-\left(\Pi_N(2f(u^n)-f(u^{n-1}))\ ,\ \delta u^{n+1}\right)\\
&=-\left(2f(u^n)-f(u^{n-1})\ ,\ \delta u^{n+1}\right)\\
&\leq -\int_{\mathbb{T}^2} F(u^{n+1})\ dx+\int_{\mathbb{T}^2} F(u^n)\ dx-\frac{1}{2}||\delta u^{n+1}||_2^2\\
&\quad+\frac{3}{2}\left(||u^n||_\infty^2+||u^{n+1}||_\infty^2\right)\cdot||\delta u^{n+1}||_2^2\\
&\quad+\frac{\left(1+3||u^n||_\infty^2+3||u^{n-1}||_\infty^2\right)^2}{\nu}\cdot||\delta u^n||_2^2+\frac{\nu}{4}||\delta u^{n+1}||_2^2\ .
\end{aligned} \tag{7.40}
$$

Combine all estimates (7.35) and (7.40) we get

$$
\begin{aligned}
&\frac{1}{\tau}||\delta u^{n+1}||_2^2+\frac{1}{4\tau}\left(||\delta u^{n+1}||_2^2-||\delta u^n||_2^2+||\delta^2 u^{n+1}||_2^2\right)\\
&+\frac{\nu}{2}\left(||\nabla u^{n+1}||_2^2-||\nabla u^n||_2^2+||\delta\nabla u^{n+1}||_2^2\right)\\
&+A\tau||\delta u^{n+1}||_2^2\\
&\leq -\int_{\mathbb{T}^2} F(u^{n+1})\ dx+\int_{\mathbb{T}^2} F(u^n)\ dx-\frac{1}{2}||\delta u^{n+1}||_2^2\\
&+\frac{3}{2}\left(||u^n||_\infty^2+||u^{n+1}||_\infty^2\right)\cdot||\delta u^{n+1}||_2^2\\
&+\frac{\left(1+3||u^n||_\infty^2+3||u^{n-1}||_\infty^2\right)^2}{\nu}\cdot||\delta u^n||_2^2+\frac{\nu}{4}||\delta u^{n+1}||_2^2\ .
\end{aligned} \tag{7.41}
$$

After simplification,

$$
\begin{aligned}
&\left(\frac{1}{\tau}+A\tau-\frac{\nu}{4}+\frac{1}{2}\right)\cdot||\delta u^{n+1}||_2^2+\tilde{E}(u^{n+1})\\
&\leq\left\{\frac{3}{2}(||u^n||_\infty^2+||u^{n+1}||_\infty^2)+\frac{\left(1+3||u^n||_\infty^2+3||u^{n-1}||_\infty^2\right)^2}{\nu}\right\}\cdot||\delta u^{n+1}||_2^2+\tilde{E}(u^n)\ .
\end{aligned} \tag{7.42}
$$

Clearly to show $\tilde{E}(u^{n+1}) \le \tilde{E}(u^n)$, it suffices to show

$$\begin{aligned} &\frac{1}{\tau} + A\tau - \frac{\nu}{4} + \frac{1}{2} \ge \\ &\frac{3}{2}(||u^n||_\infty^2 + ||u^{n+1}||_\infty^2) + \frac{\left(1 + 3||u^n||_\infty^2 + 3||u^{n-1}||_\infty^2\right)^2}{\nu} \ . \end{aligned} \tag{7.43}$$

We now prove this sufficient condition inductively. Set

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

By Lemma 7.2.1 in previous section, $B \lesssim 1$. We shall prove for every $m \ge 2$,

$$\begin{cases} \tilde{E}(u^m) \le B\ ,\ \tilde{E}(u^m) \le \tilde{E}(u^{m-1})\ , \\ ||u^m||_\infty \le \alpha_B \cdot \left[(1+\nu^{-1}) \cdot \sqrt{\log(3 + \frac{A\tau}{\nu} + \frac{1}{\tau\nu} + \nu^{-\frac{5}{2}} + \nu^{-1})} + \tau + 1\right]\ , \end{cases} \tag{7.44}$$

where $\alpha_B > 0$ is the same constant in Lemma 7.3.2.

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 we can apply Lemma 7.3.2, and hence obtain

$$||u^2||_\infty \le \alpha_B \cdot \left\{(1+\nu^{-1}) \cdot \sqrt{\log(3 + \frac{A\tau}{\nu} + \frac{1}{\tau\nu} + \nu^{-\frac{5}{2}} + \nu^{-1})} + \tau + 1\right\}\ . \tag{7.45}$$

We only need to check $\tilde{E}(u^2) \le \tilde{E}(u^1)$. By the sufficient condition (7.41), we only need to check the inequality

$$\frac{1}{\tau} + A\tau - \frac{\nu}{4} + \frac{1}{2} \geq \frac{3}{2}(||u^1||_\infty^2 + ||u^2||_\infty^2) + \frac{\left(1 + 3||u^1||_\infty^2 + 3||u^0||_\infty^2\right)^2}{\nu} \ . \tag{7.46}$$

By Lemma 7.2.1, $||u^0||_\infty$, $||u^1||_\infty \lesssim 1$, it suffices to choose A such that

$$\frac{1}{\tau} + A\tau - \frac{\nu}{4} + \frac{1}{2} \geq C \cdot (1 + \nu^{-2}) \cdot \log(3 + \frac{A\tau}{\nu} + \frac{1}{\tau\nu} + \nu^{-\frac{5}{2}} + \nu^{-1}) + C\nu^{-1} + C + C\tau \ . \tag{7.47}$$

We discuss two case and denote $X = A\tau + \frac{1}{\tau}$.

Case 1: $0 < \nu \leq 1/2$. In this case we need

$$X + \frac{1}{2} \geq C\nu^{-2} \cdot (|\log \nu| + |\log X|) \ . \tag{7.48}$$

Hence we need

$$X \geq C \cdot \nu^{-2} |\log \nu| \ . \tag{7.49}$$

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

$$X \geq C \cdot (|\log X| + 1 + \nu) \ , \tag{7.50}$$

and hence

$$X \geq C \cdot (1 + \nu) \ . \tag{7.51}$$

In conclusion, as $X \geq 2\sqrt{A}$,

$$A \geq C \cdot (1 + \nu^2 + \nu^{-4} |\log \nu|^2) \geq C \cdot (\nu^2 + \nu^{-4} |\log \nu|^2) \ . \tag{7.52}$$

Now we check the induction step. Assume the induction hypothesis hold for $2 \le m \le n$, then for $m = n+1$,

$$||u^{n+1}||_\infty \le \alpha_B \cdot \left\{ (1+\nu^{-1}) \cdot \sqrt{\log(3 + \frac{A\tau}{\nu} + \frac{1}{\tau\nu} + \nu^{-\frac{5}{2}} + \nu^{-1}) + \tau} \right\} , \tag{7.53}$$

by Lemma 7.3.2. It remains to show $\tilde{E}(u^{n+1}) \le \tilde{E}(u^n)$. It suffices to choose A such that

$$\begin{aligned} \frac{1}{\tau} + A\tau + \frac{1}{2} \ge & \frac{\nu}{4} + C \cdot (1+\nu^{-2}) \cdot \log(3 + \frac{A\tau}{\nu} + \frac{1}{\tau\nu} + \nu^{-\frac{5}{2}} + \nu^{-1}) \\ & + \frac{C(1+\nu^{-4})}{\nu} \left((\log(3 + \frac{A\tau}{\nu} + \frac{1}{\tau\nu} + \nu^{-\frac{5}{2}} + \nu^{-1}))^2 + \tau \right) . \end{aligned} \tag{7.54}$$

In terms of $X = A\tau + \frac{1}{\tau}$ again, we need to discuss two cases as well.

