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A stable and conservative finite difference scheme for the Cahn-Hilliard equation*

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Summary. We propose a stable and conservative finite difference scheme to solve numerically the Cahn-Hilliard equation which describes a phase separation phenomenon. Numerical solutions to the equation is hard to obtain because it is a nonlinear and nearly ill-posed problem. We design a new difference scheme based on a general strategy proposed recently by Furihata and Mori. The new scheme inherits characteristic properties, the conservation of mass and the decrease of the total energy, from the equation. The decrease of the total energy implies boundedness of discretized Sobolev norm of the solution. This in turn implies, by discretized Sobolev's lemma, boundedness of max norm of the solution, and hence the stability of the solution. An error estimate for the solution is obtained and the order is $O((\Delta x)^2 + (\Delta t)^2)$. Numerical examples demonstrate the effectiveness of the proposed scheme.

Mathematics Subject Classification (1991): 65M06

1. Introduction

The Cahn-Hilliard equation [1]

$$(1) \qquad \frac{\partial u}{\partial t} = \frac{\partial^2}{\partial x^2}\frac{\delta G}{\delta u}, \qquad x \in (0, L) \subset \mathbf{R}, 0 < t$$

$$(2) \qquad \frac{\delta G}{\delta u} = pu + ru^3 + q\,\frac{\partial^2 u}{\partial x^2},$$

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where p, q and r are constants with $p < 0$, $q < 0$ and $0 < r$ is a model equation to describe a phase separation phenomenon called the spinodal decomposition. The decomposition phenomenon occurs when binary solutions such as alloys, polymer mixtures are cooled down [20]. Here $u(x,t)$ is a distribution function of the concentration of one component of the binary mixture. Boundary conditions for the equation are

$$\frac{\partial u}{\partial x}\bigg|_{x=0} = \frac{\partial u}{\partial x}\bigg|_{x=L} = 0, \tag{3}$$

$$\frac{\partial}{\partial x}\frac{\delta G}{\delta u}\bigg|_{x=0} = \frac{\partial}{\partial x}\frac{\delta G}{\delta u}\bigg|_{x=L} = 0. \tag{4}$$

The functional G means a local free energy called the Ginzburg–Landau free energy. The notation $\dfrac{\delta G}{\delta u}$ defined by (2) is consistent with the variational derivative of

$$G(u(x,t)) = \frac{1}{2}pu^2 + \frac{1}{4}ru^4 - \frac{1}{2}q(\frac{\partial u}{\partial x})^2 \tag{5}$$

with respect to $u(x,t)$. In fact, the relation between G of (5) and $\dfrac{\delta G}{\delta u}$ of (2)

$$\lim_{\epsilon\to 0}\frac{1}{\epsilon}\left\{\int_0^L G(u+\epsilon v)\ dx - \int_0^L G(u)\ dx\right\} = \int_0^L v\frac{\delta G}{\delta u}\ dx \tag{6}$$

is derived through integration by parts under the boundary condition (3).

It is known that the solution $u(x,t)$ of the Cahn-Hilliard equation possesses the properties that the total mass $\int_0^L u(x,t)\ dx$ is conserved and that the total free energy $\int_0^L G(u(x,t))\ dx$ decreases with time. Steady state solutions of the Cahn-Hilliard equation were studied by Carr, Gurtin and Slemrod [2] and Novick-Cohen and Segel [18]. Elliott and Zheng [8] proved that if the initial data $u(x,0)$ belongs to $H_E^2(\Omega) \equiv \left\{ f \in H^2(\Omega);\ \dfrac{\partial f}{\partial \nu} = 0 \text{ on } \partial\Omega \right\}$ then the Cahn-Hilliard equation has a unique solution $u(x,t) \in H^{4,1}(\Omega \times (0,T))$ where Ω is a bounded domain in $\mathbf{R}^n (n \le 3)$ and $\dfrac{\partial}{\partial \nu}$ is the outward normal derivative to $\partial\Omega$. In spite of these studies, there remains a lot to be investigated.

Since we cannot hope for analytical solutions, we must resort to numerical methods to solve the Cahn-Hilliard equation. Even numerical solutions are not easy to obtain. For example, conventional difference schemes without careful choice of parameters are often unstable. This is partly because the dependency of the solution on the initial data $u(x,0)$ is very sensitive and partly because the linear stability analysis renders meaningless results. Numerical methods for this equation have been considered in several papers. Langer, Bar-on and Milners made a pioneer study [16] based on a simple ansatz for two-point distribution function. Some kinds of finite element schemes were studied with mathematical rigor by Elliott and Sonqmu [8], Elliott and French [4], Elliott, French and Milner [6], Elliott and French [5] and Elliott and Larsson [7]. Du and Nicolaides [3] proposed an interesting finite element scheme and a finite difference scheme with the property that the total energy decreases with time under the Dirichlet boundary conditions. Furihata, Onda and Mori [12] proposed a practical nonlinear stability analysis method for finite difference schemes and applied it to the Cahn-Hilliard equation. Sun [19] proposed an interesting linearized finite difference scheme which is uniquely solvable and convergent with the convergence rate of order two in a discrete L_2-norm.

The conventional strategy to obtain numerical solutions by the finite difference method is to choose appropriate mesh size based on the linear stability analysis for difference schemes. This conventional strategy, however, does not work well for the Cahn-Hilliard equation. In fact there are not many successful studies on the finite difference method for this equation. Therefore we should look for an alternative strategy. The alternative strategy, proposed for general problems in [10] by Furihata and Mori, is to design such schemes that preserve characteristic properties (e.g. mass conservation law) inherent in the Cahn-Hilliard equation. We also expect that if the designed schemes preserve characteristic properties of the original equation then the schemes are numerically stable.

It can be said that this alternative strategy was implicit in some previous works, including Du and Nicolaides [3], Greenspan [13], Hirota [14], Ward [21] and Li and Vu-Quoc [17]. Greenspan [13] discussed difference schemes for conservative initial value problem $\ddot{x} = f(x)$, $x(0) = \alpha$, $\dot{x}(0) = \beta$. Hirota [14] discretized the Hamiltonian form. Ward [21] discussed how to discretize integrable partial differential equations. Li and Vu-Quoc [17] obtained some finite difference algorithms which possess a conserved quantity to the nonlinear Klein-Gordon equation. The formalism of Li and Vu-Quoc is similar to our formalism in this paper.

In this paper we design a new difference scheme for the Cahn-Hilliard equation based on the alternative strategy. The proposed difference scheme inherits the properties of

1. the conservation of mass, and
2. the decrease of the total energy,

from the Cahn-Hilliard equation. We define $U_k^{(n)}$ $(k = -2, -1, 0, \cdots, N, N+1, N+2; n = 0, 1, 2, \cdots)$ to be the approximation to $u(x,t)$ at location $x = k\Delta x$ and time $t = n\Delta t$, where Δx is a space mesh size and Δt is a time mesh size. The concrete form of the proposed difference scheme for (1)–(2) is

$$\frac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t} = \delta_k^{\langle 2\rangle} \left(\frac{\delta G_d}{\delta U}\right)_k^{(n+\frac{1}{2})}, \qquad k = 0, 1, \cdots, N;\ n = 0, 1, \cdots, \tag{7}$$

$$\begin{aligned}\left(\frac{\delta G_d}{\delta U}\right)_k^{(n+\frac{1}{2})} = {} & p\left\{\frac{U_k^{(n+1)} + U_k^{(n)}}{2}\right\} \\ & + r\left\{\frac{(U_k^{(n+1)})^3 + (U_k^{(n+1)})^2 U_k^{(n)} + U_k^{(n+1)}(U_k^{(n)})^2 + (U_k^{(n)})^3}{4}\right\} \\ & + q\,\delta_k^{\langle 2\rangle}\left\{\frac{U_k^{(n+1)} + U_k^{(n)}}{2}\right\},\end{aligned} \tag{8}$$

where $N = L/\Delta x$ and $\delta_k^{\langle 2\rangle}$ is a second-order difference operator defined by

$$\delta_k^{\langle 2\rangle} f_k \stackrel{\text{def}}{=} \frac{1}{(\Delta x)^2}\left(f_{k-1} - 2f_k + f_{k+1}\right). \tag{9}$$

The discrete boundary conditions are

$$\left.\delta_k^{\langle 1\rangle} U_k^{(n)}\right|_{k=0} = \left.\delta_k^{\langle 1\rangle} U_k^{(n)}\right|_{k=N} = 0, \tag{10}$$

$$\left.\delta_k^{\langle 1\rangle}\left(\frac{\delta G_d}{\delta U}\right)_k^{(n+\frac{1}{2})}\right|_{k=0} = \left.\delta_k^{\langle 1\rangle}\left(\frac{\delta G_d}{\delta U}\right)_k^{(n+\frac{1}{2})}\right|_{k=N} = 0, \tag{11}$$

where $\delta_k^{\langle 1\rangle}$ is a first-order difference operator defined by

$$\delta_k^{\langle 1\rangle} f_k \stackrel{\text{def}}{=} \frac{1}{2\Delta x}\left(f_{k+1} - f_{k-1}\right). \tag{12}$$

Note that the discrete boundary conditions (10) and (11) equal

$$U_{-1}^{(n)} = U_1^{(n)},\ U_{N+1}^{(n)} = U_{N-1}^{(n)}, \tag{13}$$

$$U_{-2}^{(n)} = U_2^{(n)},\ U_{N+2}^{(n)} = U_{N-2}^{(n)}. \tag{14}$$

Besides preserving the Properties 1 and 2, if the proposed scheme has a solution subject to an initial value, there exists a constant C, dependent on the initial value but independent of Δx, Δt, and n, such that

$$\max_{0\le k\le N}\left|U_k^{(n)}\right| < C. \tag{15}$$

The proof for (15) consists of two lemmas. The first lemma shows that the decrease of the total energy implies the boundedness of the discrete Sobolev norm of a numerical solution. The second lemma (the discrete Sobolev lemma) shows that the boundedness of the discrete Sobolev norm of a numerical solution yields a bound on the maximum norm of a numerical solution.

