## Semi-implicit methods for phase field equations

#### Zhonghua Qiao

Department of Applied Mathematics, The Hong Kong Polytechnic University

Workshop on Numerical Analysis for Partial Differential Equations, Ehime University, June 26, 2018.

#### Collaborators:

Dong Li (HKUST) and Tao Tang (SUSTC)

#### Acknowledgement:

Hong Kong RGC General Research Fund: PolyU 153022/14P NSFC/RGC Joint Research Scheme: N\_HKBU204/12

#### Outline

Introduction

 ${\bf Stabilized\ semi-implicit\ schemes}$ 

Proof of unconditional energy stability for CH

Higher order time-stepping methods

## Outline

#### Introduction

Stabilized semi-implicit schemes

Proof of unconditional energy stability for CH

Higher order time-stepping methods

#### Introduction

In this work we consider two phase field models: the Cahn-Hilliard (CH) equation and the molecular beam epitaxy equation (MBE) with slope selection. The Cahn-Hilliard equation was originally developed to describe phase separation in a two-component system (such as metal alloy). It typically takes the form

$$\begin{cases} \partial_t u = \Delta(-\nu\Delta u + f(u)), & (x,t) \in \Omega \times (0,\infty), \\ u\Big|_{t=0} = u_0, \end{cases}$$
 (1)

where u = u(x, t) is a real-valued function which represents the difference between two concentrations.

In (1) the spatial domain  $\Omega$  is taken to be the usual  $2\pi$ -periodic torus  $\mathbb{T}^2 = \mathbb{R}^2/2\pi\mathbb{Z}^2$ . The free energy term f(u) is given by

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

The parameter  $\nu > 0$  is often called diffusion coefficient. Usually one is interested in the physical regime  $0 < \nu \ll 1$ . The energy functional associated with (1) is

$$E(u) = \int_{\Omega} \left( \frac{1}{2} \nu |\nabla u|^2 + F(u) \right) dx. \tag{3}$$

As is well known, Eq. (1) can be regarded as a gradient flow of E(u) in  $H^{-1}$ .

For smooth solutions to (1), the total mass is conserved:

$$\frac{d}{dt}M(t) \equiv 0, \qquad M(t) = \int_{\Omega} u(x,t)dx. \tag{4}$$

In particular  $M(t) \equiv 0$  if M(0) = 0. Throughout this work we will only consider initial data  $u_0$  with mean zero. On the Fourier side this implies the zero<sup>th</sup> mode  $\hat{u}(0) = 0$ .

One can then define fractional Laplacian  $|\nabla|^s u$  for s < 0, e.g.,  $|\nabla|^s = (-\Delta)^{s/2}$ .

The basic energy identity takes the form

$$\frac{d}{dt}E(u(t)) + \||\nabla|^{-1}\partial_t u\|_2^2 = 0.$$
 (5)

Note that  $\partial_t u$  has mean zero and  $|\nabla|^{-1}\partial_t u$  is well-defined. Alternatively to avoid using  $|\nabla|^{-1}$ , one can rewrite (5) as

$$\frac{d}{dt}E(u(t)) + \int_{\Omega} |\nabla(-\nu\Delta u + f(u))|^2 dx = 0.$$
 (6)

It follows from the energy identity that

$$E(u(t)) \le E(u(s)), \quad \forall \ t \ge s.$$
 (7)

This gives a priori control of  $H^1$ -norm of the solution.

#### Outline

Introduction

Stabilized semi-implicit schemes

Proof of unconditional energy stability for CH

Higher order time-stepping methods

## Semi-implicit scheme

A first order in time semi-implicit scheme of Eq. (1) is as follows:

$$\begin{cases} \frac{u^{n+1} - u^n}{\tau} = -\nu \Delta^2 u^{n+1} + \Delta \Pi_N(f(u^n)), & n \ge 0, \\ u^0 = \Pi_N u_0. \end{cases}$$
 (8)

where  $\tau > 0$  is the time step.

The semi-implicit scheme can generate large truncation errors. As a result smaller time steps are usually required to guarantee accuracy and energy stability.

## A stabilized first-order scheme for the CH model

To resolve this issue, a class of large time-stepping methods were proposed and analyzed. For example, Bertozzi, Ju and Lu 2011, He, Liu and Tang 2007, Shen and Yang 2010, Zhu, Chen, Shen and Tikare 1999.

