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NUMERICAL ANALYSIS OF A CONTINUUM MODEL OF PHASE TRANSITION*

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Abstract. A method for solution of the Cahn-Hilliard equation is presented. Unlike previous work, the discrete equations for the new method possess a Lyapunov function. This makes it possible to prove convergence of the approximate solutions without assumptions beyond those necessary for existence and uniqueness of the differential equation. Several consequences are explored.

Key words. parabolic equations, phase transitions, Cahn-Hilliard equation

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1. Introduction.

One form of the Cahn-Hilliard model for continuum phase transitions in a finite domain is

$$\frac{\partial u}{\partial t}+\sigma\Delta^2 u=\Delta\phi(u), \qquad 0<\sigma\ll 1, \tag{1.1}$$

with boundary conditions

$$\frac{\partial u}{\partial n}=0, \qquad \frac{\partial(\sigma\Delta u-\phi(u))}{\partial n}=0, \tag{1.2}$$

and an initial condition. The function ϕ is the derivative of a double well potential such as $\phi(u)=u^3-u$, and σ is constant. If $\sigma=0$, the resulting second-order equation can exhibit instabilities where $|u|<1/\sqrt{3}$, that is, where $\phi'<0$. When $\sigma>0$ the fourth-order term in (1.1) regularizes the equation and makes it well posed. In applications, σ is frequently very small in some suitable sense, and rapid growth in the solution can occur before the regularization takes effect. For this reason, an important part of the analysis of (1.1) is to estimate the absolute pointwise maximum value of the solution. The technique for this estimate depends on the existence of a Lyapunov function for (1.1) [EZ]. If the maximum is finite the rest of the analysis can follow familiar lines. Therefore, estimation of the maximum seems to be the key result.

Numerical methods for (1.1) are considered in [EF] and [EFM]. In [EF] the one-dimensional case is discretized using conforming finite element schemes with an implicit time discretization. In [EFM] semidiscrete schemes are used for a mixed formulation of the governing equation. Both of these papers contain a number of error estimates for the schemes they consider. In part, these estimates require similar results to the analysis of the differential equation. In particular, it turns out to be essential to know a pointwise maximum bound on the *numerical* solution. Once the bound is known, the error analysis is close to the standard linear theory for evolutionary equations. So again it seems that estimation of the maximum is the important point.

In the semidiscrete schemes, the pointwise estimate of the numerical solution follows immediately from the differential equation theory; the error analysis is then

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relatively straightforward and close to the linear case. For the fully discrete schemes of [EF] however, no Lyapunov function is known at present and the maximum cannot be estimated. To avoid this difficulty, the approach of [EF] is to hypothesize the required bound. It is not obvious that this hypothesis is valid for numerical schemes. For example, there are certainly local regions where, for short times, virtually uncontrolled growth of the exact and also the numerical solution can occur. In these regions, the error can also grow at an uncontrolled rate, thereby activating unphysical behavior in the numerics: consequently, far from being a hypothesis, an estimate of the maximum pointwise value of the numerical solution becomes an essential part of the numerical analysis of the problem.

In this report we will analyze a Dirichlet problem for the Cahn–Hilliard equation using a mixed formulation. The physical importance of the Dirichlet problem was pointed out to us by M. E. Gurtin: it governs the propagation of a solidification front into an ambient medium which is at rest relative to the front. Our analysis will be for the one-dimensional case. Extension to higher dimensions is feasible, and will be addressed in our subsequent report. In the next section, the mixed problem is formulated and existence and uniqueness theorems are proved. These proofs are based on compactness methods for a semidiscrete approximation sequence. In § 3 we present a new finite element based fully discrete scheme. The most important feature of this scheme is that it has a Lyapunov functional. This permits us to prove long time existence and uniqueness for the scheme, as well as the pointwise estimates referred to above. Error analysis for both the semidiscrete scheme using finite elements, and the fully discrete scheme are in § 4. In this section, we also give a finite difference method which is likely to be useful in some nonlinear situations. Finally, § 5 contains some additional comments.