Case 1: $0 < \nu \le 1/2$. Then

$$X \ge C \cdot \nu^{-5}(|\log \nu|^2 + |\log X|^2) . \tag{7.55}$$

As a result,

$$X \ge C \cdot \nu^{-5} |\log \nu|^2 . \tag{7.56}$$

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

$$X \ge C\nu + C \cdot (\log X + (\log X)^2 \nu^{-1}) , \tag{7.57}$$

hence $X \ge C \cdot (\nu + 1)$.

In conclusion of two cases,

$$A \geq C \cdot (\nu^2 + 1 + \nu^{-10} |\log \nu|^4) \geq C \cdot (\nu^2 + \nu^{-10} |\log \nu|^4) \, . \tag{7.58}$$

This completes the induction. Combining the estimate, we need to take

$$A \geq C \cdot (\nu^2 + \nu^{-10} |\log \nu|^4) \, , \tag{7.59}$$

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

7.4 L^2 Error Estimate of Second Order Scheme I

First we state the theorem.

Theorem 7.4.1. *(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 2D Allen-Cahn equation with initial data u_0. Let u^1 be defined according to (7.2) with initial data $u^0 = \Pi_N u_0$. Let u^m, $m \geq 2$ be defined in (7.1) with initial data u^0 and u^1. Assume A satisfies the same condition in Theorem 7.3.1. Define $t_0 = 0$, $t_1 = \tau_1$ and $t_m = \tau_1 + (m-1)\tau$ for $m \geq 2$. Then for any $m \geq 1$,*

$$||u(t_m) - u^m||_2 \leq C_1 \cdot e^{C_2 t_m} \cdot (N^{-s} + \tau^2) \, , \tag{7.60}$$

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

Remark 11. *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.*

Similar to chapter 4, we will study the auxiliary error estimate behavior and time discretization behavior of Allen-Cahn equation before proving the theorem.

7.4.1 Auxiliary L^2 Error Estimate for Near Solutions

Consider for $n \geq 1$,

$$\begin{cases} \dfrac{3u^{n+1}-4u^n+u^{n-1}}{2\tau} = \nu\Delta u^{n+1} - A\tau(u^{n+1}-u^n) - \Pi_N\left(2f(u^n)-f(u^{n-1})\right) + G^n \\ \dfrac{3v^{n+1}-4v^n+v^{n-1}}{2\tau} = \nu\Delta v^{n+1} - A\tau(v^{n+1}-v^n) - \Pi_N\left(2f(v^n)-f(v^{n-1})\right) \end{cases}, \tag{7.61}$$

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

Proposition 3. *For solutions of (7.59), assume for some $N_1 > 0$,*

$$\sup_{n\geq 0} ||u^n|| + \sup_{n\geq 0} ||v^n|| \leq N_1\ , \tag{7.62}$$

Then for any $m \geq 2$,

$$\begin{aligned} ||u^m - v^m||_2^2 &\leq C\cdot\exp\left((m-1)\tau\cdot\frac{C(1+N_1^4)}{\eta}\right) \\ &\cdot\left((1+A\tau^2)||u^1-v^1||_2^2 + ||u^0-v^0||_2^2 + \frac{\tau}{\eta}\sum_{n=1}^{m-1}||G^n||_2^2\right)\ , \end{aligned} \tag{7.63}$$

where $C > 0$ is a absolute constant that could be computed and $0 < \eta < \frac{1}{100M}$ is a constant depending only on M, 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

$$\begin{aligned}&\frac{3e^{n+1}-4e^n+e^{n-1}}{2\tau}-\nu\Delta e^{n+1}+A\tau(e^{n+1}-e^n)\\&=-\Pi_N\left(2f(u^n)-2f(v^n)\right)+\Pi_N\left(f(u^{n-1})-f(v^{n-1})\right)+G^n\end{aligned}\tag{7.64}$$

Take the L^2 inner product with e^{n+1} on both sides, we derive

$$\begin{aligned}&\frac{1}{2\tau}(3e^{n+1}-4e^n+e^{n-1},e^{n+1})+\nu||\nabla e^{n+1}||_2^2+\frac{A\tau}{2}\left(||e^{n+1}||_2^2-||e^n||_2^2+||e^{n+1}-e^n||_2^2\right)\\&=-2(f(u^n)-f(v^n),\ e^{n+1})+(f(u^{n-1})-f(v^{n-1}),\ e^{n+1})+(G^n,\ e^{n+1})\ .\end{aligned}\tag{7.65}$$

To estimate the RHS, first observe that

$$|(f(u^n)-f(v^n),e^{n+1})|\le||f(u^n)-f(v^n)||_2||e^{n+1}||_2\le\frac{||f(u^n)-f(v^n)||_2^2}{\eta}+\eta||e^{n+1}||_2^2,\tag{7.66}$$

where $\eta<\frac{1}{100M}$ is a small number only depending on M.

Moreover, use similar method in chapter 4,

$$\begin{aligned}f(u^n)-f(v^n)&=f(u^n)-f(u^n-e^n)\\&=(u^n)^3-(u^n-e^n)^3-e^n\\&=-(e^n)^3-e^n-3u^n(e^n)^2+3(u^n)^2e^n\ .\end{aligned}\tag{7.67}$$

So by assumption

$$\begin{aligned}||f(u^n)-f(v^n)||_2^2\lesssim&||e^n||_\infty^4||e^n||_2^2+||e^n||_2^2+||u^n||_\infty^2||e^n||_2^2+||u^n||_\infty^4||e^n||_2^2\\\lesssim&(1+N_1^4)||e^n||_2^2\ .\end{aligned}\tag{7.68}$$

Similarly,

$$||f(u^{n-1})-f(v^{n-1})||_2^2\lesssim(1+N_1^4)||e^{n-1}||_2^2\ .\tag{7.69}$$

As a result,

$$\text{RHS} \le \frac{C(1+N_1^4)}{\eta}\left(||e^n||_2^2 + ||e^{n-1}||_2^2\right) + \frac{1}{\eta}||G^n||_2^2 + \eta||e^{n+1}||_2^2 . \tag{7.70}$$

On the other hand,

$$\begin{aligned}(3e^{n+1} - 4e^n + e^{n-1}, e^{n+1} - e^n) &= (2\delta e^{n+1} + \delta^2 e^{n+1},\ \delta e^{n+1}) \\ &= 2||\delta e^{n+1}||_2^2 + \frac{1}{2}\left(||\delta e^{n+1}||_2^2 - ||\delta e^n||_2^2 + ||\delta^2 e^{n+1}||_2^2\right) .\end{aligned} \tag{7.71}$$

Also,

$$\begin{aligned}&(3e^{n+1} - 4e^n + e^{n-1},\ e^n) = 3(\delta e^{n+1},\ e^n) - (\delta e^n,\ e^n) \\ =&\frac{3}{2}\left(||e^{n+1}||_2^2 - ||e^n||_2^2 - ||e^{n+1} - e^n||_2^2\right) - \frac{1}{2}\left(||e^n||_2^2 - ||e^{n-1}||_2^2 + ||e^n - e^{n-1}||_2^2\right) .\end{aligned} \tag{7.72}$$

These two equations give

$$\begin{aligned}&(3e^{n+1} - 4e^n + e^{n-1},\ e^{n+1}) \\ =&\frac{3}{2}(||e^{n+1}||_2^2 - ||e^n||_2^2) - \frac{1}{2}(||e^n||_2^2 - ||e^{n-1}||_2^2) + ||\delta e^{n+1}||_2^2 - ||\delta e^n||_2^2 \\ &+ \frac{1}{2}||\delta^2 e^{n+1}||_2^2 .\end{aligned} \tag{7.73}$$