The basic idea is to add an  $O(\tau)$  stabilizing term to the numerical scheme to alleviate the time step constraint whilst keeping energy stability.

A stabilized first-order scheme for the CH model is given below:

$$\begin{cases} \frac{u^{n+1} - u^n}{\tau} = -\nu \Delta^2 u^{n+1} + A\Delta(u^{n+1} - u^n) + \Delta\Pi_N(f(u^n)), n \ge 0, \\ u^0 = \Pi_N u_0, \end{cases}$$
(9)

where  $\tau > 0$  is the time step, and A > 0 is the coefficient for the  $O(\tau)$  regularization term.

In He, Liu and Tang 2007, it is proved that under a condition on A of the form:

$$A \ge \max_{x \in \Omega} \left\{ \frac{1}{2} |u^n(x)|^2 + \frac{1}{4} |u^{n+1}(x) + u^n(x)|^2 \right\} - \frac{1}{2}, \tag{10}$$

one can obtain energy stability

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

Note that the condition (10) depends nonlinearly on the numerical solution. In other words, it implicitly uses the  $L^{\infty}$ -bound assumption on  $u^n$  in order to make A a controllable constant.

In Shen and Yang 2010, energy stability is proved with truncated nonlinear term. More precisely it is assumed that

$$\max_{u \in \mathbb{R}} |\tilde{f}'(u)| \le L \tag{11}$$

which is what we referred to as the Lipschitz assumption on the nonlinearity. Here  $\tilde{f}(u)$  is a suitable "modification" of the original function f(u).

Roughly speaking, all prior analytical developments are conditional in the sense that either one makes a Lipschitz assumption on the nonlinearity, or one assumes certain a priori  $L^{\infty}$  bounds on the numerical solution. It is very desirable to remove these technical restrictions and establish a more reasonable stability theory.

# Unconditional Energy Stability

D. Li, Z. Qiao and T. Tang, SIAM J. Numer. Anal., 2016.

Theorem 1. [Unconditional energy stability for CH] Consider (9) with  $\nu > 0$  and assume  $u_0 \in H^2(\Omega)$  with mean zero. Denote  $E_0 = E(u_0)$  the initial energy. There exists a constant  $\beta_c > 0$  depending only on  $E_0$  such that if

$$A \ge \beta \cdot (\|u_0\|_{H^2}^2 + \nu^{-1}|\log \nu|^2 + 1), \quad \beta \ge \beta_c,$$
 (12)

then

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

where E is defined by (3).

# A stabilized first-order scheme of MBE model with slope selection

$$\frac{\partial u}{\partial t} = -\nu \Delta^2 u - \nabla \cdot [(1 - |\nabla u|^2) \nabla u], \qquad (\mathbf{x}, t) \in \Omega \times (0, T]$$

A first order stabilized energy-stable scheme:

$$\frac{u^{n+1} - u^n}{\tau} + \nu \Delta^2 u^{n+1} - A \Delta u^{n+1} = -\nabla \cdot [(1 - |\nabla u^n|^2 + A)\nabla u^n]$$
(13)

i.e. an  $O(\tau)$  term is added, where A > 0 is a constant.

Property: If the constant A is sufficiently large, then

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

How large is A?

$$A \ge \max_{x \in \Omega} \{ \frac{1}{2} |\nabla u^n|^2 - \frac{1}{2} + \frac{1}{4} |\nabla u^{n+1} + \nabla u^n|^2 \}. \tag{14}$$

#### Theorem 2.[Unconditional energy stability for MBE]

Consider (13). Assume the initial value  $u_0 \in H^3(\Omega)$  with mean zero. There exists a constant  $\beta_c > 0$  depending only on  $E_0$  such that if

$$A \ge \beta \cdot (\|u_0\|_{H^3}^2 + \nu^{-1}|\log \nu|^2 + 1), \quad \beta \ge \beta_c,$$
 (15)

then

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

Here E is defined by

$$E(u) = \frac{\nu}{2} ||\Delta u||_2^2 + \int_{\Omega} G(\nabla u) dx,$$
 (16)

where  $G(z) = \frac{1}{4}(|z|^2 - 1)^2$  for  $z \in \mathbb{R}^2$ .