2. Existence and uniqueness. The problem we consider is the following:

$$\frac{\partial u}{\partial t}+\sigma\frac{\partial^4 u}{\partial x^4}=\frac{\partial^2\phi(u)}{\partial x^2},\qquad 0<x<1,\quad 0<t\leqq T,$$

$$u(0,t)=u(1,t)=0,$$

$$\frac{\partial^2 u}{\partial x^2}(0,t)=\frac{\partial^2 u}{\partial x^2}(1,t)=0,$$

$$u(x,0)=u_0(x),$$

where

$$\phi(u)=\gamma_2u^3+\gamma_1u^2+\gamma_0u,\qquad \gamma_2>0,$$

and $\sigma>0$ is constant.

Let $p=\sigma u_{xx}-\phi(u)$, $p(0,t)=p(1,t)=0$. Then, formally, we have, for any $v\in H_0^1(0,1)$,

$$\langle u_t, v\rangle+\langle p_{xx}, v\rangle=0,$$

where $\langle f,g\rangle=\int_0^1 f(x)\overline{g(x)}\,dx$, and $H_0^1(0,1)$ denotes the standard Sobolev space

$$\{u\in L^2(0,1)\,|\,u_x\in L^2(0,1),\ u(0)=u(1)=0\}$$

normed by

$$\|u\|_{1,2}^2=\int_0^1 u^2\,dx+\int_0^1 u_x^2\,dx.$$

Integrating the second term by parts, we get

$$\langle u_t, v\rangle - \langle p_x, v_x\rangle = 0.$$

Similarly, for any $w \in H_0^1(0,1)$,

$$\langle p, w\rangle = \langle \sigma u_{xx}, w\rangle - \langle \phi(u), w\rangle = -\sigma\langle u_x, w_x\rangle - \langle \phi(u), w\rangle.$$

Now, let us use $L^2[(0,T), H_0^1(0,1)]$ to denote

$$\left\{ f(\cdot, t) \in H_0^1(0,1), \int_0^T \|f(\cdot,t)\|_{1,2}^2 \, dt < \infty \right\}.$$

Let

$$L^\infty[(0,T), H_0^1(0,1)] = \left\{ f(\cdot,t) \in H_0^1(0,1), \operatorname*{ess\,sup}_{0<t<T} \|f(\cdot,t)\|_{1,2} < \infty \right\}.$$

Then, the above discussion suggests the following weak formulation.

Given $u_0 \in H_0^1(0,1)$, find $u(t) \in L^\infty[(0,T), H_0^1(0,1)]$ and $p(t) \in L^2[(0,T), H_0^1(0,1)]$ such that, for any $v, w \in H_0^1(0,1)$,

$$\frac{d}{dt}\langle u(t), v\rangle - \langle p(t)_x, v_x\rangle = 0, \tag{2.1}$$

$$\langle p(t), w\rangle + \sigma\langle u(t)_x, w_x\rangle + \langle \phi(u(t)), w\rangle = 0, \tag{2.2}$$

$$u(x,0) = u_0(x). \tag{2.3}$$

We shall use the usual Faedo–Galerkin approach to establish the existence of a solution for problem (2.1)–(2.3).

First, choose a sequence of finite-dimensional spaces $\{S_k\}$, $k = 1, 2, \cdots$, such that

$$S_k \subset H_0^1(0,1), \qquad k = 1, 2, \cdots$$

and $\bigcup_{k=1}^\infty S_k$ is dense in $H_0^1(0,1)$.

Then we formulate the following approximation problem.

Find $(U^k, P^k) : [0,T] \to [S_k]^2$ such that, for any $v, w \in S_k$,

$$\frac{d}{dt}\langle U^k(t), v\rangle - \langle D_x P^k(t), D_x v\rangle = 0, \tag{2.4}$$

$$\langle P^k(t), w\rangle + \sigma\langle D_x U^k(t), D_x w\rangle + \langle \phi(U^k(t)), w\rangle = 0, \tag{2.5}$$

$$U^k(0) = u_0^k, \tag{2.6}$$

where D_x denotes differentiation with respect to x and u_0^k is the $H_0^1(0,1)$ projection of u_0 onto S_k. Note that $\|u_0^k - u_0\|_{1,2} \to 0$ as $k \to +\infty$.