It is proven, through the fixed-point theorem for a contraction mapping, that the proposed scheme has a unique solution under a condition for Δt and Δx. It is also proven that the numerical solution by the proposed scheme converges to the true solution of the Cahn-Hilliard equation if the true solution belongs to $C^6([0,L] \times [0,T])$.

Finally some numerical examples are shown to demonstrate the effectiveness of the proposed difference scheme. It is observed that the proposed difference scheme is stable even when Δt is 1000 times as large as the stability upper limit of Δt in the conventional schemes reported in [12].

2. Properties preserved by the proposed scheme

We first note two well-known properties [8] of the solution of the Cahn-Hilliard equation, which are mentioned in the introduction. Namely,

$$\int_0^L u(x,t)\, dx = \int_0^L u(x,0)\, dx, \tag{16}$$

$$\frac{d}{dt}\int_0^L G(u(x,t))\, dx \le 0. \tag{17}$$

We call (16) the conservation of mass and (17) the decrease of the total energy. The conservation of mass (16) can be shown easily as follows:

$$\begin{aligned} \frac{d}{dt}\int_0^L u(x,t)\, dx &= \int_0^L \frac{\partial u(x,t)}{\partial t}\, dx = \int_0^L \frac{\partial^2}{\partial x^2}\frac{\delta G}{\delta u}\, dx \\ &= \left[\frac{\partial}{\partial x}\frac{\delta G}{\delta u}\right]_{x=0}^L = 0. \end{aligned} \tag{18}$$

The decrease of the total energy (17) can be shown similarly:

$$\begin{aligned} \frac{d}{dt}\int_0^L G(u(x,t))\, dx &= \int_0^L \frac{\delta G}{\delta u}\frac{\partial u}{\partial t}\, dx \\ &= -\int_0^L \left\{\frac{\partial}{\partial x}\frac{\delta G}{\delta u}\right\}^2 dx \le 0. \end{aligned} \tag{19}$$

Remark 1. From (17) we see that we can employ the total of energy as a Lyapunov functional of the system (see Du and Nicolaides [3]).

The main purpose of this section is to show that the proposed scheme (8) has properties corresponding to (16) and (17), i.e.

$$\sum_{k=0}^{N}{}'' \, U_k^{(n)} \varDelta x = \sum_{k=0}^{N}{}'' \, U_k^{(0)} \varDelta x, \tag{20}$$

$$\sum_{k=0}^{N}{}'' \, G_d\left(U_k^{(n+1)}\right) \varDelta x - \sum_{k=0}^{N}{}'' \, G_d\left(U_k^{(n)}\right) \varDelta x \leq 0. \tag{21}$$

Here $\displaystyle\sum_{k=0}^{N}{}''$ is a summation operator defined by

$$\sum_{k=0}^{N}{}'' \, f_k \stackrel{\text{def}}{=} \frac{1}{2} f_0 + \sum_{k=1}^{N-1} f_k + \frac{1}{2} f_N, \tag{22}$$

and

$$G_d(U_k) \stackrel{\text{def}}{=} \frac{1}{2} p U_k^2 + \frac{1}{4} r U_k^4 - \frac{1}{2} q \frac{(\delta_k^+ U_k)^2 + (\delta_k^- U_k)^2}{2} \tag{23}$$

is the discrete local free energy, where δ_k^+ is the forward difference operator defined by $\delta_k^+ f_k = \dfrac{1}{\varDelta x}(f_{k+1} - f_k)$ and δ_k^- is the backward difference operator defined by $\delta_k^- f_k = \dfrac{1}{\varDelta x}(f_k - f_{k-1})$. The relation between G_d of (23) and $\left(\dfrac{\delta G_d}{\delta U}\right)_k^{(n+\frac{1}{2})}$ of (9) is given by

$$\begin{aligned}
&\sum_{k=0}^{N}{}'' \, G_d\left(U_k^{(n+1)}\right) \varDelta x - \sum_{k=0}^{N}{}'' \, G_d\left(U_k^{(n)}\right) \varDelta x \\
&= \sum_{k=0}^{N}{}'' \left(U_k^{(n+1)} - U_k^{(n)}\right) \left(\frac{\delta G_d}{\delta U}\right)_k^{(n+\frac{1}{2})} \varDelta x \\
&\quad - \frac{q}{2} \Big[(s_k^{\langle 1 \rangle} U_k^{(n+1)} - U_k^{(n)}) \delta_k^{\langle 1 \rangle} U_k^{(n+1)} \\
&\quad + (U_k^{(n+1)} - s_k^{\langle 1 \rangle} U_k^{(n)}) \delta_k^{\langle 1 \rangle} U_k^{(n)} \Big]_{k=0}^{N} \qquad \text{by (26) below} \\
&= \sum_{k=0}^{N}{}'' \left(U_k^{(n+1)} - U_k^{(n)}\right) \left(\frac{\delta G_d}{\delta U}\right)_k^{(n+\frac{1}{2})} \varDelta x \qquad \text{by (10),}
\end{aligned} \tag{24}$$

where $s_k^{\langle 1 \rangle}$ is an averaging operator defined by

$$s_k^{\langle 1 \rangle} f_k \stackrel{\text{def}}{=} \frac{f_{k+1} + f_{k-1}}{2}. \tag{25}$$

In the derivation above we used the following general identity (summation by parts)

$$
\begin{aligned}
(26)\quad & \sum_{k=0}^{N}{}'' \left\{ \frac{(\delta_k^+ f_k)^2 + (\delta_k^- f_k)^2}{2} \right\} \Delta x - \sum_{k=0}^{N}{}'' \left\{ \frac{(\delta_k^+ g_k)^2 + (\delta_k^- g_k)^2}{2} \right\} \Delta x \\
&= \left[(s_k^{\langle 1 \rangle} f_k - g_k) \delta_k^{\langle 1 \rangle} f_k + (f_k - s_k^{\langle 1 \rangle} g_k) \delta_k^{\langle 1 \rangle} g_k \right]_{k=0}^{N} \\
&\quad -2 \sum_{k=0}^{N}{}'' \left\{ (f_k - g_k)\, \delta_k^{\langle 2 \rangle} \left(\frac{f_k + g_k}{2} \right) \right\} \Delta x.
\end{aligned}
$$

We call (20) the discrete conservation of mass and (21) the discrete decrease of the total energy. The discrete conservation of mass (20) can be shown as

$$
\begin{aligned}
(27)\quad & \frac{1}{\Delta t} \left\{ \sum_{k=0}^{N}{}'' U_k^{(n+1)} \Delta x - \sum_{k=0}^{N}{}'' U_k^{(n)} \Delta x \right\} \\
&= \sum_{k=0}^{N}{}'' \left\{ \frac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t} \right\} \Delta x \\
&= \sum_{k=0}^{N}{}'' \left\{ \delta_k^{\langle 2 \rangle} \left(\frac{\delta G_d}{\delta U} \right)_k^{(n+\frac{1}{2})} \right\} \Delta x \\
&= \left[\delta_k^{\langle 1 \rangle} \left(\frac{\delta G_d}{\delta U} \right)_k^{(n+\frac{1}{2})} \right]_{k=0}^{N} \\
&= 0
\end{aligned}
$$

since

$$
(28)\quad \sum_{k=0}^{N}{}'' \left\{ \delta_k^{\langle 2 \rangle} f_k \right\} \Delta x = \left[\delta_k^{\langle 1 \rangle} f_k \right]_{k=0}^{N}
$$

holds true in general.