Collecting all estimates (7.70) and (7.73), (7.63) becomes

$$\begin{aligned}&\frac{1}{2\tau}\left(\frac{3}{2}||e^{n+1}||_2^2 - \frac{1}{2}||e^n||_2^2 + ||e^{n+1} - e^n||_2^2\right) + \frac{A\tau}{2}||e^{n+1}||_2^2 \\ \le&\frac{1}{2\tau}\left(\frac{3}{2}||e^n||_2^2 - \frac{1}{2}||e^{n-1}||_2^2 + ||e^n - e^{n-1}||_2^2\right) + \frac{A\tau}{2}||e^n||_2^2 \\ &+\frac{C(1+N_1^4)}{\eta}\left(||e^n||_2^2 + ||e^{n-1}||_2^2\right) + \frac{1}{\eta}||G^n||_2^2 + \eta||e^{n+1}||_2^2 .\end{aligned} \tag{7.74}$$

Now 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

$$X^{n+1} = \begin{cases} \frac{1}{2}||e^{n+1}||_2^2 + \frac{1}{2}||2e^{n+1} - e^n||_2^2 \\ \frac{1}{10}||e^n||_2^2 + \frac{5}{2}||e^{n+1} - \frac{2}{5}e^n||_2^2 \, . \end{cases} \tag{7.75}$$

This shows

$$X^{n+1} \geq \frac{1}{10} \max\left\{||e^{n+1}||_2^2,\ ||e^n||_2^2\right\} \, . \tag{7.76}$$

Making use of X^{n+1}, (7.72) becomes

$$\begin{aligned} &\frac{\left(X^{n+1} + A\tau^2||e^{n+1}||_2^2\right) - \left(X^n + A\tau^2||e^n||_2^2\right)}{2\tau} \\ \leq &\frac{C(1+N_1^4)}{\eta}\left(||e^n||_2^2 + ||e^{n-1}||_2^2\right) + \frac{1}{\eta}||G^n||_2^2 + \eta||e^{n+1}||_2^2 \, . \end{aligned} \tag{7.77}$$

This leads to

$$\begin{aligned} &\frac{\left(X^{n+1} - 2\eta\tau||e^{n+1}||_2^2 + A\tau^2||e^{n+1}||_2^2\right) - \left(X^n - 2\eta\tau||e^n||_2^2 + A\tau^2||e^n||_2^2\right)}{2\tau} \\ \leq &\frac{C(1+N_1^4)}{\eta}\left(||e^n||_2^2 + ||e^{n-1}||_2^2\right) + \frac{1}{\eta}||G^n||_2^2 + \eta||e^n||_2^2 \\ \leq &\left(\frac{C(1+N_1^4)}{\eta} + C\eta\right) \cdot \left(X^n - 2\eta\tau||e^n||_2^2\right) + \frac{1}{\eta}||G^n||_2^2 \, . \end{aligned} \tag{7.78}$$

Define

$$\begin{aligned} y_n &= X^n - 2\eta\tau||e^n||_2^2 + A\tau^2||e^n||_2^2 \, , \\ \alpha &= \frac{C(1+N_1^4)}{\eta} + C\eta \, , \\ \beta_n &= \frac{||G_n||_2^2}{\eta} \, . \end{aligned} \tag{7.79}$$

This shows for ν small,

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

Applying discrete Gronwall's inequality, we have for $m \geq 2$,

$$||e^m||_2^2 \leq C\left(X^m - 2\eta\tau||e^m||_2^2\right) \leq Ce^{(m-1)\tau\cdot\frac{C(1+N_1^4)}{\eta}}\left(X^1 + A\tau^2||e^1||_2^2 + \frac{\tau}{\eta}\sum_{n=1}^{m-1}||G^n||_2^2\right), \tag{7.80}$$

which gives

$$\begin{aligned}
&||u^m - v^m||_2^2 \\
\leq& C\cdot\exp\left((m-1)\tau\cdot\frac{C(1+N_1^4)}{\eta}\right)\cdot\left(\frac{3}{2}||e^1||_2^2 - \frac{1}{2}||e^0||_2^2 + ||e^1 - e^0||_2^2\right. \\
&\left. + A\tau^2||e^1||_2^2 + \frac{\tau}{\eta}\sum_{n=1}^{m-1}||G^n||_2^2\right) \\
\leq& C\cdot\exp\left((m-1)\tau\cdot\frac{C(1+N_1^4)}{\eta}\right)\cdot\left((1+A\tau^2)||u^1 - v^1||_2^2 + ||u^0 - v^0||_2^2\right. \\
&\left. + \frac{\tau}{\eta}\sum_{n=1}^{m-1}||G^n||_2^2\right).
\end{aligned} \tag{7.81}$$

□

7.4.2 Time Discretization of Allen-Cahn Equation

In this section, we will rewrite the PDE in terms of the second order scheme.

Lemma 7.4.2. *(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 $n \geq 1$,

$$\begin{aligned} &\frac{3u(t_{n+1}) - 4u(t_n) + u(t_{n-1})}{2\tau} \\ &= \nu\Delta u(t_{n+1}) - A\tau\left(u(t_{n+1}) - u(t_n)\right) - \Pi_N\left[2f(u(t_n)) - f(u(t_{n-1}))\right] + G^n \ . \end{aligned} \tag{7.82}$$

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

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

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

$$h(t) = h(t_0) + h'(t_0)(t-t_0) + \frac{1}{2}h''(t_0)(t-t_0)^2 + \frac{1}{2}\int_{t_0}^{t} h'''(s)(s-t)^2\ ds \ . \tag{7.83}$$

We then apply this to AC,

$$\begin{cases} u(t_n) = u(t_{n+1}) - \partial_t u(t_{n+1})\cdot\tau + \frac{1}{2}\partial_{tt}u(t_{n+1})\tau^2 + \frac{1}{2}\int_{t_{n+1}}^{t_n} \partial_{ttt}u(s)(s-t_n)^2\ ds \\ u(t_{n-1}) = u(t_{n+1}) - \partial_t u(t_{n+1})\cdot 2\tau + 2\partial_{tt}u(t_{n+1})\tau^2 + \frac{1}{2}\int_{t_{n+1}}^{t_{n-1}} \partial_{ttt}u(s)(s-t_{n-1})^2\ ds. \end{cases} \tag{7.84}$$

As a result, we use second equation above-4×first equation and hence get

$$
\begin{aligned}
&\frac{3u(t_{n+1})-4u(t_n)+u(t_{n-1})}{2\tau}\\
&=\frac{1}{2\tau}\left(2\tau\cdot\partial_t u(t_{n+1})-2\int_{t_{n+1}}^{t_n}\partial_{ttt}u(s)(s-t_n)^2\,ds\right.\\
+&\left.\frac{1}{2}\int_{t_{n+1}}^{t_{n-1}}\partial_{ttt}u(s)(s-t_{n-1})^2\,ds\right)\\
&=\partial_t u(t_{n+1})+\frac{1}{\tau}\int_{t_n}^{t_{n+1}}\partial_{ttt}u(s)(s-t_n)^2\,ds-\frac{1}{4\tau}\int_{t_{n-1}}^{t_{n+1}}\partial_{ttt}u(s)(s-t_{n-1})^2\,ds\\
&=\nu\Delta u(t_{n+1})-A\tau(u(t_{n+1})-u(t_n))-\Pi_N[2f(u(t_n))-f(u(t_{n-1}))]\\
+&A\tau(u(t_{n+1})-u(t_n))-\Pi_{>N}[2f(u(t_n))-f(u(t_{n-1}))]\\
+&2f(u(t_n))-f(u(t_{n-1}))-f(u(t_{n+1})\\
+&\frac{1}{\tau}\int_{t_n}^{t_{n+1}}\partial_{ttt}u(s)(s-t_n)^2\,ds-\frac{1}{4\tau}\int_{t_{n-1}}^{t_{n+1}}\partial_{ttt}u(s)(s-t_{n-1})^2\,ds\;.
\end{aligned}
\tag{7.85}
$$

Clearly,

$$
\begin{aligned}
G^n=&\underbrace{A\tau(u(t_{n+1})-u(t_n))}_{I_1}-\underbrace{\Pi_{>N}[2f(u(t_n))-f(u(t_{n-1}))]}_{I_2}\\
&+\underbrace{2f(u(t_n))-f(u(t_{n-1}))-f(u(t_{n+1})}_{I_3}\\
&+\underbrace{\frac{1}{\tau}\int_{t_n}^{t_{n+1}}\partial_{ttt}u(s)(s-t_n)^2\,ds}_{I_4}-\underbrace{\frac{1}{4\tau}\int_{t_{n-1}}^{t_{n+1}}\partial_{ttt}u(s)(s-t_{n-1})^2\,ds}_{I_5}\;.
\end{aligned}
\tag{7.86}
$$

Step 2: We will estimate $||I_1||_2 \sim ||I_5||_2$.