Later, we will use finite element spaces to replace S_k. The resulting schemes are called finite element semidiscrete schemes. The same semidiscrete scheme is also introduced in a recent work [EFM].

An important feature of (2.1)–(2.2) is that we can define a Lyapunov functional

$$\mathscr{F}(u) = \int_0^1 \left(\frac{\sigma}{2}|D_x u|^2 + \mathscr{H}(u) \right) dx,$$

where

$$\mathscr{H}(u) = \int_0^u \phi(u)\, du. \tag{2.7}$$

In a similar way, we have for (2.4)–(2.6), the following lemma.

LEMMA 2.1. *Let* $u_0^k \in H_0^1(0,1)$; *then*

$$\frac{d}{dt}\mathscr{F}(U^k) = \int_0^1 \sigma D_x U^k D_x U_t^k + \phi(U^k) U_t^k \, dx$$
$$= -\int_0^1 P^k U_t^k \, dx$$
$$= -\int_0^1 D_x P^k D_x P^k \, dx$$
$$= -\|D_x P^k\|_{0,2}^2.$$

From this follows Corollary 2.1.

COROLLARY 2.1. *If* $u_0^k \in H_0^1(0,1)$, *then*

$$\|U^k\|_{1,2} \leqq C \quad \text{a.e. for } t \in (0, T).$$

Consequently, $\|U^k\|_{0,\infty} \leqq C'$ *where the constants* C *and* C' *depend only on* $\|u_0\|_{1,2}$.

From this pointwise boundedness of U^k, it follows that ϕ' becomes uniformly bounded and hence ϕ is Lipschitz continuous. Consequently, Picard's classical theorem, e.g., [BD, § 2.12] on the existence and uniqueness of solutions for ordinary differential equations gives Theorem 2.1.

THEOREM 2.1. *For any* $T > 0$, *if* $u_0^k \in H_0^1(0,1)$, *then* (2.4)–(2.6) *has a unique solution* $(U^k(t), P^k(t))$ *in* $L^\infty[(0,T), H_0^1(0,1)] \times L^2[(0,T), H_0^1(0,1)]$.

Next, using the Fourier transform we establish some estimates on the time derivatives of U^k.

Let $U^k(t)$, $P^k(t)$ be extended by zero outside the time interval $[0, T]$.

LEMMA 2.2. *Let* $(\hat{U}^k, \hat{P}^k)$ *be the Fourier transform in time of* (U^k, P^k). *Then, for* $0 < \alpha < \frac{1}{4}$, *there exists* $C > 0$, *depending only on* α, T, *and* $\|u_0\|_{1,2}$, *such that*

$$\int_{-\infty}^{+\infty} |\tau|^{2\alpha} \|\hat{U}^k(\tau)\|_{0,2}^2 \, d\tau \leqq C.$$

Proof. Taking the Fourier transform of the weak forms (2.4)–(2.5), we have

$$i\tau\langle \hat{U}^k(\tau), v\rangle - \langle D_x\hat{P}^k(\tau), D_x v\rangle = \langle u_0^k, v\rangle - e^{i\tau T}\langle U^k(T), v\rangle$$

and

$$\langle \hat{P}^k(\tau), w\rangle + \langle \sigma D_x \hat{U}^k(\tau), D_x w\rangle + \langle \hat{\phi}(U^k), w\rangle = 0.$$

Then, letting $v = \sigma\hat{U}^k$ and $w = \hat{P}^k$, and adding the equations together, we get

$$i\sigma\tau\langle \hat{U}^k(\tau), \hat{U}^k(\tau)\rangle + \langle \hat{P}^k(\tau), \hat{P}^k(\tau)\rangle$$
$$= \langle -\hat{\phi}(U^k), \hat{P}^k(\tau)\rangle + \sigma\langle u_0, \hat{U}^k(\tau)\rangle - \sigma\, e^{i\tau T}\langle U^k(T), \hat{U}^k(\tau)\rangle.$$