The decrease of the discrete total energy (21) can be shown as

$$
\begin{aligned}
(29)\quad & \frac{1}{\Delta t} \left\{ \sum_{k=0}^{N}{}'' G_d \left(U_k^{(n+1)} \right) \Delta x - \sum_{k=0}^{N}{}'' G_d \left(U_k^{(n)} \right) \Delta x \right\} \\
&= \sum_{k=0}^{N}{}'' \left\{ \left(\frac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t} \right) \left(\frac{\delta G_d}{\delta U} \right)_k^{(n+\frac{1}{2})} \right\} \Delta x \qquad \text{by (25)} \\
&= \sum_{k=0}^{N}{}'' \left\{ \left(\frac{\delta G_d}{\delta U} \right)_k^{(n+\frac{1}{2})} \delta_k^{\langle 2 \rangle} \left(\frac{\delta G_d}{\delta U} \right)_k^{(n+\frac{1}{2})} \right\} \Delta x \qquad \text{by (8)}
\end{aligned}
$$

$$
\begin{aligned}
&= \left[s_k^{\langle 1 \rangle} \left(\frac{\delta G_d}{\delta U} \right)_k^{(n+\frac{1}{2})} \delta_k^{\langle 1 \rangle} \left(\frac{\delta G_d}{\delta U} \right)_k^{(n+\frac{1}{2})} \right]_{k=0}^{N} \\
&\quad - \frac{1}{2} \sum_{k=0}^{N}{}'' \left[\left\{ \delta_k^{+} \left(\frac{\delta G_d}{\delta U} \right)_k^{(n+\frac{1}{2})} \right\}^2 + \left\{ \delta_k^{-} \left(\frac{\delta G_d}{\delta U} \right)_k^{(n+\frac{1}{2})} \right\}^2 \right] \Delta x \\
&= - \frac{1}{2} \sum_{k=0}^{N}{}'' \left[\left\{ \delta_k^{+} \left(\frac{\delta G_d}{\delta U} \right)_k^{(n+\frac{1}{2})} \right\}^2 + \left\{ \delta_k^{-} \left(\frac{\delta G_d}{\delta U} \right)_k^{(n+\frac{1}{2})} \right\}^2 \right] \Delta x \\
&\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \text{by (11)} \\
&\leq 0.
\end{aligned}
$$

In the derivation above we used summation by parts like (26).

In Sect. 3 the stability of the proposed difference scheme is derived from the decrease of the discrete total energy.

Remark 2. The lengthy calculations like (29) could be put into neater forms by introducing new discrete operators [9] rather than by using the conventional ones such as $\delta_k^{\langle 1 \rangle}$, $\delta_k^{\langle 2 \rangle}$ and $s_k^{\langle 1 \rangle}$. In this paper, however, we stick to the conventional expressions for readers' convenience.

3. Stability of the proposed scheme

The purpose of this section is to show that, if the proposed scheme has a solution, it is bounded in the maximum norm. The proof consists of two lemmas. The first lemma shows that the discrete Sobolev norm of the solution of the proposed difference scheme is bounded. The second (the discrete Sobolev lemma) shows that if the discrete Sobolev norm of a discrete function is bounded, the maximum norm of the function is bounded.

Lemma 1.

$$
\text{(30)} \quad \left\| U^{(n)} \right\|_{\text{d-}(1,2)}^2 \leq \frac{1}{\min(-p, -\frac{1}{2}q)} \left\{ \sum_{k=0}^{N}{}'' G_d \left(U_k^{(0)} \right) \Delta x + \frac{9}{4} \frac{p^2}{r} L \right\},
$$

where $\|\bullet\|_{\text{d-}(1,2)}$ *is a discrete first-order Sobolev–Hilbert norm which is defined as*

$$
\text{(31)} \qquad \|f\|_{\text{d-}(1,2)}^2 \stackrel{\text{def}}{=} \sum_{k=0}^{N}{}'' (f_k)^2 \Delta x + \sum_{k=0}^{N-1} (\delta_k^{+} f_k)^2 \Delta x,
$$

$$
f = (f_k)_{k=-l}^{N+l} \in \mathbf{R}^{N+1+2l}; \ 0 \leq l.
$$

Proof. From the decrease of the total energy (21) we can show

$$
\begin{aligned}
(32)\quad & \sum_{k=0}^{N}{}'' \, G_d\left(U_k^{(0)}\right) \Delta x \\
& \geq \sum_{k=0}^{N}{}'' \, G_d\left(U_k^{(n)}\right) \Delta x \\
& \geq \sum_{k=0}^{N}{}'' \left\{ -p(U_k^{(n)})^2 - \frac{9}{4}\frac{p^2}{r} - \frac{1}{2}q \frac{(\delta_k^+ U_k^{(n)})^2 + (\delta_k^- U_k^{(n)})^2}{2} \right\} \Delta x \\
& \qquad\qquad \left(\text{since } \frac{1}{2}pX^2 + \frac{1}{4}rX^4 \geq -pX^2 - \frac{9}{4}\frac{p^2}{r} \right) \\
& \geq \min(-p, -\frac{1}{2}q) \sum_{k=0}^{N}{}'' \left\{ (U_k^{(n)})^2 + \frac{(\delta_k^+ U_k^{(n)})^2 + (\delta_k^- U_k^{(n)})^2}{2} \right\} \Delta x \\
& \quad - \frac{9}{4}\frac{p^2}{r} L \\
& = \min(-p, -\frac{1}{2}q) \left\| U^{(n)} \right\|_{\text{d-}(1,2)}^2 - \frac{9}{4}\frac{p^2}{r} L,
\end{aligned}
$$

where we have used the B.C. (10) in the last equality.

Lemma 2 (Discrete Sobolev Lemma).

$$
(33)\qquad \max_{0 \leq k \leq N} |f_k| \leq 2 \max\left(\frac{1}{\sqrt{L}}, \sqrt{L} \right) \|f\|_{\text{d-}(1,2)} .
$$

Proof. We can obtain this inequality through the proof by John[15, Sect. 8.6] for a similar statement with a slightly different discrete Sobolev norm.

Applying Lemma 2 to (30) we obtain the following inequality.

Theorem 1.

$$
\max_{0 \leq k \leq N} \left| U_k^{(n)} \right| \leq 2 \sqrt{ \frac{\max(\frac{1}{L}, L)}{\min(-p, -\frac{1}{2}q)} \left\{ \sum_{k=0}^{N}{}'' \, G_d\left(U_k^{(0)}\right) \Delta x + \frac{9}{4}\frac{p^2}{r} L \right\} }.
$$
(34)

This inequality implies that the proposed difference scheme (8)–(9) is stable for any time step n.

Corollary 1. *If* $U_k^{(0)} = u^{(0)}(k\Delta x)$ *for a function* $u^{(0)}(x) \in C^3[0, L]$, *then it holds that*

$$
\max_{0 \leq k \leq N} \left| U_k^{(n)} \right| \leq 2 \sqrt{ \frac{\max(\frac{1}{L}, L)}{\min(-p, -\frac{1}{2}q)} \left\{ \int_0^L G(u^{(0)}) dx + C_0 L^2 + \frac{9}{4}\frac{p^2}{r} L \right\} },
$$
(35)

where

$$C_0 = \frac{1}{8}\int_0^L \left|\frac{\partial^2 G(u^{(0)})}{\partial x^2}\right| dx + \frac{-q}{2} L \left(\frac{1}{4}A_2^2 + \frac{1}{3}A_1A_3 + \frac{L^2}{576}A_3^2\right), \tag{36}$$

$$A_m = \max_{x\in[0,L]} \left|\frac{\partial^m}{\partial x^m} u^{(0)}\right|, \qquad 1 \le m \le 3. \tag{37}$$

Proof. We see

$$\begin{aligned} &\left|\int_0^L G(u^{(0)})dx - \sum_{k=0}^{N}{}'' \, G_d(u_k^{(0)})\Delta x\right| \\ &\le \left|\int_0^L G(u^{(0)})dx - \sum_{k=0}^{N}{}'' \, G(u_k^{(0)})\Delta x\right| \\ &\quad + \left|\sum_{k=0}^{N}{}'' \left\{G(u_k^{(0)}) - G_d(u_k^{(0)})\right\} \Delta x\right| \end{aligned} \tag{38}$$

where $u_k^{(0)} = u^{(0)}(k\Delta x)$.

For the first term on the right-hand side, representing the error of the trapezoidal rule for quadrature, we have

$$\begin{aligned} &\left|\int_0^L G(u^{(0)})dx - \sum_{k=0}^{N}{}'' \, G(u_k^{(0)})\Delta x\right| \\ &\le \frac{1}{8}(\Delta x)^2 \int_0^L \left|\frac{\partial^2}{\partial x^2} G(u^{(0)})\right| dx \end{aligned} \tag{39}$$

from the Euler-Maclaurin summation formula, since $G(u^{(0)}) \in C^2[0,L]$.