I_1:

$$\begin{aligned}||I_1||_2^2 =&||A\tau(u(t_{n+1})-u(t_n))||_2^2 \\ \lesssim&\tau^2||u(t_{n+1})-u(t_n)||_2^2 \\ \lesssim&\tau^2||\int_{t_n}^{t_{n+1}}\partial_t u(s)\ ds||_2^2 \\ \lesssim&\tau^2\int_{\mathbb{T}^2}\left(\int_{t_n}^{t_{n+1}}\partial_t u(s)\ ds\right)^2 \\ \lesssim&\tau^2\int_{\mathbb{T}^2}\left((\int_{t_n}^{t_{n+1}}|\partial_t u(s)|^2\ ds)^{1/2}\cdot\sqrt{\tau}\right)^2 \\ \lesssim&\tau^2\cdot\tau\cdot\int_{t_n}^{t_{n+1}}||\partial_t u(s)||_2^2\ ds \\ \lesssim&\tau^3\int_{t_n}^{t_{n+1}}||\partial_t u(s)||_2^2\ ds\ .\end{aligned} \tag{7.87}$$

I_2: By the maximum principle Lemma 4.2.2 proved in chapter 4 and $u \in L_t^\infty H_x^s$,

$$\begin{aligned}||I_2||_2 \lesssim&N^{-s}\cdot(||f(u(t_n))||_{H^s}+||f(u(t_{n-1}))||_{H^s}) \\ \lesssim&N^{-s}\ .\end{aligned} \tag{7.88}$$

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

$$h(t)=h(t_0)+h'(t_0)(t-t_0)-\int_{t_0}^{t}h''(s)\cdot(s-t)\ ds\ . \tag{7.89}$$

Then,

$$\begin{cases} f(u(t_n))=f(u(t_{n+1}))-\partial_t(f(u))(t_{n+1})\cdot\tau+\displaystyle\int_{t_n}^{t_{n+1}}\partial_{tt}(f(u))\cdot(s-t_n)\ ds \\ f(u(t_{n-1}))=f(u(t_{n+1}))-\partial_t(f(u))(t_{n+1})\cdot 2\tau+\displaystyle\int_{t_{n-1}}^{t_{n+1}}\partial_{tt}(f(u))\cdot(s-t_{n-1})\ ds\ . \end{cases} \tag{7.90}$$

Then we use second equation above-2×first equation and derive:

$$
\begin{aligned}
& f(u(t_{n+1}))-2f(u(t_n))+f(u(t_{n-1})) \\
=& -2\int_{t_n}^{t_{n+1}} \partial_{tt}(f(u))\cdot(s-t_n)\,ds+\int_{t_{n-1}}^{t_{n+1}} \partial_{tt}(f(u))\cdot(s-t_{n-1})\,ds\ .
\end{aligned}
\tag{7.91}
$$

As a result,

$$
\begin{aligned}
||I_3||_2^2 =& ||f(u(t_{n+1}))-2f(u(t_n))+f(u(t_{n-1}))||_2^2 \\
\lesssim& ||\int_{t_n}^{t_{n+1}} \partial_{tt}(f(u))\cdot(s-t_n)\,ds||_2^2+||\int_{t_{n-1}}^{t_{n+1}} \partial_{tt}(f(u))\cdot(s-t_{n-1})\,ds||_2^2 \\
\lesssim& \tau^2\cdot||\int_{t_n}^{t_{n+1}} \partial_{tt}(f(u))\,ds||_2^2+\tau^2\cdot||\int_{t_{n-1}}^{t_{n+1}} \partial_{tt}(f(u))\,ds||_2^2 \\
\lesssim& \tau^3\int_{t_{n-1}}^{t_{n+1}} ||\partial_{tt}(f(u))||_2^2\,ds\ ,
\end{aligned}
\tag{7.92}
$$

by a similar estimate in I_1.

I_4&I_5:

$$
\begin{aligned}
& ||I_4||_2^2+||I_5||_2^2 \\
\lesssim& \left\|\frac{1}{\tau}\int_{t_n}^{t_{n+1}} \partial_{ttt}u(s)(s-t_n)^2\,ds\right\|_2^2+\left\|\frac{1}{\tau}\int_{t_{n-1}}^{t_{n+1}} \partial_{ttt}u(s)(s-t_{n-1})^2\,ds\right\|_2^2 \\
\lesssim& \left\|\frac{1}{\tau}\int_{t_{n-1}}^{t_{n+1}} \partial_{ttt}u(s)\cdot\tau^2\,ds\right\|_2^2 \\
\lesssim& \tau^2\cdot\left\|\int_{t_{n-1}}^{t_{n+1}} \partial_{ttt}u(s)\,ds\right\|_2^2 \\
\lesssim& \tau^3\int_{t_{n-1}}^{t_{n+1}} ||\partial_{ttt}u(s)||_2^2\,ds\ .
\end{aligned}
\tag{7.93}
$$

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

Collecting estimates above, we have

$$\begin{aligned}\tau\cdot\sum_{n=1}^{m-1}||G^n||_2^2 =&\tau\cdot\sum_{n=1}^{m-1}(||I_1||_2^2+||I_2||_2^2+||I_3||_2^2+||I_4||_2^2+||I_5||_2^2)\\ &\lesssim m\tau\cdot N^{-2s}+\tau^4\cdot\int_0^{t_m}||\partial_t u||_2^2+||\partial_{tt}(f(u))||_2^2+||\partial_{ttt}u||_2^2\;d\tilde{s}\;.\end{aligned}\tag{7.94}$$

Note that

$$\begin{cases}\partial_{tt}u=\nu\partial_t\Delta u-\partial_t(f(u))\\ \partial_{ttt}u=\nu\partial_{tt}\Delta u-\partial_{tt}(f(u))\\ \partial_t(f(u))=f'(u)\partial_t u\\ \partial_{tt}(f(u))=f'(u)\partial_{tt}u+f''(u)(\partial_t u)^2\;,\end{cases}\tag{7.95}$$

hence together with maximum principle and higher Sobolev bounds proved in chapter 4, one has

$$\begin{aligned}\tau\cdot\sum_{n=1}^{m-1}||G^n||_2^2&\lesssim m\tau\cdot N^{-2s}+\tau^4\cdot\int_0^{t_m}||\partial_t u||_2^2+||\partial_{tt}(f(u))||_2^2+||\partial_{ttt}u||_2^2\;d\tilde{s}\\ &\lesssim t_m\cdot N^{-2s}+\tau^4\cdot\int_0^{t_m}||u||_{H^s}^2\;d\tilde{s}\\ &\lesssim t_m\cdot N^{-2s}+\tau^4\cdot(1+t_m)\\ &\lesssim(1+t_m)\cdot(\tau^4+N^{-2s})\;.\end{aligned}\tag{7.96}$$