Taking imaginary parts, we see that

$$\sigma|\tau| \, \|\hat{U}^k(\tau)\|_{0,2}^2 \leqq C\{\|\hat{\phi}(U^k)\|_{0,2}^2 + \|\hat{P}^k(\tau)\|_{0,2}^2 + \|\hat{U}^k(\tau)\|_{0,2}\}.$$

Note that $\int_{-\infty}^{+\infty} \|\hat{U}^k(\tau)\|_{0,2}^2 \leqq C$, $\int_{-\infty}^{+\infty} \|\hat{P}^k(\tau)\|_{0,2}^2 \leqq C$, and $\int_{|\tau|\geqq 1} \tau^{4\alpha-2} \leqq C$ if $\alpha < \frac{1}{4}$, where C is a constant independent of k. Then, for $|\tau| \leqq 1$, $\int_{|\tau|\leqq 1} |\tau|^{2\alpha} \|\hat{U}^k(\tau)\|_{0,2}^2 \leqq \int_{|\tau|\leqq 1} \|\hat{U}^k(\tau)\|_{0,2}^2 \leqq C$ and, for $|\tau| \geqq 1$ and $0 < \alpha < \frac{1}{4}$,

$$|\tau|^{2\alpha} \|\hat{U}^k(\tau)\|_{0,2}^2 \leqq C\{|\tau|^{2\alpha-1}(\|\hat{\phi}(U^k)\|_{0,2}^2 + \|\hat{P}^k(\tau)\|_{0,2}^2) + |\tau|^{2\alpha-1}\|\hat{U}^k(\tau)\|_{0,2}\}$$
$$\leqq C'\{\|\hat{\phi}(U^k)\|_{0,2}^2 + \|\hat{P}^k(\tau)\|_{0,2}^2 + |\tau|^{4\alpha-2} + \|\hat{U}^k(\tau)\|_{0,2}^2\}.$$

Since $\|U^k(t)\|_{0,\infty} \leqq C$ almost everywhere for $t \in (0, T)$,

$$\int_{|\tau| \geqq 1} \|\hat{\phi}(U^k(\tau))\|_{0,2}^2 \, d\tau \leqq C \int_0^T \|U^k(t)\|_{0,2}^2 \, dt.$$

Hence

$$\int_{|\tau| \geqq 1} |\tau|^{2\alpha} \|\hat{U}^k(\tau)\|_{0,2}^2 \, d\tau \leqq C \left[\int_0^T \|U^k(t)\|_{0,2}^2 \, dt + \int_{|\tau| \geqq 1} |\tau|^{4\alpha - 2} \, d\tau \right] + C$$
$$\leqq C. \qquad \square$$

Let

$$H^\alpha[\mathbb{R}, L^2(0,1)] = \left\{ f(x,t) \,\middle|\, \int_{\mathbb{R}} (\|\hat{f}(\cdot, \tau)\|_{0,2}^2 + |\tau|^{2\alpha} \|\hat{f}(\cdot, \tau)\|_{0,2}^2) \, d\tau < \infty \right\},$$

and

$$H^\alpha[(0,T), L^2(0,1)] = \{ f(x,t) \mid \exists g \in H^\alpha[\mathbb{R}, L^2(0,1)], \text{ such that } f = g|_{(0,T)} \}.$$

Then, Lemma 2.2 implies that for $k = 1, 2, \cdots$, the solutions $(U^k(t), P^k(t))$ satisfy

$$U^k \in L^\infty[(0,T), H_0^1(0,1)] \cap H^\alpha((0,T), L^2(0,1)], \qquad 0 < \alpha < \tfrac{1}{4}, \tag{2.8}$$

and

$$P^k \in L^2[(0,T), H_0^1(0,1)], \tag{2.9}$$

and in addition, they are uniformly bounded with respect to k in these spaces. Hence, we can extract a subsequence weakly (or weakly *) convergent to a pair (U, P).

By Lions' compactness lemma [LM, § 16, Chap. 1], we can extract a further subsequence $\{U^{k_l}\}$ such that $U^{k_l} \to U$ almost everywhere for $(x,t) \in (0,1) \times (0,T)$ as $l \to \infty$. Thus, by passing to the limit, we see that the weak limit (U, P) satisfies (2.1)–(2.3). We now have the following theorem.