For the second term we obtain

$$G(u_k^{(0)}) - G_d(u_k^{(0)}) = \begin{cases} \dfrac{-q}{2}\left(\dfrac{-(\Delta x)^2}{4}\right)\dfrac{\partial^2 u_{\alpha_0}^{(0)}}{\partial x^2} & : k = 0, \\ \dfrac{-q}{2}\left(\dfrac{-(\Delta x)^2}{4}\right)\dfrac{\partial^2 u_{N-\alpha_N}^{(0)}}{\partial x^2} & : k = N, \end{cases} \tag{40}$$

and

$$\begin{aligned} &G(u_k^{(0)}) - G_d(u_k^{(0)}) \\ &= \frac{-q}{2}\left[-\frac{\Delta x^2}{8}\frac{\partial^2}{\partial x^2}\left(\left(\frac{\partial u_{k+\frac{1}{2}\gamma_k}^{(0)}}{\partial x}\right)^2\right)\right. \end{aligned} \tag{41}$$

$$
\begin{aligned}
&-\frac{\Delta x^2}{24}\left(\frac{\partial u^{(0)}_{k+\frac{1}{2}}}{\partial x}\frac{\partial^3 u^{(0)}_{k+\alpha_k^+}}{\partial x^3}+\frac{\partial u^{(0)}_{k-\frac{1}{2}}}{\partial x}\frac{\partial^3 u^{(0)}_{k+\alpha_k^-}}{\partial x^3}\right)\\
&-\frac{\Delta x^4}{1152}\left(\left(\frac{\partial^3 u^{(0)}_{k+\alpha_k^+}}{\partial x^3}\right)^2+\left(\frac{\partial^3 u^{(0)}_{k+\alpha_k^-}}{\partial x^3}\right)^2\right)\Bigg]\\
&: 1 \le k \le (N-1)
\end{aligned}
$$

where $0 \le \alpha_0 \le 1$, $0 \le \alpha_N \le 1$, $0 \le \alpha_k^{\pm} \le 1$ and $-1 \le \gamma_k \le 1$ since

(42)
$$\delta_k^{\pm} u_k^{(0)} = \frac{\partial u^{(0)}_{k\pm\frac{1}{2}}}{\partial x} + \frac{(\Delta x)^2}{24}\frac{\partial^3 u^{(0)}_{k\pm\alpha_k^{\pm}}}{\partial x^3}$$

and

(43)
$$v_{k+\frac{1}{2}} - 2v_k + v_{k-\frac{1}{2}} = \frac{(\Delta x)^2}{4}\frac{\partial^2 v_{k+\frac{1}{2}\gamma_k}}{\partial x^2} \quad \text{for} \quad v(x) \in C^2[0, L].$$

From (39), (40), (41) and $\Delta x \le L$ we obtain (35). This completes the proof.

4. Unique existence of the solution to the proposed scheme

This section is to prove, through the fixed-point theorem for a contraction mapping, that the proposed scheme (8) has a unique solution under a certain condition on Δt and Δx.

In connection with the scheme (8) we define a mapping $\mathcal{T}_{U^{(n)}} : \mathbf{R}^{N+1} \to \mathbf{R}^{N+1}$ in terms of the following equation:

(44)
$$
\begin{aligned}
&\left(1 - \frac{q\Delta t}{2}\delta_k^{\langle 4\rangle}\right)\{\mathcal{T}_{U^{(n)}}V\}_k\\
&= U_k^{(n)} + \frac{\Delta t}{2}\delta_k^{\langle 2\rangle}\left\{pV_k + r\{\mathcal{Q}_{U^{(n)}}V\}_k\right\},
\end{aligned}
$$

where $V = \{V_k\}_{k=0}^{N}$, the mapping $\mathcal{Q}_{U^{(n)}} : \mathbf{R}^{N+1} \to \mathbf{R}^{N+1}$ is defined as

(45)
$$\{\mathcal{Q}_{U^{(n)}}V\}_k \stackrel{\text{def}}{=} (V_k)^3 + V_k\left(V_k - U_k^{(n)}\right)^2,$$

and operators in the above equation are defined under the boundary condition (10) and (11), i.e., (13), (14) and

(46)
$$V_{-1} = V_1,\ \ V_{N+1} = V_{N-1},$$

(47)
$$V_{-2} = V_2,\ \ V_{N+2} = V_{N-2}.$$

If the mapping $\mathcal{T}_{U^{(n)}}$ has a fixed-point V^*, then $2V^* - U^{(n)}$ is the solution $U^{(n+1)}$ of the proposed scheme (8).

The following lemma implies that the mapping $\mathcal{T}_{U^{(n)}}$ is well-defined for any $U^{(n)}$.

Lemma 3. *The operator* $\left(1 - \dfrac{q\Delta t}{2}\delta_k^{\langle 4\rangle}\right)$ *is nonsingular.*

Proof. The $(N+1) \times (N+1)$ matrix expression of $\left(1 - \dfrac{q\Delta t}{2}\delta_k^{\langle 4\rangle}\right)$ is $\left(I - \dfrac{q\Delta t}{2}D_2^2\right)$, where I is the identity matrix of order $N+1$ and

$$D_2 \stackrel{\text{def}}{=} \frac{1}{(\Delta x)^2}\begin{pmatrix} -2 & 2 & & & 0 \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ 0 & & & 2 & -2 \end{pmatrix} \tag{48}$$

under the boundary condition (10). Eigenvalues of D_2 are

$$\lambda_k \stackrel{\text{def}}{=} \frac{2}{(\Delta x)^2}\left\{\cos\left(\frac{k}{N}\pi\right) - 1\right\}, \qquad k = 0, 1, \cdots, N \tag{49}$$

and eigenvalues of $\left(I - \dfrac{q\Delta t}{2}D_2^2\right)$ are $1 - \dfrac{q\Delta t}{2}(\lambda_k)^2$, $k = 0, 1, \cdots, N$. Positiveness of the eigenvalues implies the nonsingularity of $\left(I - \dfrac{q\Delta t}{2}D_2^2\right)$.

Next, we prove the existence and uniqueness of the solution for the proposed scheme (8) on the basis of the fixed-point theorem for a contraction mapping.

Theorem 2. *If*

$$\Delta t < \min\left(\frac{-q}{2\left(-p + 41rM^2\right)^2}, \frac{-2q}{\left(-p + 113rM^2\right)^2}\right), \tag{50}$$

then the mapping $\mathcal{T}_{U^{(n)}}$ *has a unique fixed-point in the closed ball* $\mathcal{K}$*, where*

$$M \stackrel{\text{def}}{=} \left\|U^{(n)}\right\|_2, \tag{51}$$

$$\mathcal{K} \stackrel{\text{def}}{=} \left\{ v \in \mathbf{R}^{N+1} \,\middle|\, \|v\|_2 \leq 4M \right\}, \tag{52}$$

$$\|v\|_2 \stackrel{\text{def}}{=} \sqrt{\sum_{k=0}^{N}(v_k)^2}. \tag{53}$$

Remark 3. For the solution $U_k^{(n)}$ of the scheme (8) M is bounded as

$$M \le 2\sqrt{\frac{(N+1)\max(\frac{1}{L},L)}{\min(-p,-\frac{1}{2}q)}\left\{\sum_{k=0}^{N}{}'' G_d\left(U_k^{(0)}\right)\Delta x + \frac{9}{4}\frac{p^2}{r}L\right\}} \tag{54}$$

from the Theorem 1.

Remark 4. Since

$$M \sim \frac{\left\|U^{(n)}\right\|_{\text{d-}(0,2)}}{\sqrt{\Delta x}} \sim \frac{\|u(n\Delta t,\cdot)\|_{L^2(0,L)}}{\sqrt{\Delta x}}, \tag{55}$$

(50) implies that $\Delta t = O(\Delta x^2)$.

Proof. By the fixed-point theorem for a contraction mapping it suffices to show that $\mathcal{T}_{U^{(n)}}$ is a contraction mapping on $\mathcal{K}$.

First, we prove that $\mathcal{T}_{U^{(n)}}$ is a mapping $\mathcal{K} \to \mathcal{K}$. We diagonalize the matrix D_2 as

$$D_2 = X\Lambda X^{-1}, \tag{56}$$

where X and Λ are matrices order $N+1$ as

$$X \stackrel{\text{def}}{=} \left(\cos\left(\frac{ij\pi}{N}\right)\right)_{i,j=0}^{N}, \tag{57}$$

$$\Lambda \stackrel{\text{def}}{=} \operatorname{diag}(\lambda_k), \tag{58}$$

where λ_k is given by (49). Then the matrix expression of $\mathcal{T}_{U^{(n)}}$ is given by

$$\begin{aligned}\mathcal{T}_{U^{(n)}}V &= X\left(I - \frac{q\Delta t}{2}\Lambda^2\right)^{-1} X^{-1}\, U^{(n)} \\ &\quad + \frac{\Delta t}{2}X\left(I - \frac{q\Delta t}{2}\Lambda^2\right)^{-1}\Lambda X^{-1}\left\{pV + r\mathcal{Q}_{U^{(n)}}V\right\}.\end{aligned} \tag{59}$$