#### Outline

Introduction

Stabilized semi-implicit schemes

Proof of unconditional energy stability for CH

Higher order time-stepping methods

We use the following interpolation inequality on  $\mathbb{T}^2$ : for s > 1 and any  $f \in H^s(\mathbb{T}^2)$  with mean zero, we have

$$||f||_{L^{\infty}(\mathbb{T}^2)} \le 1 + C_s ||f||_{\dot{H}^1(\mathbb{T}^2)} \log(3 + ||f||_{H^s(\mathbb{T}^2)}),$$
 (17)

where  $C_s > 0$  is a constant depending only on s.

Rewrite (9) as

$$u^{n+1} = \frac{1 - A\tau\Delta}{1 + \nu\tau\Delta^2 - A\tau\Delta}u^n + \frac{\tau\Delta\Pi_N}{1 + \nu\tau\Delta^2 - A\tau\Delta}f(u^n).$$
 (18)

**Lemma 1** There is an absolute constant  $c_1 > 0$  such that for any  $n \ge 0$ ,

$$||u^{n+1}||_{H^{\frac{3}{2}}(\mathbb{T}^2)} \le c_1 \cdot \left(\frac{A+1}{\nu} + \frac{1}{A\tau}\right) \cdot (E_n+1),$$
 (19)

$$||u^{n+1}||_{\dot{H}^{1}(\mathbb{T}^{2})} \le \left(1 + \frac{1}{A} + \frac{3}{A}||u^{n}||_{\infty}^{2}\right) \cdot ||u^{n}||_{\dot{H}^{1}(\mathbb{T}^{2})},\tag{20}$$

where  $E_n = E(u^n)$ .

#### **Proof:**

First note that on the Fourier side, we have for each  $0 \neq k \in \mathbb{Z}^d$ ,

$$\frac{(1+A\tau|k|^2)|k|^{\frac{3}{2}}}{1+\nu\tau|k|^4+A\tau|k|^2} \lesssim \frac{1}{A\tau} + \frac{A}{\nu},$$
$$\frac{\tau|k|^2 \cdot |k|^{\frac{3}{2}}}{1+\nu\tau|k|^4+A\tau|k|^2} \lesssim \frac{1}{\nu}|k|^{-\frac{1}{2}}.$$

Thus

$$||u^{n+1}||_{H^{\frac{3}{2}}} \lesssim \left(\frac{A}{\nu} + \frac{1}{A\tau}\right) ||u^{n}||_{2} + \frac{1}{\nu} ||\langle\nabla\rangle^{-\frac{1}{2}} (f(u^{n}))||_{2}$$
$$\lesssim \left(\frac{A}{\nu} + \frac{1}{A\tau}\right) ||u^{n}||_{2} + \frac{1}{\nu} ||(u^{n})^{3} - u^{n}||_{\frac{4}{3}}$$
$$\lesssim \left(\frac{A+1}{\nu} + \frac{1}{A\tau}\right) (E_{n} + 1).$$

In the second inequality above we have used the Sobolev imbedding  $\|\langle \nabla \rangle^{-1/2} h\|_{L^2(\mathbb{T}^2)} \lesssim \|h\|_{L^{4/3}(\mathbb{T}^2)}$ .

For  $||u^{n+1}||_{\dot{H}^1}$ , we have

$$||u^{n+1}||_{\dot{H}^{1}} \leq ||u^{n}||_{\dot{H}^{1}} + \frac{1}{A}||(u^{n})^{3} - u^{n}||_{\dot{H}^{1}}$$
$$\leq (1 + \frac{1}{A} + \frac{3}{A}||u^{n}||_{\infty}^{2}) \cdot ||u^{n}||_{\dot{H}^{1}}.$$

This completes the proof of Lemma 1.

#### Lemma 2

For any  $n \geq 0$ ,

$$E_{n+1} - E_n + \left(A + \frac{1}{2} + \sqrt{\frac{2\nu}{\tau}}\right) \|u^{n+1} - u^n\|_2^2$$

$$\leq \|u^{n+1} - u^n\|_2^2 \cdot \left(\|u^n\|_{\infty}^2 + \frac{1}{2}\|u^{n+1}\|_{\infty}^2\right). \tag{21}$$