THEOREM 2.2. *Let $T > 0$, $u_0 \in H_0^1(0,1)$. Then, there exists a unique solution of* (2.1)–(2.3), (U, P), *and moreover,*

$$U \in L^\infty[(0,T), H_0^1(0,1)] \cap H^\alpha[(0,T), L^2(0,1)], \qquad P \in L^2[(0,T), H_0^1(0,1)]$$

and

$$\mathcal{F}(U(t)) \leqq \mathcal{F}(u_0) \quad \text{a.e. for } t \in (0,T).$$

Proof. We note first that bounds on the solutions can be obtained as in Lemmas 2.1 and Lemma 2.2. Thus, only the uniqueness remains to be proved. But this can be verified by an energy estimate following from the fact that U is bounded in $L^\infty[(0,1) \times (0,T)]$ and $\phi(U)$ is locally Lipschitz continuous. $\square$

As a consequence of the uniqueness, we see that the weak limit is independent of the choice of the subsequence. Hence, the convergence of the whole sequence follows.

COROLLARY 2.2. *Let $T > 0$, $u_0 \in H_0^1(0,1)$ be given, and $u_0^k \to u_0$ in $H_0^1(0,1)$ as $k \to +\infty$. Then, the sequence $\{(U^k, P^k)\}$ converges weakly (or weakly *) to the solution of* (2.1)–(2.3) *in*

$$[L^\infty((0,T), H_0^1(0,1)) \cap H^\alpha((0,T), L^2(0,1))] \times L^2((0,T), H_0^1(0,1)).$$

In particular, if we let the spaces $\{S_k\}$ be finite element spaces $\{S_{h_k}^r\}$ defined for a regular partition $0 = x_0 < x_1 < \cdots < x_{n_k - 1} < x_{n_k} = 1$, with $h_k = \max_{0 \leqq i \leqq n_k - 1} |x_{i+1} - x_i|$, by

$$S_h^r = \{ g \in C^0[0,1], g|_{[x_i, x_{i+1}]} \in P_r([x_i, x_{i+1}]), g(0) = g(1) = 0 \},$$

and we let u_0^k be the H_0^1 projection of u_0 onto $S_{h_k}^r$, then, as $h_k \to 0$ $(k \to +\infty)$, we see that the finite element solutions have the weak convergence property as above. Error estimates for them will be given later.

3. A fully discrete scheme. For practical computations, fully discrete methods are used most. In this section, we shall present a fully discrete scheme and establish its solvability and the existence of a Lyapunov functional.

A different fully discrete scheme is given in [EF] based on a direct formulation using C^1-finite element spaces. Except for the error estimate of [EF], which is given under the hypothesis that the discrete solutions are pointwise bounded, there seems to be no other rigorous analysis available for fully discrete schemes.

To introduce the fully discrete scheme we first define the following function:

$$\tilde{\phi}(u, v) := \begin{cases} [\mathcal{H}(u) - \mathcal{H}(v)]/(u - v) & \text{if } u \neq v, \\ \phi(u) & \text{if } u = v \end{cases}$$

where $\mathcal{H}$ is defined by (2.7).

We can write $\tilde{\phi}(u, v)$ explicitly, as follows:

$$\tilde{\phi}(u, v) = \frac{\gamma_2}{4}(u^3 + u^2 v + u v^2 + v^3) + \frac{1}{3}\gamma_1(u^2 + uv + v^2) + \frac{\gamma_0}{2}(u + v).$$

It is obvious that

$$\tilde{\phi}(u, v) \to \phi(u) \quad \text{as } v \to u.$$

Next, let $\Delta t = T/N$, for a positive integer N. Then we formulate the following fully discrete problem.