Hence

$$\begin{aligned}&\left\|\mathcal{T}_{U^{(n)}}V\right\|_2 \\ &\le \|X\|_2\left\|\left(I - \frac{q\Delta t}{2}\Lambda^2\right)^{-1}\right\|_2 \left\|X^{-1}\right\|_2\left\|U^{(n)}\right\|_2 \\ &\quad + \frac{\Delta t}{2}\|X\|_2\left\|\left(I - \frac{q\Delta t}{2}\Lambda^2\right)^{-1}\Lambda\right\|_2\left\|X^{-1}\right\|_2 \\ &\quad \left\{-p\|V\|_2 + r\left\|\mathcal{Q}_{U^{(n)}}V\right\|_2\right\}\end{aligned} \tag{60}$$

$$\leq 2 \max_{0\leq k\leq N} \left| \frac{1}{1-\frac{q\Delta t}{2}\lambda_k^2} \right| \left\| U^{(n)} \right\|_2$$
$$+2\frac{\Delta t}{2} \max_{0\leq k\leq N} \left| \frac{\lambda_k}{1-\frac{q\Delta t}{2}\lambda_k^2} \right| \left\{ -p \left\| V \right\|_2 + r \left\| \mathcal{Q}_{U^{(n)}} V \right\|_2 \right\}$$
$$\leq 2M \left\{ 1 + \sqrt{\frac{2\Delta t}{-q}} \left(-p + 41rM^2 \right) \right\}$$

because

$$\left\| \mathrm{diag}(d_k) \right\|_2 = \max_k |d_k|, \tag{61}$$

$$\max_{0\leq k\leq N} \left| \frac{1}{1-\frac{q\Delta t}{2}\lambda_k^2} \right| \leq 1, \tag{62}$$

$$\max_{0\leq k\leq N} \left| \frac{\lambda_k}{1-\frac{q\Delta t}{2}\lambda_k^2} \right| \leq \frac{1}{\sqrt{-2q\Delta t}}, \tag{63}$$

$$\left\| \mathcal{Q}_{U^{(n)}} V \right\|_2 \leq 164\ M^3, \tag{64}$$

$$\left\| X \right\|_2 \leq \sqrt{2N}, \tag{65}$$

$$\left\| X^{-1} \right\|_2 \leq \sqrt{\frac{2}{N}}, \tag{66}$$

when $\left\| U^{(n)} \right\|_2 = M$ and $\left\| V \right\|_2 \leq 4M$. From (60) we see that $\mathcal{T}_{U^{(n)}}$ is a mapping $\mathcal{K} \to \mathcal{K}$ if

$$\Delta t \leq \frac{-q}{2\left(-p + 41\ rM^2\right)^2}. \tag{67}$$

Next we prove that $\mathcal{T}_{U^{(n)}}$ is a contraction mapping. Using (59) and the estimates above we can show

$$\begin{aligned} &\left\| \mathcal{T}_{U^{(n)}} V - \mathcal{T}_{U^{(n)}} V' \right\|_2 \\ &\leq \sqrt{\frac{\Delta t}{-2q}} \left\{ -p \left\| V - V' \right\|_2 + r \left\| \mathcal{Q}_{U^{(n)}} V - \mathcal{Q}_{U^{(n)}} V' \right\|_2 \right\} \\ &\leq \sqrt{\frac{\Delta t}{-2q}} \left(-p + 113rM^2 \right) \left\| V - V' \right\|_2 \end{aligned} \tag{68}$$

because

$$\left\| \mathcal{Q}_{U^{(n)}} V - \mathcal{Q}_{U^{(n)}} V' \right\|_2 \leq 113M^2 \left\| V - V' \right\|_2. \tag{69}$$

Therefore $\mathcal{T}_{U^{(n)}}$ is a contraction mapping if

$$\Delta t < \frac{-2q}{\left(-p + 113rM^2\right)^2}. \tag{70}$$

5. Error estimates for the proposed scheme

The purpose of this section is to show an error estimate (Theorem 3 below) of numerical solutions of the proposed scheme. We define the error as

$$\mathrm{e}_k^{(n)} \stackrel{\text{def}}{=} U_k^{(n)} - u(k\Delta x, n\Delta t), \quad k = -1, 0, 1, \cdots, N, N+1, \tag{71}$$

where $u(x,t)$ is the solution to the Cahn-Hilliard equation. We define an extension of u by

$$u(x,t) \stackrel{\text{def}}{=} \begin{cases} u(x-2lL,t) : 2lL \le x \le (2l+1)L, \\ u(2lL-x,t) : (2l-1)L < x < 2lL, \end{cases} \tag{72}$$

where $l \in \mathbf{Z}$. The error is measured in terms of the discrete L_2-norm,

$$\|f\|^2_{\text{d-}(0,2)} \stackrel{\text{def}}{=} \sum_{k=0}^{N}{}'' (f_k)^2 \Delta x, \quad f = (f_k)_{k=-l}^{N+l} \in \mathbf{R}^{N+1+2l};\ 0 \le l. \tag{73}$$

We use two time difference operators and a time averaging operator,

$$\delta_n^{\langle 1 \rangle} f^{(n)} \stackrel{\text{def}}{=} \frac{f^{(n+\frac{1}{2})} - f^{(n-\frac{1}{2})}}{\Delta t}, \tag{74}$$

$$\delta_n^{\langle 2 \rangle} f^{(n)} \stackrel{\text{def}}{=} \frac{f^{(n+\frac{1}{2})} - 2f^{(n)} + f^{(n-\frac{1}{2})}}{(\frac{1}{2}\Delta t)^2}, \tag{75}$$

$$s_n^{\langle 1 \rangle} f^{(n)} \stackrel{\text{def}}{=} \frac{f^{(n+\frac{1}{2})} + f^{(n-\frac{1}{2})}}{2}. \tag{76}$$

Lemma 4.

$$\begin{aligned} &\frac{1}{\Delta t}\left\{ \left\|\mathrm{e}^{(n+1)}\right\|^2_{\text{d-}(0,2)} - \left\|\mathrm{e}^{(n)}\right\|^2_{\text{d-}(0,2)} \right\} \\ &\le \frac{1}{2}\left\{ \left\|\mathrm{e}^{(n+1)}\right\|^2_{\text{d-}(0,2)} + \left\|\mathrm{e}^{(n)}\right\|^2_{\text{d-}(0,2)} \right\} \\ &\quad -\frac{1}{q}\left\| \tilde{\phi}(U^{(n+1)}; U^{(n)}) - \phi^{(n+\frac{1}{2})} \right\|^2_{\text{d-}(0,2)} \\ &\quad + \left\| \zeta_1^{(n+\frac{1}{2})} \right\|^2_{\text{d-}(0,2)} + \left\| \zeta_2^{(n+\frac{1}{2})} \right\|^2_{\text{d-}(0,2)} \end{aligned} \tag{77}$$

where

$$\begin{aligned} \tilde{\phi}(f_k; g_k) \stackrel{\text{def}}{=} &\, p\left\{ \frac{f_k + g_k}{2} \right\} \\ &+ r\left\{ \frac{(f_k)^3 + (f_k)^2 g_k + f_k (g_k)^2 + (g_k)^3}{4} \right\}, \end{aligned} \tag{78}$$

(79) $$\phi_k^{(n+\frac{1}{2})} \stackrel{\text{def}}{=} \left\{ pu + ru^3 \right\}\Big|_{(x,t)=(k\Delta x,(n+\frac{1}{2})\Delta t)},$$

(80) $$\zeta_{1,k}^{(n+\frac{1}{2})} = \left\{ \left(\frac{\partial}{\partial t} - \delta_n^{\langle 1\rangle} \right) u - \left(\frac{\partial^2}{\partial x^2} - \delta_k^{\langle 2\rangle} \right) \frac{\delta G}{\delta u} \right\}\Bigg|_{(x,t)=(k\Delta x,(n+\frac{1}{2})\Delta t)},$$

(81) $$\zeta_{2,k}^{(n+\frac{1}{2})} = \sqrt{-q} \left\{ \left(s_n^{\langle 1\rangle} \delta_k^{\langle 2\rangle} - \frac{\partial^2}{\partial x^2} \right) u \right\}\Bigg|_{(x,t)=(k\Delta x,(n+\frac{1}{2})\Delta t)},$$

for $k = 0, 1, \cdots, N$.

In (80) the term $\delta_n^{\langle 1\rangle} u \Big|_{(x,t)=(k\Delta x,(n+\frac{1}{2})\Delta t)}$, e.g., is defined as follows:

(82) $$\begin{aligned} &\delta_n^{\langle 1\rangle} u \Big|_{(x,t)=(k\Delta x,(n+\frac{1}{2})\Delta t)} \\ &\stackrel{\text{def}}{=} \delta_n^{\langle 1\rangle} u(k\Delta x, (n+\frac{1}{2})\Delta t) \\ &= \frac{u(k\Delta x, (n+1)\Delta t) - u(k\Delta x, n\Delta t)}{\Delta t}. \end{aligned}$$

Similarly (81) is defined.