**Proof:** In this proof we denote by  $(\cdot, \cdot)$  the usual  $L^2$  inner product. Recall

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

Taking the  $L^2$  inner product with  $(-\Delta)^{-1}(u^{n+1}-u^n)$  on both sides, we get

$$\frac{1}{\tau} \||\nabla|^{-1} (u^{n+1} - u^n)\|_2^2 + \frac{\nu}{2} (\|\nabla u^{n+1}\|_2^2 - \|\nabla u^n\|_2^2 + \|\nabla (u^{n+1} - u^n)\|_2^2) 
+ A \|u^{n+1} - u^n\|_2^2 = (\Delta \Pi_N f(u^n), (-\Delta)^{-1} (u^{n+1} - u^n)).$$
(22)

Since all  $u^n$  have Fourier modes supported in  $|k|_{\infty} \leq N$ , we have

$$(\Delta \Pi_N f(u^n), (-\Delta)^{-1} (u^{n+1} - u^n)) = -(f(u^n), u^{n+1} - u^n).$$
 (23)

By the Fundamental Theorem of Calculus, we have (recall f = F')

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

Thus

$$\frac{1}{\tau} \| |\nabla|^{-1} (u^{n+1} - u^n) \|_2^2 + E_{n+1} - E_n + \frac{\nu}{2} \| \nabla (u^{n+1} - u^n) \|_2^2 + (A + \frac{1}{2}) \| u^{n+1} - u^n \|_2^2 
= \frac{1}{4} ((u^{n+1} - u^n)^2, 3(u^n)^2 + (u^{n+1})^2 + 2u^n u^{n+1}) 
\leq \| u^{n+1} - u^n \|_2^2 \cdot \frac{1}{4} (3 \| u^n \|_{\infty}^2 + \| u^{n+1} \|_{\infty}^2 + 2 \| u^n \|_{\infty} \| u^{n+1} \|_{\infty}) 
\leq \| u^{n+1} - u^n \|_2^2 \cdot (\| u^n \|_{\infty}^2 + \frac{1}{2} \| u^{n+1} \|_{\infty}^2).$$
(24)

Finally observe

$$\begin{split} &\frac{1}{\tau} \||\nabla|^{-1} (u^{n+1} - u^n)\|_2^2 + \frac{\nu}{2} \|\nabla(u^{n+1} - u^n)\|_2^2 \\ &\geq \sqrt{\frac{2\nu}{\tau}} \||\nabla|^{-1} (u^{n+1} - u^n)\|_2 \|\nabla(u^{n+1} - u^n)\|_2 \geq \sqrt{\frac{2\nu}{\tau}} \|u^{n+1} - u^n\|_2^2. \end{split}$$

The desired inequality then follows easily.

#### Proof of Theorem 1

We inductively prove for all  $n \geq 1$ ,

$$E_n \le E_0, \tag{25}$$

$$||u^n||_{H^{\frac{3}{2}}} \le c_1 \cdot \left(\frac{A+1}{\nu} + \frac{1}{A\tau}\right) \cdot (E_0 + 1),$$
 (26)

where  $c_1 > 0$  is the same absolute constant in Lemma 1. We proceed in two steps.

In Step 1 below, we first verify that if the statement holds for some  $n \geq 1$ , then it holds for n + 1.

In Step 2, we check the "base" case, namely for n=1 the statement holds.

Step 1: the induction step  $n \Rightarrow n+1$ . Assume the induction holds for some  $n \geq 1$ . We now verify the statement for n+1. By Lemma 1, we have

$$||u^{n+1}||_{H^{\frac{3}{2}}} \le c_1 \cdot \left(\frac{A+1}{\nu} + \frac{1}{A\tau}\right) \cdot (E_n+1) \le c_1 \cdot \left(\frac{A+1}{\nu} + \frac{1}{A\tau}\right) \cdot (E_0+1).$$

Thus we only need to check  $E_{n+1} \leq E_0$ . In fact we shall show  $E_{n+1} \leq E_n$ .