Find $(U_n, P_n) \in S_h^r \times S_h^r$, $n = 0, 1, 2, \cdots, N$, such that, for all v^h, $w^h \in S_h^r$,

$$U^0 = u_0^h, \tag{3.1}$$

$$\langle \delta_t U_{n+(1/2)}, v^h \rangle - \langle D_x P_{n+1}, D_x v^h \rangle = 0, \tag{3.2}$$

$$\langle P_{n+1}, w^h \rangle + \sigma \langle D_x U_{n+(1/2)}, D_x w^h \rangle + \langle \tilde{\phi}(U_n, U_{n+1}), w^h \rangle = 0, \tag{3.3}$$

where $U_{n+(1/2)} = \frac{1}{2}(U_n + U_{n+1})$ and $\delta_t U_{n+(1/2)} = (1/\Delta t)(U_{n+1} - U_n)$.

For now, we assume (3.1)-(3.3) is well posed, although the well posedness will be discussed shortly. It is interesting to note that $\mathcal{F}(u)$ remains a discrete Lyapunov functional for (3.1)-(3.3). In fact, if (U_n, P_n) solves (3.1)-(3.3), then we have Lemma 3.1.

LEMMA 3.1. $(1/\Delta t)[\mathcal{F}(U_{n+1}) - \mathcal{F}(U_n)] + \|D_x P_{n+1}\|_{0,2}^2 = 0$ *for* $n = 0, 1, 2, \cdots, N$.

Proof. By using (3.2)-(3.3) and the definition of $\mathcal{F}(\cdot)$, we obtain

$$\begin{aligned} \frac{1}{\Delta t}[\mathcal{F}(U_{n+1}) - \mathcal{F}(U_n)] &= \sigma \langle D_x U_{n+(1/2)}, D_x \delta_t U_{n+(1/2)} \rangle + \langle \tilde{\phi}(U_n, U_{n+1}), \delta_t U_{n+(1/2)} \rangle \\ &= -\langle P_{n+1}, \delta_t U_{n+(1/2)} \rangle \\ &= -\langle \delta_t U_{n+(1/2)}, P_{n+1} \rangle \\ &= -\langle D_x P_{n+1}, D_x P_{n+1} \rangle. \qquad \square \end{aligned}$$

Note that this proof is similar to the proof of Lemma 2.1.

From Lemma 3.1, if the solutions exist, then their boundedness follows.

COROLLARY 3.1. *Let T be given, and $u_0 \in H_0^1(0, 1)$. If (U_n, P_n) exists, then*

$$\|U_n\|_{1,2} \leqq C; \quad \textit{moreover, } \|U_n\|_{0,\infty} \leqq C' \quad \textit{for } 0 < n \leqq N,$$

where C and C' are constants.

We now present an existence theorem for the solutions (U_n, P_n), which also provides a constructive approach to finding them.

First, we define mappings $\mathcal{T}_v: S_h^r \to S_h^r$, $v \in S_h^r$, such that for $u \in S_h^r$, $U = \mathcal{T}_v(u)$ satisfies, for any q^h, $w^h \in S_h^r$,

$$\langle U, q^h\rangle - \Delta t\langle D_x P, D_x q^h\rangle = \langle v, q^h\rangle, \tag{3.4}$$

$$\langle P, w^h\rangle + \frac{\sigma}{2}\langle D_x U, D_x w^h\rangle = -\frac{\sigma}{2}\langle D_x v, D_x w^h\rangle - \langle \tilde{\phi}(u, v), w^h\rangle \tag{3.5}$$

for some $P \in S_h^r$.

LEMMA 3.2. *$\mathcal{T}_v$ is well defined for any $\Delta t > 0$ and $v \in S_h^r$.*

Proof. Let $\{w_i\}_{i=1}^M$ be a basis for S_h^r,

$$A_{ij} = \langle w_i, w_j\rangle, \qquad B_{ij} = \langle D_x w_i, D_x w_j\rangle,$$

and $A = (A_{ij})$, $B = (B_{ij})$. Then U and P can be written as $U = \sum_{i=1}^n U_i w_i$, $P = \sum_{i=1}^n P_i w_i$. Let

$$\tilde{U} = \begin{pmatrix} U_1 \\ \vdots \\ U_n \end{pmatrix} \text{ and } \tilde{P} = \begin{pmatrix} P_1 \\ \vdots \\ P_n \end{pmatrix}.$$

We have from (3.4) and (3.5) that for some vector $\tilde{f}$,

$$\begin{pmatrix} A & -\Delta t B \\ (\sigma/2)B & A \end{pmatrix}\begin{pmatrix} \tilde{U} \\ \tilde{P} \end{pmatrix} = \tilde{f}.$$

$$M = \begin{pmatrix} A & -\Delta t B \\ (\sigma/2)B & A \end{pmatrix}$$

is invertible since A and $A + (\sigma/2)\Delta t B A^{-1} B$ are invertible for any $\Delta t > 0$, so $\mathcal{T}_v$ is well defined. □

$\mathcal{T}_v$ will be used to investigate the well posedness of the fully discrete scheme (3.1)-(3.3).