□

7.4.3 Proof of L^2 Error Estimate of Second Order Scheme I (7.1)

First, assumptions in Proposition 3 are satisfied by the unconditional Theorem 7.3.1 and maximum principle of Allen-Cahn equation. Thus we apply the auxiliary estimate Proposition 3. Then

$$||u(t_m)-u^m||_2^2 \lesssim e^{Cm\tau}\cdot\left((1+A\tau^2)||u^1-v^1||_2^2+||u^0-v^0||_2^2+\tau\sum_{n=1}^{m-1}||G^n||_2^2\right). \tag{7.97}$$

By Lemma 7.2.2 and Lemma 7.4.2,

$$\begin{aligned}||u(t_m)-u^m||_2^2 &\lesssim e^{Cm\tau}\cdot\left((1+A\tau^2)||u^1-v^1||_2^2+||u^0-v^0||_2^2+\tau\sum_{n=1}^{m-1}||G^n||_2^2\right)\\ &\lesssim e^{Ct_m}\cdot\big((1+A\tau^2)(N^{-2s}+\tau^4)+N^{-2s}+(1+t_m)\cdot(\tau^4+N^{-2s})\big)\\ &\lesssim e^{Ct_m}\cdot(N^{-2s}+\tau^4)\,.\end{aligned} \tag{7.98}$$

Thus for $m\geq 2$,

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

Remark 12. *For the error estimate, we actually do not need that high regularity of initial data because of a smoothing effect of Allen-Cahn equation.*

7.5 Introduction of Scheme II

In this section, we will introduce another second order scheme.

$$\frac{3u^{n+1}-4u^n+u^{n-1}}{2\tau}=\nu\Delta u^{n+1}-A(u^{n+1}-2u^n+u^{n-1})-\Pi_N\left(2f(u^n)-f(u^{n-1})\right), \tag{7.99}$$

where $\tau>0$ is the time step and $n\geq 1$.

To start the iteration, we again need to derive u^1 according to the following first order scheme:

$$\begin{cases}\dfrac{u^1-u^0}{\tau_1}=\nu\Delta u^1-\Pi_N f(u^0)\ , \\ u^0=\Pi_N u_0\ ,\end{cases} \tag{7.100}$$

where $\tau_1=\min\{\tau^{\frac{4}{3}}\ ,\ 1\ ,\frac{1}{\sqrt{A+1}}\}$. The choice of such τ is to guarantee the error estimate as proved in section 7.2, and to ensure that the new modified energy function can be controlled by initial data.

7.6 Estimate of the First Order Scheme (7.100)

In this section we will still estimate some bounds of u^1 which will be used to prove the stability of the second order scheme. It is slightly different from scheme (7.2).

Lemma 7.6.1. *Consider the scheme (7.100).*

$$\begin{cases}\dfrac{u^1-u^0}{\tau_1}=\nu\Delta u^1-\Pi_N f(u^0)\ , \\ u^0=\Pi_N u_0\ ,\end{cases} \tag{7.101}$$

where $\tau_1 = \min\{\tau^{\frac{4}{3}}\ ,\ 1\ ,\ \frac{1}{\sqrt{A+1}}\}$*. Assume* $u_0 \in H^2(\mathbb{T}^2)$*, then*

$$\begin{aligned} E(u^1) + \frac{\|u^1 - u^0\|_2^2}{\tau_1} + &\lesssim_{E(u_0)\ ,\ \|u_0\|_{H^2}} 1 \\ (1+A)\|u^1 - u^0\|_2^2 &\lesssim_{\|u_0\|_{H^2}} (1+\nu)^2\ . \end{aligned} \tag{7.102}$$

Proof. The first inequality shares the same proof as in section 7.2, as the scheme (7.100) is a refined version of (7.2).

For the second inequality, recall that $\|u^1\|_{H^2} \lesssim_{\|u_0\|_{H^2}}$, hence by (7.101)

$$\frac{1}{\tau_1}\|u^1 - u^0\|_2 \le \nu\|u^1\|_{H^2} + \|f(u^0)\|_2 \lesssim_{\|u_0\|_{H^2}} 1 + \nu\ . \tag{7.103}$$

This implies

$$(A+1)\|u^1 - u^0\|_2^2 \lesssim_{\|u_0\|_{H^2}} (1+\nu)^2\ . \tag{7.104}$$

□

7.7 Conditional Stability of the Second Order Scheme II (7.99) & (7.100)

In this section we will prove a conditional stability theorem for the second order scheme (7.99) combining (7.100). To get started, we state the theorem first.

Theorem 7.7.1. *(Conditional Stability) Consider the scheme (7.99)-(7.100) with* $\nu > 0$*,* $\tau > 0$ *and* $N \ge 2$*. Assume* $u_0 \in H^2(\mathbb{T}^2)$*. The initial energy is denoted by* $E_0 = E(u_0)$*. There exist constants* $C_i > 0$*,* $i = 1,\ 2,\ 3,\ 4$ *depending only on* E_0 *and* $\|u_0\|_{H^2}$*, such that the following holds:*

Case 1: $A = 0$. *If*

$$\tau \leq \begin{cases} C_1 \dfrac{\nu^4}{1+|\log\nu|^2}, & when\ 0<\nu<1\ ; \\ C_2 \dfrac{\nu^{-2}}{1+|\log\nu|^2}, & when\ \nu \geq 1\ . \end{cases} \tag{7.105}$$

then

$$\mathring{E}(u^{n+1}) \leq \mathring{E}(u^n)\ .$$

Case 2: $A = constant \cdot (\nu^{-4} + \nu^2)$. *If*

$$\tau \leq \begin{cases} C_3 \dfrac{\nu^2}{1+|\log\nu|}, & when\ 0<\nu<1\ ; \\ C_4 \dfrac{\nu^{-1}}{1+|\log\nu|}, & when\ \nu \geq 1\ . \end{cases} \tag{7.106}$$

then

$$\mathring{E}(u^{n+1}) \leq \mathring{E}(u^n)\ .$$

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

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

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

Lemma 7.7.2. *Consider (7.99) for* $n \geq 1$. *Suppose* $E(u^n) \leq B\cdot(1+\nu)^2$ *and* $E(u^{n-1}) \leq B\cdot(1+\nu)^2$ *for some* $B > 0$. *Then*

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

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

Proof. For simplicity we write $\lesssim$ instead of $\lesssim_B$.

First note by the energy estimate,

$$||\nabla u^{n-1}||_2 + ||\nabla u^n||_2 \lesssim \nu^{-\frac{1}{2}}(1+\nu)\ ,\ ||u^{n-1}||_4 + ||u^n||_4 \lesssim (1+\nu)^{\frac{1}{2}}\ . \tag{7.107}$$

Now rewrite the scheme (7.99) as

$$\begin{aligned} u^{n+1} = & \frac{4+4A\tau}{3+2A\tau-2\nu\tau\Delta}u^n - \frac{1+2A\tau}{3+2A\tau-2\nu\tau\Delta}u^{n-1} \\ & - \frac{2\tau\Pi_N}{3+2A\tau-2\nu\tau\Delta}\left(2f(u^n)-f(u^{n-1})\right)\ . \end{aligned} \tag{7.108}$$

For Fourier mode $k=0$,

$$\begin{cases} \dfrac{4+4A\tau}{3+2A\tau} \lesssim 1 \\ \dfrac{1+2A\tau}{3+2A\tau} \lesssim 1 \\ \dfrac{2\tau}{3+2A\tau} \lesssim \dfrac{1}{A} \lesssim 1\ . \end{cases} \tag{7.109}$$