Proof. Define

(83) $$F_k^{(n+\frac{1}{2})} \stackrel{\text{def}}{=} \left(\frac{\delta G_d}{\delta U} \right)_k^{(n+\frac{1}{2})} - \frac{\delta G}{\delta u}\Bigg|_{(x,t)=(k\Delta x,(n+\frac{1}{2})\Delta t)},$$

for $k = -1, 0, 1, \cdots, N, N+1$. From (1), (8), (71) and (83) we obtain

(84) $$\frac{\mathrm{e}_k^{(n+1)} - \mathrm{e}_k^{(n)}}{\Delta t} = \delta_k^{\langle 2\rangle} F_k^{(n+\frac{1}{2})} + \zeta_{1,k}^{(n+\frac{1}{2})},$$

for $k = 0, 1, \cdots, N$. From (2), (9) and (83) we obtain

(85) $$\begin{aligned} F_k^{(n+\frac{1}{2})} &= \tilde{\phi}(U_k^{(n+1)}; U_k^{(n)}) - \phi_k^{(n+\frac{1}{2})} \\ &\quad + q\delta_k^{\langle 2\rangle} \frac{\mathrm{e}_k^{(n+1)} + \mathrm{e}_k^{(n)}}{2} - \sqrt{-q}\, \zeta_{2,k}^{(n+\frac{1}{2})}, \end{aligned}$$

for $k = 0, 1, \cdots, N$. From (84) and (85) we have

(86) $$\begin{aligned} &\frac{1}{2} \sum_{k=0}^{N}{}'' \left\{ \frac{(\mathrm{e}_k^{(n+1)})^2 - (\mathrm{e}_k^{(n)})^2}{\Delta t} \right\} \Delta x - \frac{1}{q} \sum_{k=0}^{N}{}'' \left(F_k^{(n+\frac{1}{2})} \right)^2 \Delta x \\ &= \sum_{k=0}^{N}{}'' \left\{ \frac{\mathrm{e}_k^{(n+1)} + \mathrm{e}_k^{(n)}}{2} \times \mathrm{RHS}(84) \right\} \Delta x \end{aligned}$$

$$
\begin{aligned}
&-\frac{1}{q}\sum_{k=0}^{N}{}'' \left\{ F_k^{(n+\frac{1}{2})} \times \mathrm{RHS}(85) \right\} \Delta x \\
&= \sum_{k=0}^{N}{}'' \left\{ \frac{\mathrm{e}_k^{(n+1)} + \mathrm{e}_k^{(n)}}{2} \delta_k^{\langle 2\rangle} F_k^{(n+\frac{1}{2})} - F_k^{(n+\frac{1}{2})} \delta_k^{\langle 2\rangle} \frac{\mathrm{e}_k^{(n+1)} + \mathrm{e}_k^{(n)}}{2} \right\} \Delta x \\
&\quad -\frac{1}{q}\sum_{k=0}^{N}{}'' \left\{ \left(\tilde{\phi}(U_k^{(n+1)}; U_k^{(n)}) - \phi_k^{(n+\frac{1}{2})} \right) F_k^{(n+\frac{1}{2})} \right\} \Delta x \\
&\quad +\sum_{k=0}^{N}{}'' \left\{ \frac{\mathrm{e}_k^{(n+1)} + \mathrm{e}_k^{(n)}}{2} \zeta_{1,k}^{(n+\frac{1}{2})} \right\} \Delta x \\
&\quad -\frac{1}{q}\sum_{k=0}^{N}{}'' \left\{ F_k^{(n+\frac{1}{2})} (-\sqrt{-q}) \zeta_{2,k}^{(n+\frac{1}{2})} \right\} \Delta x.
\end{aligned}
$$

Here the first term

$$
\begin{aligned}
(87)\quad &\sum_{k=0}^{N}{}'' \left\{ \frac{\mathrm{e}_k^{(n+1)} + \mathrm{e}_k^{(n)}}{2} \delta_k^{\langle 2\rangle} F_k^{(n+\frac{1}{2})} - F_k^{(n+\frac{1}{2})} \delta_k^{\langle 2\rangle} \frac{\mathrm{e}_k^{(n+1)} + \mathrm{e}_k^{(n)}}{2} \right\} \Delta x \\
&= \left[\frac{\mathrm{e}_k^{(n+1)} + \mathrm{e}_k^{(n)}}{2} \delta_k^{\langle 1\rangle} F_k^{(n+\frac{1}{2})} - F_k^{(n+\frac{1}{2})} \delta_k^{\langle 1\rangle} \frac{\mathrm{e}_k^{(n+1)} + \mathrm{e}_k^{(n)}}{2} \right]_{k=0}^{N}
\end{aligned}
$$

vanishes since

$$
(88)\qquad \left. \delta_k^{\langle 1\rangle} F_k^{(n+\frac{1}{2})} \right|_{k=0} = \left. \delta_k^{\langle 1\rangle} F_k^{(n+\frac{1}{2})} \right|_{k=N} = 0,
$$

$$
(89)\qquad \left. \delta_k^{\langle 1\rangle} e_k^{(n)} \right|_{k=0} = \left. \delta_k^{\langle 1\rangle} e_k^{(n)} \right|_{k=N} = 0
$$

under the boundary condition (10) and definition (72), whereas the remaining terms can be bounded from the above by the inequality $ab \leq \frac{1}{2}(a^2 + b^2)$. Hence we obtain the inequality (77).

Lemma 5.

$$
\begin{aligned}
(90)\quad &\left\| \tilde{\phi}(U^{(n+1)}; U^{(n)}) - \phi^{(n+\frac{1}{2})} \right\|_{\text{d-}(0,2)}^2 \\
&\leq \left\{ -p + 3r(C_2)^2 \right\}^2 \left\{ \left\| \mathrm{e}^{(n+1)} \right\|_{\text{d-}(0,2)}^2 + \left\| \mathrm{e}^{(n)} \right\|_{\text{d-}(0,2)}^2 \right\} \\
&\quad -q \left\{ \left\| \zeta_3^{(n+\frac{1}{2})} \right\|_{\text{d-}(0,2)}^2 + \left\| \zeta_4^{(n+\frac{1}{2})} \right\|_{\text{d-}(0,2)}^2 \right\},
\end{aligned}
$$

where

$$C_2 \stackrel{\text{def}}{=} \max_{0\le l\le n+1} \left\{ \max_{0\le k\le N} \left| U_k^{(l)} \right|, \sup_{x\in[0,L]} |u(x, l\Delta t)| \right\}, \tag{91}$$

and

$$\zeta_{3,k}^{(n+\frac{1}{2})} \stackrel{\text{def}}{=} \frac{r}{2\sqrt{-q}} C_2 \left\{ u(k\Delta x, (n+1)\Delta t) - u(k\Delta x, n\Delta t) \right\}^2, \tag{92}$$

$$\zeta_{4,k}^{(n+\frac{1}{2})} \stackrel{\text{def}}{=} \frac{2}{\sqrt{-q}} \left\{ -p + 3r(C_2)^2 \right\} (s_n^{\langle 1\rangle} - 1) u(k\Delta x, (n+\frac{1}{2})\Delta t), \tag{93}$$

for $k = 0, 1, \cdots, N$.

Remark 5. Note that C_2 is finite since the proposed scheme is unconditionally stable (Corollary 1) and the solution $u \in C^0([0, L])$.

Proof. We represent $\tilde{\phi} - \phi = \sum_{i=m}^{4} I_m$ where $I_m = (I_{m,k})_{k=0}^N$ with

$$I_{1,k} \stackrel{\text{def}}{=} \tilde{\phi}(U_k^{(n+1)}; U_k^{(n)}) - \tilde{\phi}(u(k\Delta x, (n+1)\Delta t); U_k^{(n)}), \tag{94}$$

$$\begin{aligned} I_{2,k} \stackrel{\text{def}}{=}\ & \tilde{\phi}(u(k\Delta x, (n+1)\Delta t); U_k^{(n)}) \\ & - \tilde{\phi}(u(k\Delta x, (n+1)\Delta t); u(k\Delta x, n\Delta t)), \end{aligned} \tag{95}$$

$$\begin{aligned} I_{3,k} \stackrel{\text{def}}{=}\ & \tilde{\phi}(u(k\Delta x, (n+1)\Delta t); u(k\Delta x, n\Delta t)) \\ & - \phi(\frac{u(k\Delta x, (n+1)\Delta t) + u(k\Delta x, n\Delta t)}{2}), \end{aligned} \tag{96}$$

$$\begin{aligned} I_{4,k} \stackrel{\text{def}}{=}\ & \phi(\frac{u(k\Delta x, (n+1)\Delta t) + u(k\Delta x, (n+1)\Delta t)}{2}) \\ & - \phi(u(k\Delta x, (n+\frac{1}{2})\Delta t)). \end{aligned} \tag{97}$$

The following estimates are easy to show:

$$|I_{1,k}| \le \frac{1}{2} \left(-p + 3r(C_2)^2 \right) \left| \mathrm{e}_k^{(n+1)} \right|, \tag{98}$$

$$|I_{2,k}| \le \frac{1}{2} \left(-p + 3r(C_2)^2 \right) \left| \mathrm{e}_k^{(n)} \right|, \tag{99}$$

$$|I_{4,k}| \le \left(-p + 3r(C_2)^2 \right) (s_n^{\langle 1\rangle} - 1) u(k\Delta x, (n+\frac{1}{2})\Delta t). \tag{100}$$