LEMMA 3.3. *For any integer $n \geqq 0$, (3.1)-(3.3) has a solution (U^{n+1}, P^{n+1}) if and only if $\mathcal{T}_v$ has a fixed point for $v = U^n$.*

The proof is straightforward and is omitted. Next, we give a sufficient condition under which $\mathcal{T}_v$ is a contractive mapping. For that, we assume that the standard inverse estimates hold for the finite element spaces S_h^r [C].

LEMMA 3.4. *Fix $\alpha > 0$. Assume that $v \in S_h^r$ and $\|v\|_{0,2} \leqq \alpha$; then there exists a constant $\beta > 0$ such that, if $\Delta t/h^2 < \beta$, then $\mathcal{T}_v$ is a contraction mapping from the ball $K = \{u \in S_h^r: \|u\|_{0,2} \leqq 2\alpha\}$ into itself.*

Proof. Let $q^h = (\sigma/2)(U + v)$ and $w^h = \Delta t P$ in (3.4) and (3.5), respectively. We get

$$\frac{\sigma}{2}\|U\|_{0,2}^2 - \frac{\sigma(\Delta t)}{2}\langle D_x P, D_x(U+v)\rangle = \frac{\sigma}{2}\|v\|_{0,2}^2$$

and

$$\Delta t\|P\|_{0,2}^2 + \frac{\sigma(\Delta t)}{2}\langle D_x(U+v), D_x P\rangle = -\langle \tilde{\phi}(u, v), \Delta t P\rangle.$$

Adding these two equations together,

$$\frac{\sigma}{2}\|U\|_{0,2}^2 + \Delta t\|P\|_{0,2}^2 = \frac{\sigma}{2}\|v\|_{0,2}^2 - \Delta t\langle \tilde{\phi}(u, v), P\rangle,$$

so that

$$\|U\|_{0,2}^2 \leqq \|v\|_{0,2}^2 + \frac{\Delta t}{\sigma}\|\tilde{\phi}(u, v)\|_{0,2}^2.$$

By inverse estimates, we have that there exists a constant $C > 0$, independent of h and α, such that, for $\|u\|_{0,2} \leqq 2\alpha$,

$$\|u\|_{0,\infty} \leqq C\alpha h^{-1/2} \quad \text{and} \quad \|v\|_{0,\infty} \leqq C\alpha h^{-1/2}.$$

This gives that for some constant $d > 0$,

$$\|\tilde{\phi}(u, v)\|_{0,2} \leqq d h^{-1}\alpha^3,$$

so,

$$\begin{aligned}\|U\|_{0,2}^2 &\leqq \|v\|_{0,2}^2 + \frac{\Delta t}{\sigma}\cdot d^2\alpha^6 h^{-2}\\ &\leqq \alpha^2 + \frac{\Delta t}{\sigma} d^2\alpha^4 h^{-2}\alpha^2.\end{aligned}$$

If we let $\beta_1 = 3\sigma/d^2\alpha^4$, then for $\Delta t/h^2 < \beta_1$, we have

$$\|U\|_{0,2}^2 \leqq 4\alpha^2,$$

i.e.,

$$\|U\|_{0,2} \leqq 2\alpha.$$

Thus, we see that $\mathcal{T}_v$ maps K into itself.