Thus

$$|\widehat{u^{n+1}}(0)| \lesssim 1\ . \tag{7.110}$$

For $|k| \geq 1$,

$$\begin{cases} \dfrac{4+4A\tau}{3+2A\tau+2\nu\tau|k|^2} \lesssim 1 \\ \dfrac{1+2A\tau}{3+2A\tau+2\nu\tau|k|^2} \lesssim 1 \\ \dfrac{2\tau}{3+2A\tau+2\nu\tau|k|^2} \lesssim \dfrac{1}{\nu|k|^2}\ . \end{cases} \tag{7.111}$$

This implies,

$$
\begin{aligned}
||u^{n+1}||_{\dot{H}^1} \lesssim & ||u^n||_{\dot{H}^1} + ||u^{n-1}||_{\dot{H}^1} + \frac{1}{\nu}||\langle\nabla\rangle^{-1}(2f(u^n) - f(u^{n-1}))||_2 \\
\lesssim & \nu^{-\frac{1}{2}}(1+\nu) + \nu^{-1}\cdot\left(||(u^n)^3||_{4/3} + ||(u^{n-1})^3||_{4/3} + ||u^n||_2 + ||u^{n-1}||_2\right) \\
\lesssim & \nu^{-\frac{1}{2}}(1+\nu) + \nu^{-1}\cdot\left((1+\nu)^{\frac{3}{2}} + (1+\nu)^{\frac{1}{2}}\right) \\
\lesssim & \nu^{-1} + \nu^{\frac{1}{2}} \ .
\end{aligned}
\tag{7.112}
$$

Similarly,

$$
\begin{cases}
\dfrac{4+4A\tau}{3+2A\tau+2\nu\tau|k|^2} \lesssim \left(\dfrac{1}{\nu\tau} + \dfrac{A}{\nu}\right)\cdot\dfrac{1}{|k|^2} \\
\dfrac{1+2A\tau}{3+2A\tau+2\nu\tau|k|^2} \lesssim \left(\dfrac{1}{\nu\tau} + \dfrac{A}{\nu}\right)\cdot\dfrac{1}{|k|^2} \\
\dfrac{2\tau}{3+2A\tau+2\nu\tau|k|^2} \lesssim \dfrac{1}{\nu|k|^2} \ .
\end{cases}
\tag{7.113}
$$

Thus,

$$
\begin{aligned}
||u^{n+1}||_{\dot{H}^2} \lesssim & \left(\frac{1}{\nu\tau} + \frac{A}{\nu}\right)\cdot\left(||u^n||_2 + ||u^{n-1}||_2\right) + \frac{1}{\nu}||(2f(u^n) - f(u^{n-1}))||_2 \\
\lesssim & \left(\frac{1}{\nu\tau} + \frac{A}{\nu}\right)\cdot(1+\nu)^{\frac{1}{2}} + \nu^{-1}\left(||u^n||_6^3 + ||u^{n-1}||_6^3 + ||u^n||_2 + ||u^{n-1}||_2\right) \\
\lesssim & \left(\frac{1}{\nu\tau} + \frac{A}{\nu}\right)\cdot(1+\nu)^{\frac{1}{2}} + \nu^{-1}(\nu^{-\frac{3}{2}}(1+\nu)^3 + (1+\nu)^{\frac{1}{2}}) \\
\lesssim & \frac{1}{\nu\tau} + \frac{A}{\nu} + \frac{1}{\nu^{\frac{1}{2}}\tau} + \frac{A+1}{\nu^{\frac{1}{2}}} + \nu^{-\frac{5}{2}} + \nu^{\frac{1}{2}} \ ,
\end{aligned}
\tag{7.114}
$$

by a standard Sobolev's inequality.

As a result, by the log interpolation inequality again,

$$
||u^{n+1}||_\infty \lesssim (\nu^{\frac{1}{2}} + \nu^{-1})\cdot\sqrt{1+\log(A+1)+|\log\nu|+|\log\tau|} + 1 \ . \tag{7.115}
$$

□

7.7.1 Proof of Conditional Stability (Theorem 7.7.1)

Recall that

$$\begin{aligned}\frac{3u^{n+1}-4u^n+u^{n-1}}{2\tau} &- \nu\Delta u^{n+1}+A(u^{n+1}-2u^n+u^{n-1}) \\ &= -\Pi_N\left(2f(u^n)-f(u^{n-1})\right).\end{aligned} \tag{7.116}$$

We apply L^2 inner product with $\delta u^{n+1}=u^{n+1}-u^n$ on both sides of (7.116).

Recall that

$$\begin{aligned}&\left(3u^{n+1}-4u^n+u^{n-1}\ ,\ u^{n+1}-u^n\right) \\ &=2||\delta u^{n+1}||_2^2+\frac{1}{2}\left(||\delta u^{n+1}||_2^2-||\delta u^n||_2^2+||\delta^2u^{n+1}||_2^2\right)\ .\end{aligned} \tag{7.117}$$

Estimate of the LHS:

$$\begin{aligned}\text{LHS} =& \frac{1}{\tau}||\delta u^{n+1}||_2^2+\frac{1}{4\tau}\left(||\delta u^{n+1}||_2^2-||\delta u^n||_2^2+||\delta^2u^{n+1}||_2^2\right) \\ &+\frac{\nu}{2}\left(||\nabla u^{n+1}||_2^2-||\nabla u^n||_2^2+||\delta\nabla u^{n+1}||_2^2\right) \\ &+\frac{A}{2}\left(||\delta u^{n+1}||_2^2-||\delta u^n||_2^2+||\delta^2u^{n+1}||_2^2\right) \\ \geq& \left[\frac{\nu}{2}||\nabla u^{n+1}||_2^2+\frac{1}{4\tau}||\delta u^{n+1}||_2^2+\frac{A}{2}||\delta u^{n+1}||_2^2\right] \\ &-\left[\frac{\nu}{2}||\nabla u^n||_2^2+\frac{1}{4\tau}||\delta u^n||_2^2+\frac{A}{2}||\delta u^n||_2^2\right] \\ &+\frac{1}{\tau}||\delta u^{n+1}||_2^2+\frac{A}{2}||\delta^2u^{n+1}||_2^2\ .\end{aligned} \tag{7.118}$$

Now it remains to estimate the RHS:

$$\begin{aligned} \text{RHS} &= -\left(2f(u^n) - f(u^{n-1}) \;,\; \delta u^{n+1}\right) \\ &= \underbrace{\left(2u^n - u^{n-1} \;,\; \delta u^{n+1}\right)}_{I_1} + \underbrace{\left((u^{n-1})^3 - 2(u^n)^3 \;,\; \delta u^{n+1}\right)}_{I_2} \;. \end{aligned} \tag{7.119}$$

$$\begin{aligned} I_1 &= \left(-\delta^2 u^{n+1} \;,\; \delta u^{n+1}\right) + \left(u^{n+1} \;,\; \delta u^{n+1}\right) \\ &= -\frac{1}{2}\left(||\delta u^{n+1}||_2^2 - ||\delta u^n||_2^2 + ||\delta^2 u^{n+1}||_2^2\right) \\ &\quad + \frac{1}{2}\left(||u^{n+1}||_2^2 - ||u^n||_2^2 + ||\delta u^{n+1}||_2^2\right) \;. \end{aligned} \tag{7.120}$$

For I_2, we use the identity $u^{n-1} = \delta^2 u^{n+1} + 2u^n - u^{n+1}$, then

$$\begin{aligned} (u^{n-1})^3 - 2(u^n)^3 =& (\delta^2 u^{n+1} + 2u^n - u^{n+1})^3 - 2(u^n)^3 \\ =& (\delta^2 u^{n+1})^3 + 3(\delta^2 u^{n+1})^2(2u^n - u^{n+1}) + 3\delta^2 u^{n+1}(2u^n - u^{n+1})^2 \\ &+ (2u^n - u^{n+1})^3 - 2(u^n)^3 \;. \end{aligned} \tag{7.121}$$