The estimate for $(I_{3,k})_{k=0}^N$,

$$|I_{3,k}| \le \frac{r}{4} C_2 \left\{ u(k\Delta x, (n+1)\Delta t) - u(k\Delta x, n\Delta t) \right\}^2, \tag{101}$$

is derived from

$$\frac{u^3+u^2v+uv^2+v^3}{4}-\left(\frac{u+v}{2}\right)^3=\frac{1}{8}(u+v)(u-v)^2. \tag{102}$$

From these inequalities we obtain

$$\|I_1\|^2_{\text{d-}(0,2)} \le \frac{1}{4}\left(-p+3r(C_2)^2\right)^2\left\|\mathrm{e}^{(n+1)}\right\|^2_{\text{d-}(0,2)}, \tag{103}$$

$$\|I_2\|^2_{\text{d-}(0,2)} \le \frac{1}{4}\left(-p+3r(C_2)^2\right)^2\left\|\mathrm{e}^{(n)}\right\|^2_{\text{d-}(0,2)}, \tag{104}$$

$$\|I_3\|^2_{\text{d-}(0,2)} \le \frac{1}{16}r^2\left(C_2\right)^2 \left\|\{u(\cdot,(n+1)\Delta t)-u(\cdot,n\Delta t)\}^2\right\|^2_{\text{d-}(0,2)}, \tag{105}$$

$$\|I_4\|^2_{\text{d-}(0,2)} \le \left(-p+3r(C_2)^2\right)^2 \left\|(s_n^{\langle 1\rangle}-1)u(\cdot,(n+\frac{1}{2})\Delta t)\right\|^2_{\text{d-}(0,2)}. \tag{106}$$

We obtain (90) by substituting (103)–(106) into

$$\left\|\tilde{\phi}(U^{(n+1)};U^{(n)})-\phi^{(n+\frac{1}{2})}\right\|^2_{\text{d-}(0,2)} \le 4\sum_{m=1}^{4}\|I_m\|^2_{\text{d-}(0,2)}. \tag{107}$$

Lemma 6. *If*

$$\Delta t<\frac{1}{2+4\frac{\{-p+3r(C_2)^2\}^2}{-q}}, \tag{108}$$

then

$$\left\|\mathrm{e}^{(n)}\right\|^2_{\text{d-}(0,2)} \le \Delta t\sum_{l=1}^{n}(C_3)^l\sum_{m=1}^{4}\left\|\zeta_m^{(n+\frac{1}{2}-l)}\right\|^2_{\text{d-}(0,2)}, \tag{109}$$

where

$$C_3 \stackrel{\text{def}}{=} 1+\left(2+4\frac{\{-p+3r(C_2)^2\}^2}{-q}\right)\Delta t. \tag{110}$$

Proof. From Lemma 4 and Lemma 5 we obtain

$$\left\{1-2\Delta t\left(\frac{1}{2}+\frac{\{-p+3r(C_2)^2\}^2}{-q}\right)\right\}\left\|\mathrm{e}^{(n+1)}\right\|^2_{\text{d-}(0,2)} \le \left\|\mathrm{e}^{(n)}\right\|^2_{\text{d-}(0,2)}+\Delta t\sum_{m=1}^{4}\left\|\zeta_m^{(n+\frac{1}{2})}\right\|^2_{\text{d-}(0,2)}. \tag{111}$$

If the inequality (108) is satisfied, from (111) we obtain

$$\begin{aligned}(112)\quad \left\|\mathrm{e}^{(n)}\right\|^2_{\text{d-}(0,2)} &\le C_3\left[\left\|\mathrm{e}^{(n-1)}\right\|^2_{\text{d-}(0,2)} + \Delta t\sum_{m=1}^{4}\left\|\zeta_m^{(n-\frac{1}{2})}\right\|^2_{\text{d-}(0,2)}\right]\\ &\le (C_3)^n\left\|\mathrm{e}^{(0)}\right\|^2_{\text{d-}(0,2)}\\ &\quad +\Delta t\sum_{l=1}^{n}(C_3)^l\sum_{m=1}^{4}\left\|\zeta_m^{(n+\frac{1}{2}-l)}\right\|^2_{\text{d-}(0,2)}.\end{aligned}$$

The first term of this inequality vanishes since the error of the initial data is zero.

The main result of this section is now stated.

Theorem 3. *Suppose that Δt is small enough to satisfy the condition (50) and (108). If (1) and (2) have a solution such that $u(x,t) \in C^6([0,L]\times[0,T])$, then the solution of the difference scheme (8) and (9) converges to the solution of (1) and (2) in the sense of discrete L_2-norm(73), and the convergence rate is $O((\Delta x)^2 + (\Delta t)^2)$.*

Proof. From Lemma 6 we obtain

$$(113)\qquad \left\|\mathrm{e}^{(n)}\right\|^2_{\text{d-}(0,2)} \le \Delta t(C_3)^n\sum_{l=1}^{n}\sum_{m=1}^{4}\left\|\zeta_m^{(n+\frac{1}{2}-l)}\right\|^2_{\text{d-}(0,2)}.$$

If (1) and (2) have a solution such that $u(x,t) \in C^6([0,L]\times[0,T])$, then

$$(114)\quad \zeta_{1,k}^{(n+\frac{1}{2})} = -\frac{\Delta t^2}{24}\frac{\partial^3 u}{\partial t^3}\bigg|_{\substack{x=k\Delta x\\ t=t_1}} + \frac{\Delta x^2}{12}\frac{\partial^4}{\partial x^4}\left(\frac{\delta G}{\delta u}\right)\bigg|_{\substack{x=x_1\\ t=(n+\frac{1}{2})\Delta t}},$$

$$(115)\quad \zeta_{2,k}^{(n+\frac{1}{2})} = \sqrt{-q}\left(\frac{\Delta x^2}{12}\frac{\partial^4 u}{\partial x^4}\bigg|_{\substack{x=x_2\\ t=(n+\frac{1}{2})\Delta t}} + \frac{\Delta t^2}{8}\frac{\partial^4 u}{\partial t^2\partial x^2}\bigg|_{\substack{x=x_3\\ t=t_2}}\right),$$

$$(116)\quad \zeta_{3,k}^{(n+\frac{1}{2})} = \frac{r}{2\sqrt{-q}}C_2(\Delta t)^2\left(\frac{\partial u}{\partial t}\bigg|_{\substack{x=k\Delta x\\ t=t_3}}\right)^2,$$

$$(117)\quad \zeta_{4,k}^{(n+\frac{1}{2})} = \frac{r}{\sqrt{-q}}\left\{-p+3r(C_2)^2\right\}^2\frac{\Delta t^2}{8}\,\frac{\partial^2 u}{\partial t^2}\bigg|_{\substack{x=k\Delta x\\ t=t_4}},$$

where $t_1, t_2, t_3, t_4 \in [n\Delta t, (n+1)\Delta t]$ and $x_1, x_2, x_3 \in [(k-1)\Delta x, (k+1)\Delta x]$. From these there is a constant C_4 such that

$$(118)\qquad \sum_{m=1}^{4}\left\|\zeta_m^{(n+\frac{1}{2})}\right\|^2_{\text{d-}(0,2)} \le C_4 L\left(\Delta x^2 + \Delta t^2\right)^2.$$

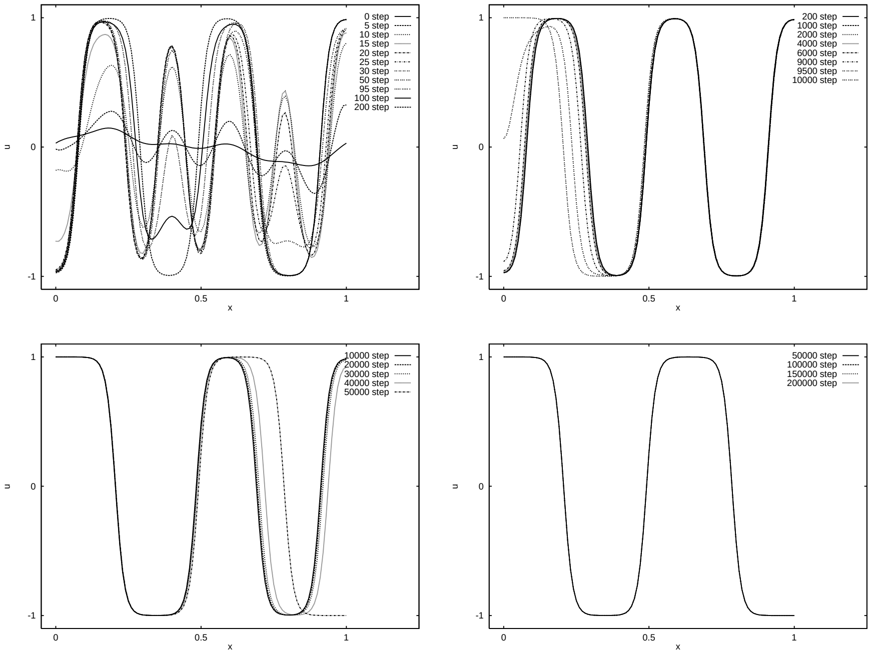

Fig. 1. Numerical solution to the Cahn-Hilliard equation ($p = -1.0$, $q = -0.0005$, $r = 1.0$) obtained by the proposed scheme (8) and (9) with $\Delta x = 1/100$ and $\Delta t = 1/1200$. The initial state is (120)

From (113) and (118) we obtain the following evaluation of the error,

$$\left\|\mathrm{e}^{(n)}\right\|_{\text{d-}(0,2)} \le \sqrt{C_4 L T}\exp\left[\left(1+\frac{2\left\{-p+3r(C_2)^2\right\}^2}{-q}\right)T\right] \left(\Delta x^2+\Delta t^2\right), \tag{119}$$

where $T = n\Delta t$.