By Lemma 2, we only need to show the inequality

$$A + \frac{1}{2} + \sqrt{\frac{2\nu}{\tau}} \ge \|u^n\|_{\infty}^2 + \frac{1}{2} \|u^{n+1}\|_{\infty}^2.$$
 (27)

We shall use the log-interpolation inequality (see (17) and choose  $s = \frac{3}{2}$ ) for any f with mean zero:

$$||f||_{L^{\infty}(\mathbb{T}^2)} \le 1 + d_1 \cdot ||f||_{\dot{H}^1(\mathbb{T}^2)} \cdot \log(||f||_{\dot{H}^{\frac{3}{2}}(\mathbb{T}^2)} + 3),$$
 (28)

where  $d_1 > 0$  is an absolute constant. In the rest of this proof, to ease the notation we shall use  $X \lesssim_{E_0} Y$  to denote  $X \leq C_{E_0} Y$  where  $C_{E_0}$  is a constant depending only on  $E_0$ . Clearly

$$||u^{n}||_{\infty} \leq 1 + d_{1}||u^{n}||_{\dot{H}^{1}} \log\left(||u^{n}||_{\dot{H}^{\frac{3}{2}}} + 3\right)$$

$$\leq 1 + d_{1} \cdot \sqrt{\frac{2E_{0}}{\nu}} \cdot \log\left(3 + c_{1} \cdot \left(\frac{A+1}{\nu} + \frac{1}{A\tau}\right) \cdot (E_{0}+1)\right)$$

$$\lesssim_{E_{0}} \underbrace{\nu^{-\frac{1}{2}}(1 + \log A + |\log \nu|)}_{=:m_{0}} + \nu^{-\frac{1}{2}} |\log(2 + \frac{1}{\tau})| + 1. \tag{29}$$

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

By (28) and Lemma 1, we have (below in the third inequality we drop 1/A since  $A \ge 1$ )

$$||u^{n+1}||_{\infty} \lesssim 1 + ||u^{n+1}||_{\dot{H}^{1}} \log \left( ||u^{n+1}||_{\dot{H}^{\frac{3}{2}}} + 3 \right)$$

$$\lesssim 1 + \left( 1 + \frac{1}{A} + \frac{||u^{n}||_{\infty}^{2}}{A} \right) ||u^{n}||_{\dot{H}^{1}} \log \left( ||u^{n+1}||_{\dot{H}^{\frac{3}{2}}} + 3 \right)$$

$$\lesssim 1 + \left( 1 + \frac{||u^{n}||_{\infty}^{2}}{A} \right) ||u^{n}||_{\dot{H}^{1}} \log \left( ||u^{n+1}||_{\dot{H}^{\frac{3}{2}}} + 3 \right)$$

$$\lesssim_{E_{0}} 1 + \left( 1 + \frac{m_{0}^{2} + \nu^{-1} |\log \tau|^{2}}{A} \right) \cdot \left( m_{0} + \nu^{-\frac{1}{2}} |\log \tau| \right)$$

$$\lesssim_{E_{0}} 1 + m_{0} + \nu^{-\frac{1}{2}} |\log \tau| + \frac{m_{0}^{3} + \nu^{-\frac{3}{2}} |\log \tau|^{3}}{A}$$

$$\lesssim_{E_{0}} m_{0} + \frac{m_{0}^{3}}{A} + 1 + \nu^{-\frac{3}{2}} |\log \tau|^{3}. \tag{30}$$

Therefore

$$||u^n||_{\infty}^2 + ||u^{n+1}||_{\infty}^2 \lesssim_{E_0} \left(m_0 + \frac{m_0^3}{A}\right)^2 + 1 + \nu^{-3}|\log \tau|^6.$$

Therefore to show the inequality (27), it suffices to prove

$$A + \sqrt{\frac{\nu}{\tau}} \ge C_{E_0} \cdot \left( \left( m_0 + \frac{m_0^3}{A} \right)^2 + 1 + \nu^{-3} |\log \tau|^6 \right), \quad (31)$$

where

$$m_0 = \nu^{-\frac{1}{2}} (1 + \log A + |\log \nu|).$$

Now we discuss two cases.

Case 1:  $\sqrt{\frac{\nu}{\tau}} \ge C_{E_0} \nu^{-3} |\log \tau|^6$ . In this case we choose A such that

$$A \gg_{E_0} m_0^2 = \nu^{-1} (1 + \log A + |\log \nu|)^2.$$

Clearly for  $\nu \gtrsim 1$ , we just need to choose  $A \gg_{E_0} 1$ . On the other hand, for  $0 < \nu \ll 1$ , it suffices to take

$$A = \beta \cdot \nu^{-1} |\log \nu|^2,$$

with  $\beta$  sufficiently large depending only on  $E_0$ . Thus in both cases if we take

$$A = \beta \cdot \max\{\nu^{-1} |\log \nu|^2, 1\},\,$$

with  $\beta \gg_{E_0} 1$ , then (31) holds.