Note that,

$$\begin{aligned} 3\delta^2 u^{n+1}(2u^n - u^{n+1})^2 &= 3\delta^2 u^{n+1}(\delta^2 u^{n+1} - u^{n-1})^2 \\ &= 3(\delta^2 u^{n+1})^3 - 6(\delta^2 u^{n+1})^2 u^{n-1} + 3\delta^2 u^{n+1}(u^{n-1})^2 \;. \end{aligned} \tag{7.122}$$

As a result,

$$\begin{aligned}
&(u^{n-1})^3 - 2(u^n)^3 \\
=&4(\delta^2 u^{n+1})^3 + (\delta^2 u^{n+1})^2(6u^n - 3u^{n+1} - 6u^{n-1}) \\
&+ 3\delta^2 u^{n+1}(u^{n-1})^2 + (2u^n - u^{n+1})^3 - 2(u^n)^3 \\
=&(\delta^2 u^{n+1})^2 \cdot \left[4(u^{n+1} - 2u^n + u^{n-1}) + 6u^n - 3u^{n+1} - 6u^{n-1}\right] \\
&+ 3\delta^2 u^{n+1}(u^{n-1})^2 + 6(u^n)^3 - 12(u^n)^2 u^{n+1} + 6u^n(u^{n+1})^2 - (u^{n+1})^3 \\
=&(\delta^2 u^{n+1})^2 \cdot (u^{n+1} - 2u^n - 2u^{n-1}) + 3\delta^2 u^{n+1}(u^{n-1})^2 \\
&+ 6u^n(u^{n+1} - u^n)^2 - (u^{n+1})^3 \ .
\end{aligned} \tag{7.123}$$

Therefore we have,

$$\begin{aligned}
|I_2| \le&||\delta^2 u^{n+1}||_\infty \cdot ||\delta^2 u^{n+1}||_2 \cdot ||\delta u^{n+1}||_2 \\
&\cdot \left(||u^{n+1}||_\infty + 2||u^n||_\infty + 2||u^{n-1}||_\infty\right) \\
&+ ||\delta^2 u^{n+1}||_2 \cdot ||\delta u^{n+1}||_2 \cdot 3||u^{n-1}||_\infty^2 \\
&+ \left((\delta u^{n+1})^2 \ , \ 6u^n(u^{n+1} - u^n)\right) - \left((u^{n+1})^3 \ , \ \delta u^{n+1}\right) \ .
\end{aligned} \tag{7.124}$$

Now note that

$$\begin{aligned}
&\frac{(u^n)^4}{4} \\
=&\frac{1}{4}(u^{n+1} - \delta u^{n+1})^4 \\
=&\frac{1}{4}\left[(u^{n+1})^4 - 4(u^{n+1})^3 \delta u^{n+1} + 6(u^{n+1})^2(\delta u^{n+1})^2 - 4u^{n+1}(\delta u^{n+1})^3 + (\delta u^{n+1})^4\right] \\
=&\frac{(u^{n+1})^4}{4} - (u^{n+1})^3 \delta u^{n+1} + \frac{1}{4}(\delta u^{n+1})^2\left[6(u^{n+1})^2 - 4u^{n+1}(u^{n+1} - u^n) + (u^{n+1} - u^n)^2\right] \\
=&\frac{(u^{n+1})^4}{4} - (u^{n+1})^3 \delta u^{n+1} + \frac{(\delta u^{n+1})^2}{4}\left[(u^n)^2 + 2u^n u^{n+1} + 3(u^{n+1})^2\right] \ .
\end{aligned} \tag{7.125}$$

Applying this identity,

$$
\begin{aligned}
&\left((\delta u^{n+1})^2\ ,\ 6u^n(u^{n+1}-u^n)\right)-\left((u^{n+1})^3\ ,\ \delta u^{n+1}\right)\\
&=\int_{\mathbb{T}^2}\frac{(u^n)^4}{4}-\int_{\mathbb{T}^2}\frac{(u^{n+1})^4}{4}-\left((\delta u^{n+1})^2\ ,\ \frac{25}{4}(u^n)^2-\frac{11}{2}u^nu^{n+1}+\frac{3}{4}(u^{n+1})^2\right)\\
&=\int_{\mathbb{T}^2}\frac{(u^n)^4}{4}-\int_{\mathbb{T}^2}\frac{(u^{n+1})^4}{4}-\left((\delta u^{n+1})^2\ ,\ \frac{25}{4}(u^n-\frac{11}{25}u^{n+1})^2\right)\\
&\quad+\frac{23}{50}\left((\delta u^{n+1})^2\ ,\ (u^{n+1})^2\right)\ .
\end{aligned}
\tag{7.126}
$$

Note that

$$
\|\delta^2u^{n+1}\|_\infty\le 4\max\left\{\|u^{n-1}\|_\infty,\ \|u^n\|_\infty,\ \|u^{n+1}\|_\infty\right\},
$$

$$
\begin{aligned}
&\text{RHS}\\
&\le-\frac{1}{4}\|u^{n+1}\|_4^4+\frac{1}{2}\|u^{n+1}\|_2^2-\frac{1}{2}\|\delta u^{n+1}\|_2^2\\
&\quad+\frac{1}{4}\|u^n\|_4^4-\frac{1}{2}\|u^n\|_2^2+\frac{1}{2}\|\delta u^n\|_2^2\\
&\quad-\frac{1}{2}\|\delta^2u^{n+1}\|_2^2+\|\delta u^{n+1}\|_2^2\cdot\left(\frac{1}{2}+\frac{23}{50}\|u^{n+1}\|_\infty^2\right)\\
&\quad+\|\delta^2u^{n+1}\|_2\cdot\|\delta u^{n+1}\|_2\cdot 23\max\left\{\|u^{n-1}\|_\infty^2,\ \|u^n\|_\infty^2,\ \|u^{n+1}\|_\infty^2\right\}\ .
\end{aligned}
\tag{7.127}
$$

Recall that

$$
E(u)=\frac{\nu}{2}\|\nabla u\|_2^2+\frac{1}{4}\|u\|_4^4-\frac{1}{2}\|u\|_2^2+\frac{1}{4}\cdot m(\mathbb{T}^2)\ ,
$$

where $m(\mathbb{T}^2)$ is the measure of $\mathbb{T}^2$. Hence by comparing the LHS and the RHS of (7.126), we get

$$\begin{aligned}
&E(u^{n+1})+\frac{1}{4\tau}\|\delta u^{n+1}\|_2^2+\frac{A+1}{2}\|\delta u^{n+1}\|_2^2\\
\le &E(u^n)+\frac{1}{4\tau}\|\delta u^n\|_2^2+\frac{A+1}{2}\|\delta u^n\|_2^2\\
&+\|\delta^2 u^{n+1}\|_2\cdot\|\delta u^{n+1}\|_2\cdot 23\max\left\{\|u^{n-1}\|_\infty^2,\ \|u^n\|_\infty^2,\ \|u^{n+1}\|_\infty^2\right\}\\
&-\left\{\frac{A+1}{2}\|\delta^2 u^{n+1}\|_2^2+\left(\frac{1}{\tau}-\frac{1}{2}-\frac{23}{50}\|u^{n+1}\|_\infty^2\right)\cdot\|\delta u^{n+1}\|_2^2\right\}\ .
\end{aligned} \tag{7.128}$$

Clearly, to show the desired energy decay, it suffices to require

$$\begin{aligned}
&2(A+1)\left(\frac{1}{\tau}-\frac{1}{2}-\frac{23}{50}\|u^{n+1}\|_\infty^2\right)\\
&\qquad\ge 529\max\left\{\|u^{n-1}\|_\infty^4,\ \|u^n\|_\infty^4,\ \|u^{n+1}\|_\infty^4\right\}\ .
\end{aligned} \tag{7.129}$$

As usual, we will prove inductively. Set

$$B=\max\left\{\mathring{E}(u^1)\ .\ E(u^0)\right\}\ ,$$

By Lemma 7.6.1 in previous section, $B\lesssim 1$. We shall prove for every $m\ge 2$,

$$\begin{cases}\mathring{E}(u^m)\le B\cdot(1+\nu)^2\ ,\ \mathring{E}(u^m)\le\mathring{E}(u^{m-1})\ ,\\ \|u^m\|_\infty\le\alpha_B\cdot\left[(\nu^{\frac{1}{2}}+\nu^{-1})\cdot\sqrt{1+\log(A+1)+|\log\nu|+|\log\tau|}+1\right]\ ,\end{cases} \tag{7.130}$$

where $\alpha_B>0$ is the same constant in Lemma 7.7.2.