6. Examples of numerical solution

The purpose of this section is to demonstrate through numerical experiments that the proposed difference scheme is stable and gives reasonable numerical solutions.

The dependence of the numerical solution on the parameter q is demonstrated in Fig. 1–3. Recall [1] that the parameter q represents (the effect of) the “interfacial energy” in a phase separation phenomenon described by the Cahn-Hilliard equation. Figure 1 shows a numerical result for $p = -1.0$, $q = -0.0005$ and $r = 1.0$ obtained by the proposed scheme with $\Delta x =$

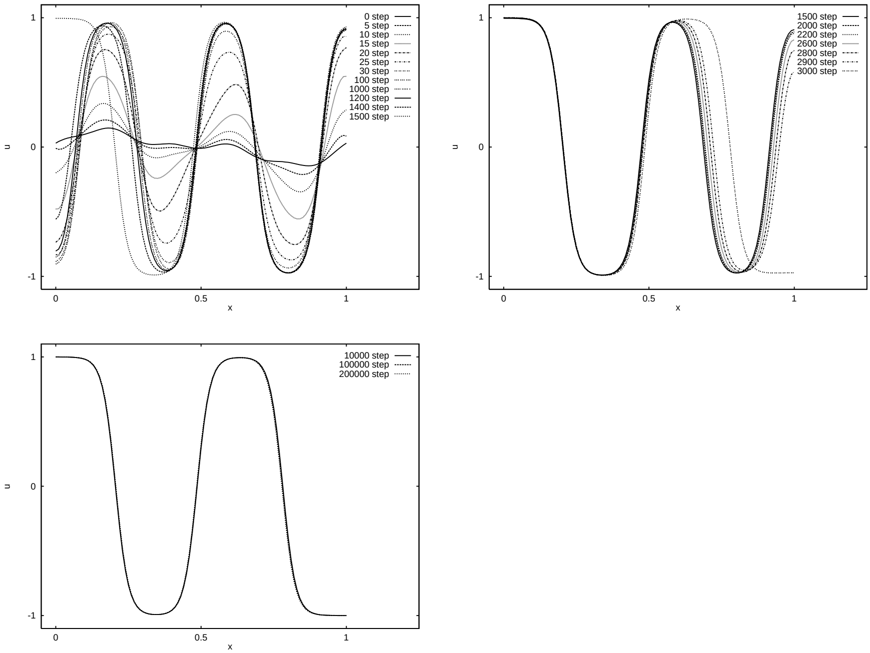

Fig. 2. Numerical solution to the Cahn-Hilliard equation ($p = -1.0, q = -0.001, r = 1.0$) obtained by the proposed scheme (8) and (9) with $\Delta x = 1/100$ and $\Delta t = 1/1200$. The initial state is (120)

$1/100$ and $\Delta t = 1/1200$. The initial state in Fig. 1 is

$$u(x,0) = 0.1\sin(2\pi x) + 0.01\cos(4\pi x) \\ +0.06\sin(4\pi x) + 0.02\cos(10\pi x). \tag{120}$$

Figure 2 shows a numerical result for the same parameters and an initial state as in Fig. 1 but for $q = -0.001$. In Fig. 3 the parameter q is changed to -0.002. The closer value of the parameter q to zero means the decrease of the "interfacial energy" of the system [1]. Spatial patterns represented by the numerical solutions in Figs. 1–3 correspond to the physical phenomenon that they become finer as the effect of the interfacial energy is smaller.

Figure 4 shows a numerical result for the same p, q and r obtained by the proposed scheme with the same Δx and Δt. The initial state is different and is

$$u(x,0) = 100x^2(x-1)^2(x-\frac{1}{2}). \tag{121}$$

The numerical results in this paper stand in virtual agreement with the results in [11] which were obtained by an explicit finite difference scheme. However, we must set Δt as small as $5.9360656\cdots \times 10^{-7} \cong 1/1685000$ in the scheme of the preceding paper [11], whereas we obtained a stable

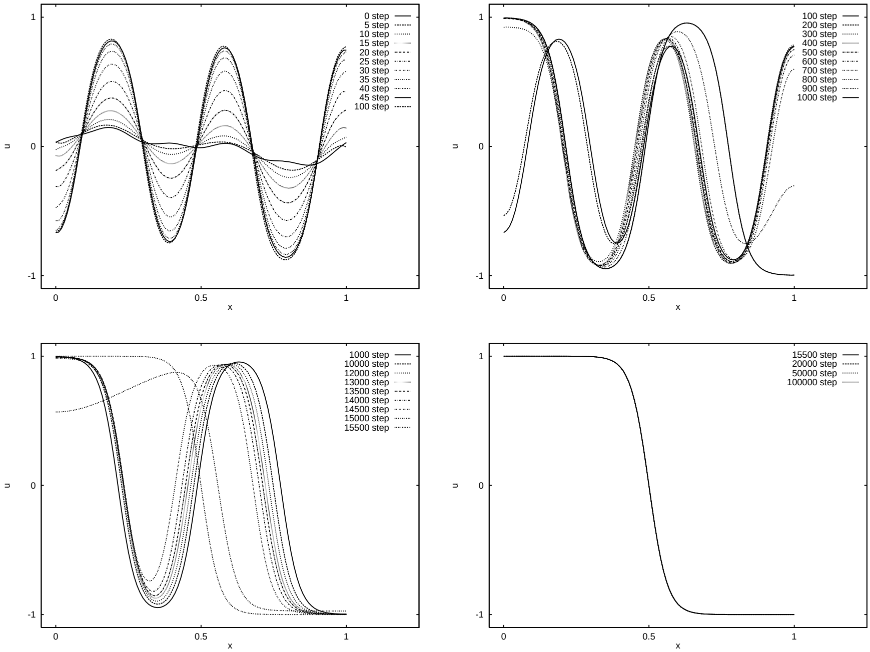

Fig. 3. Numerical solution to the Cahn-Hilliard equation ($p = -1.0, q = -0.002, r = 1.0$) obtained by the proposed scheme (8) and (9) with $\Delta x = 1/100$ and $\Delta t = 1/1200$. The initial state is (120)

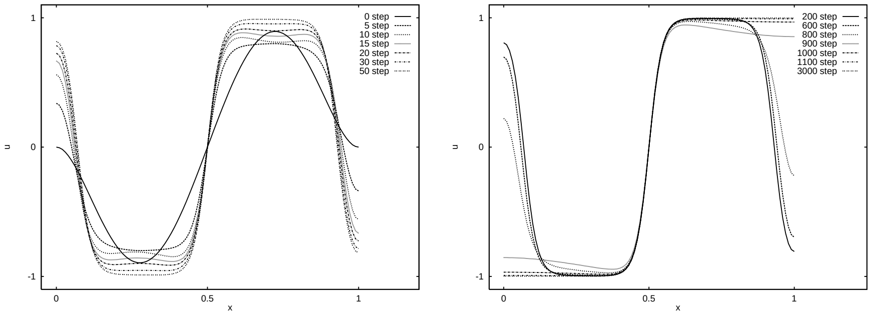

Fig. 4. Numerical solution to the Cahn-Hilliard equation ($p = -1.0, q = -0.001, r = 1.0$) obtained by the proposed scheme (8) and (9) with $\Delta x = 1/100$ and $\Delta t = 1/1200$. The initial state is (121)

solution with a mesh size as large as $\Delta t = 1/1200$ by utilizing the present scheme. Although from the point of stability we can make Δt even larger, we have chosen $\Delta t = 1/1200$ in view of accuracy.

We can see that the final numerical solutions of Fig. 3 and Fig. 4 correspond exactly to the monotone solution that is the global minimizer of the total free energy [2].

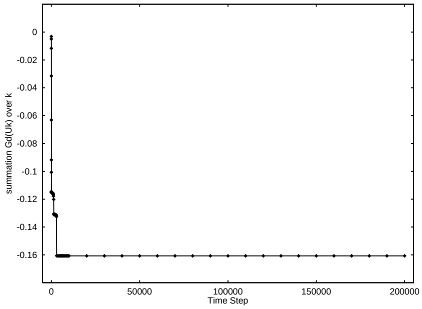

Fig. 5. The discrete total energy of the numerical solution in Fig. 2 to the Cahn-Hilliard equation

Figure 5 shows the total discrete energy of numerical solution $\sum_{k=0}^{N}{}'' G_d(U_k^{(n)})\Delta x$ in Fig. 2. This graph shows that the decrease of the total energy (21) is preserved numerically.

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