Case 2:  $\sqrt{\frac{\nu}{\tau}} \leq C_{E_0} \nu^{-3} |\log \tau|^6$ . In this case we have

$$|\log \tau| \lesssim_{E_0} 1 + |\log \nu|.$$

In this case we will not prove (31) but prove (27) directly. We first go back to the bound on  $||u^n||_{\infty}$ . Easy to check that

$$||u^n||_{\infty} \lesssim_{E_0} m_0,$$
  
 $||u^{n+1}||_{\infty} \lesssim_{E_0} \left(1 + \frac{m_0^2}{A}\right) m_0.$ 

The needed inequality on A then takes the form

$$A \ge C_{E_0} \cdot \left(1 + m_0 + \frac{m_0^3}{A}\right)^2.$$

Again we only need to choose A such that  $A \gg_{E_0} m_0^2$ . The same choice of A as in Case 1 (with  $\beta$  larger if necessary) works. Concluding from both cases, we have proved the inequality (27) holds. This completes the induction step for  $n \Rightarrow n+1$ .

Step 2: verification of the base step n = 1. By Lemma 1 we have

$$||u^1||_{H^{\frac{3}{2}}} \le c_1 \cdot \left(\frac{A+1}{\nu} + \frac{1}{A\tau}\right) \cdot (E_0 + 1).$$

Therefore we only need to check  $E_1 \leq E_0$ . This amounts to checking the inequality

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

By Lemma 1,

$$||u^{1}||_{\dot{H}^{1}} \leq \left(1 + \frac{1}{A} + \frac{3}{A} ||\Pi_{N} u_{0}||_{\infty}^{2}\right) \cdot ||u_{0}||_{\dot{H}^{1}}$$
$$\leq \left(1 + \frac{1}{A} + \frac{3}{A} ||\Pi_{N} u_{0}||_{\infty}^{2}\right) \cdot \sqrt{\frac{2E_{0}}{\nu}}.$$

#### Therefore

$$||u^{1}||_{\infty} \lesssim 1 + ||u^{1}||_{\dot{H}^{1}} \log(||u^{1}||_{\dot{H}^{\frac{3}{2}}} + 3)$$

$$\lesssim 1 + (1 + \frac{1}{A} + \frac{3}{A} ||\Pi_{N} u_{0}||_{\infty}^{2}) \cdot \sqrt{\frac{2E_{0}}{\nu}} \cdot \log(3 + c_{1}(\frac{A+1}{\nu} + \frac{1}{A\tau})(E_{0} + 1))$$

$$\lesssim_{E_{0}} 1 + (1 + \frac{1}{A} + \frac{3}{A} ||\Pi_{N} u_{0}||_{\infty}^{2}) \cdot \nu^{-\frac{1}{2}} \cdot (1 + \log A + |\log \nu| + |\log \tau|).$$

Thus we need to choose A such that

$$A + \frac{1}{2} + \sqrt{\frac{2\nu}{\tau}} \ge \|\Pi_N u_0\|_{\infty}^2 + 1$$
$$+ \tilde{C}_{E_0} \cdot (1 + \frac{1}{A} + \frac{3}{A} \|\Pi_N u_0\|_{\infty}^2)^2 \cdot \nu^{-1} \cdot (1 + \log A + |\log \nu| + |\log \tau|)^2,$$

where  $\tilde{C}_{E_0}$  is a constant depending only on  $E_0$ .

By Sobolev embedding, we have

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

Thus it suffices to take A such that

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

This completes the proof of Theorem 1.

#### Remarks

In this work we considered stabilized semi-implicit schemes for the phase field models such as the Cahn-Hilliard equation and the thin film equation with fourth order dissipation.

We analyzed the representative case (see (9) and (13)) which is first order in time and Fourier-spectral in space, with a stabilization  $O(\Delta t)$  term of the form

$$A\Delta(u^{n+1}-u^n).$$

For A sufficiently large  $(A \ge O(\nu^{-1}|\log \nu|^2))$ , we proved unconditional energy stability independent of the time step.