It suffices to verify the main inequality (7.129):

$$\begin{aligned}
&2(A+1)\left(\frac{1}{\tau}-\frac{1}{2}-C_1-C_1\cdot(\nu^{-2}+\nu)\cdot(1+\log(A+1)+|\log\nu|+|\log\tau|)\right)\\
&>C_2(\nu^{-4}+\nu^2)\cdot\left(1+|\log(A+1)|^2+|\log\nu|^2+|\log\tau|^2\right)+C_2\ .
\end{aligned} \tag{7.131}$$

Case 1: $A = 0$. Then we need

$$\frac{1}{\tau} \gg (\nu^{-4} + \nu^2) \cdot \left(1 + |\log \nu|^2 + |\log \tau|^2\right) + 1 . \tag{7.132}$$

If $0 < \nu < 1$, then we need

$$\tau \ll \frac{\nu^4}{1 + |\log \nu|^2} ; \tag{7.133}$$

If $\nu \geq 1$, then we need

$$\tau \ll \frac{\nu^{-2}}{1 + |\log \nu|^2} . \tag{7.134}$$

Case 2: $A = const \cdot (\nu^2 + \nu^{-4})$. In this case,

$$\frac{1}{\tau} \gg (\nu^{-2} + \nu) \cdot (1 + |\log(A+1)| + |\log \nu| + |\log \tau|) + |\log \nu|^2 + |\log \tau|^2 + 1 . \tag{7.135}$$

If $0 < \nu < 1$, then we need

$$\tau \ll \frac{\nu^2}{1 + |\log \nu|} ; \tag{7.136}$$

If $\nu \geq 1$, then we need

$$\tau \ll \frac{\nu^{-1}}{1 + |\log \nu|} . \tag{7.137}$$

This completes the proof.

Chapter 8

Conclusion & Future Work

Throughout this thesis, we discussed first order and second order semi-implicit Fourier spectral methods on Allen-Cahn equation and fractional Cahn-Hilliard equation in both two dimensional and three dimensional cases. We proved the stability of the first order numerical scheme by adding a stabilizing term $A(u^{n+1}-u^n)$ and $A(-\Delta)^{\alpha}(u^{n+1}-u^n)$ with a large constant A at least of size $O(\nu^{-1}|\log(\nu)|)$ for 2D case and $O(\nu^{-3})$ for 3D case. 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. We proved stability results and L^2 error estimates for two second order schemes as well.

Future work could be done in other gradient cases such as $\mathcal{G} = \Pi_0$, the zero-mass projected Allen-Cahn equation and $\mathcal{G} = -\Delta(id-\Delta)^{-1}$, the normalized Cahn-Hilliard equation could be studied as well.

Bibliography

[1] Stefan Banach. *Sur les opérations dans les ensembles abstraits et leur application aux équations intégralesa.*, Fund. Math., 3 (1922), no.1, pp. 133–181.

[2] John W. Cahn, and John E. Hilliard. *Free Energy of a Nonuniform System. I. Interfacial Free Energy.*, The Journal of Chemical Physics., 28 (1958), no.2, pp. 258-267.

[3] Lennart Carleson. *On convergence and growth of partial sums of Fourier series.*, Acta Math., 116 (1966), no.1, pp. 135–157.

[4] Andrew Christlieb, Jaylan Jones, Keith Promislow, Brian Wetton, and Mark Willoughby. *High accuracy solutions to energy gradient flows from material science models.*, Journal of computational physics., 257 (2014), pp. 193-215.

[5] Charles M. Elliott, and Songmu Zheng. *On the Cahn-Hilliard equation.*, Archive for Rational Mechanics and Analysis., 96 (1986), no.4, pp. 339-357.

[6] Lawrence C. Evans. *Partial Differential Equations: Second Edition* ., (2010), American Mathematical Society Providence, Rhode Island.

[7] Thomas H. Grönwall. *Note on the derivatives with respect to a parameter of the solutions of a system of differential equations*., Ann. of Math., 20 (1919), no.4, pp. 292-296.

[8] Yinnian He, Yunxian Liu, and Tao Tang. *On large time-stepping methods for the Cahn–Hilliard equation*., Applied Numerical Mathematics., 57 (2007), no. 5-7, pp. 616–628.

[9] Dong Li, and Zhonghua Qiao. *On second order semi-implicit fourier spectral methods for 2D Cahn–Hilliard equations*., Journal of Scientific Computing., 70 (2017), pp. 1-41.

[10] Dong Li, and Zhonghua Qiao. *On the stabilization size of semi-implicit Fourier-spectral methods for 3D Cahn-Hilliard equations*., Comm. Math. Sci., 15 (2017), no. 6, pp. 1489-1506.

[11] Dong Li, Zhonghua Qiao, and Tao Tang. *Characterizing the stabilization size for semi-implicit Fourier-spectral method to phase field equations*., SIAM J. Numer. Anal., 54 (2016), no.3, pp. 1653–1681.

[12] Dong Li, Zhonghua Qiao, and Tao Tang. *Gradient bounds for a thin film epitaxy equation*., Journal of Differential Equations., 262 (2017), no.3, pp. 1720-1746.

[13] Louis Nirenberg. *On elliptic partial differential equations*., Ann. Scuola Norm. Sup. Pisa., 13 (1959), no.2, pp. 115-162.

[14] Jie Shen, and Xiaofeng Yang. *Numerical approximations of Allen-Cahn*

and Cahn-Hilliard equations., Discrete Contin. Dyn. Syst. A., 28 (2010), no.4, pp. 1669–1691.

[15] Alan D. Sokal. *A really simple elementary proof of the uniform boundedness theorem.*, The American Mathematical Monthly., 118 (2011), no.5, pp. 450-452.

[16] Terence Tao. *Nonlinear dispersive equations: local and global analysis.*, (2006), American Mathematical Soc.

[17] Chuanju Xu, and Tao Tang. *Stability analysis of large time-stepping methods for epitaxial growth models.*, SIAM J. Numer. Anal., 44 (2006), no.4, pp. 1759–1779.

[18] Jingzhi Zhu, Long-Qing Chen, Jie Shen, and Veena Tikare. *Coarsening kinetics from a variable-mobility Cahn-Hilliard equation: Application of a semi-implicit Fourier spectral method.*, Phys. Rev. E, 60 (1999), no.4, pp. 3564–3572.

[19] [fabiogarofalophd]. *Spectral simulation of the Cahn-Hilliard equation in a two dimensional box.*, [video File] (2011)., Retrieved June 20th, 2017, from https://www.youtube.com/watch?v=od8Rb7awiOQ.

[20] [ogbash]. *Simulation of 2D waves using implicit scheme of Finite Difference Method.*, [video File] (2009)., Retrieved June 19th, 2017, from https://www.youtube.com/watch?v=QKSUaRbgpSM.