#### Further remarks

- ➤ Similar results hold for MBE (settles the open problems in Xu-Tang '06)
- ▶ 3D Cahn-Hilliard case settled recently (Li-Qiao '17, CMS)
- ▶ Difficulty in 3D:  $H^1$ -supercritical

## 3D CH: Li-Qiao '17, CMS

**Thm**: [Unconditional energy stability for 3D CH] Consider stabilized semi-implicit with  $\nu > 0$ . Assume  $u_0 \in H^2(\Omega)$  with mean zero. Denote  $E_0 = E(u_0)$  the initial energy. There exists a constant  $\beta_c > 0$  depending only on  $E_0$  such that if

$$A \ge \beta \cdot (\|u_0\|_{H^2}^2 + \nu^{-3} + 1), \quad \beta \ge \beta_c,$$

then

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

where

$$E(u) = \int_{\Omega} \left( \frac{1}{2} \nu |\nabla u|^2 + \frac{1}{4} (u^2 - 1)^2 \right) dx.$$

#### Outline

Introduction

Stabilized semi-implicit schemes

Proof of unconditional energy stability for CH

Higher order time-stepping methods

## Higher order time-stepping methods

The situation with higher order in time methods are far more complex since it is known that energy is only approximately preserved over moderately long time intervals. This brings the question of how to design robust stabilized high order in time methods with good energy conservation. A further problem is to investigate the issue of conditional or unconditional energy stability, characterize the stabilization parameter and identify the stability region in various situations.

## Second order: Xu-Tang '06

Assumes a priori  $L^{\infty}$  bounds on the numerical solution.

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

Xu and Tang proved

$$\tilde{E}^{n+1} \le \tilde{E}^n + O(\Delta t^2),$$

and

$$E(h^n) < E(h^1) + O(1)\Delta t,$$

where the O(1) term is given by

$$O(1) = \left\| \frac{h^1 - h^0}{\Delta t} \right\|_2^2 + \frac{A}{2} \Delta t \left\| \frac{\nabla (h^1 - h^0)}{\Delta t} \right\|_2^2 + \sum_{i=0}^{n-1} \Delta t \left\| \frac{\nabla (h^i - h^{i-1})}{\Delta t} \right\|_2^2.$$

## Li-Qiao '17, JSC

**Thm**: For any  $\theta_0 > 0$  the following holds: Let  $\nu > 0$ ,  $\tau > 0$  satisfy

$$\sqrt{\frac{2\nu}{\tau}} \ge \frac{1}{2} + \theta_0.$$

Let  $u_0 \in H^6(\mathbb{T}^2)$  with mean zero. There exists a constant  $\beta_c > 0$  depending only  $(\theta_0, E(u_0), ||u_0||_{H^6})$  such that if

$$A \ge \beta \cdot (1 + \nu^{-4} (1 + \nu)^6 |\log \nu|^2), \quad \beta \ge \beta_c,$$

then

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

$$\leq E(u^n) + \frac{1}{4\tau} \||\nabla|^{-1} (u^n - u^{n-1})\|_2^2 + \frac{A+1}{2} \|u^n - u^{n-1}\|_2^2, \quad \forall n \geq 1.$$

▶ Rem: roughly  $\tau < 8\nu$  suffices for stability!

#### Case A=0

thm[Case A = 0] Set A = 0. Let  $u_0 \in H^6(\mathbb{T}^2)$  with mean zero. There exist constants  $C_1 > 0$ ,  $C_2 > 0$  depending only on  $(E(u_0), ||u_0||_{H^6})$  such that if

$$\tau \le \begin{cases} C_1 \frac{\nu^9}{1 + |\log \nu|^4}, & \text{when } 0 < \nu \le 1, \\ C_2 \frac{\nu^{-3}}{1 + |\log \nu|^4}, & \text{when } \nu > 1, \end{cases}$$

then for all  $n \geq 1$ ,

$$\begin{split} &E(u^{n+1}) + \frac{1}{4\tau} \||\nabla|^{-1}(u^{n+1} - u^n)\|_2^2 + \frac{1}{2} \|u^{n+1} - u^n\|_2^2 \\ &\leq E(u^n) + \frac{1}{4\tau} \||\nabla|^{-1}(u^n - u^{n-1})\|_2^2 + \frac{1}{2} \|u^n - u^{n-1}\|_2^2. \end{split}$$

#### Further remarks

▶ Recently Song-Shu' 18 JSC, made a remarkable extension to a second-order in time IMEX Local discontinuous Galerkin method and proved unconditional energy stability with

$$A \ge O(\epsilon^{-36} |\log \epsilon|^8).$$

**.**..

# Thank You!