Similarly, for $u, u' \in K$, we can get for $U = \mathcal{T}_v(u)$ and $U' = \mathcal{T}_v(u')$:

$$\|U - U'\|_{0,2}^2 \leqq \frac{2\Delta t}{\sigma}\|\tilde{\phi}(u, v) - \tilde{\phi}(u', v)\|_{0,2}^2.$$

Since there exists constant d' satisfying

$$\|\tilde{\phi}(u, v) - \tilde{\phi}(u', v)\|_{0,2} \leqq d'\alpha^2 h^{-1}\|u - u'\|_{0,2},$$

we have

$$\|U - U'\|_{0,2}^2 \leqq \frac{2d'^2\alpha^4\Delta t}{\sigma h^2}\|u - u'\|_{0,2}^2.$$

If we let $\beta_2 = \sigma/2d'^2\alpha^4$ and $\Delta t/h^2 < \beta_2$, then there exists a constant γ, $0 < \gamma < 1$, such that

$$\|U - U'\|_{0,2} \leqq \gamma\|u - u'\|_{0,2},$$

i.e., $\mathcal{T}_v$ is a contraction mapping if $\Delta t/h^2 < \beta = \min(\beta_1, \beta_2)$. □

COROLLARY 3.2. *Let $U^n \in S_h^r$, $\|U^n\|_{0,2} \leqq C$ for some integer $n \geqq 0$; then there exists a unique solution for problem* (3.1)–(3.3), *provided that Δt is sufficiently small.*

Finally, we combine the above results to give a concrete theorem regarding the well posedness of the fully discrete scheme.

THEOREM 3.1. *Let u_0 belong to $H_0^1(0, 1)$. There exists a constant $C > 0$, depending only on u_0 and constants in the inverse estimates, such that for $\Delta t/h^2 < C$, problem* (3.1)–(3.3) *has a unique solution for all $n \geqq 0$.*

Proof. By Corollary 3.2, we know there exists $C_n > 0$ such that (3.1)-(3.3) has a unique solution for the corresponding integer n, if $\Delta t/h^2 < C_n$. The only dependence of C_n on the integer n is the dependence of C_n on $\|U^n\|_{0,2}$. However, by Corollary 3.1, $\|U^n\|_{0,2}$ can be uniformly bounded, independently of n. Thus, the choice of C_n can also be made independent of n. □

We remark that, after the above discussion, we could take nonuniform timesteps. In addition, the condition $\Delta t/h^2 < C$ is sufficient but not necessary. Problem (3.1)-(3.3) may have a solution for much larger Δt.[1]

4. Error estimates for the approximation schemes. First, we consider the semidiscrete finite element schemes that can be obtained from (2.4)-(2.6) with the superscript k being replaced by the subscript h, where the modification has been explained at the end of § 2. The convergence also follows from the discussion there. We now present error estimates for such schemes.

Let us define $\Pi_h : H_0^1(0,1) \to S_h^r$ to be a linear mapping such that for all $w \in H_0^1(0,1)$, $\Pi_h w$ satisfies

$$\langle D_x \Pi_h w, D_x V^h \rangle = \langle D_x w, D_x V^h \rangle \quad \forall V^h \in S_h^r.$$

The following is well known.

LEMMA 4.1. *Π_h is a bounded mapping, and its bound is independent of h. Moreover, for $w \in H_0^1(0,1)$,*

$$\|\Pi_h w - w\|_{1,2} \leqq \inf_{w^h \in S_h^r} \|w^h - w\|_{1,2} \leqq ch^r \|w\|_{r+1,2} \quad \text{if } w \in H^{r+1}(0,1).$$

From a standard duality argument we also have

$$\|\Pi_h w - w\|_{0,2} \leqq ch^{r+1}\|w\|_{r+1,2}.$$

LEMMA 4.2. *There exists a constant $C > 0$ which depends only on $\|U^0\|_{1,2}$ such that $\|\phi(U^h(t)) - \phi(u(t))\|_{0,2} \leqq C\|U^h(t) - u(t)\|_{0,2}$.*

Proof. This follows from the local Lipschitz continuity of ϕ and the pointwise boundedness of U_h and u.

THEOREM 4.1. *There exists a constant C which depends only on T and u_0 but not h, such that, for all $t \in (0, T)$,*

$$\|U^h(t) - u(t)\|_{L^2}^2 \leqq \|u(t) - \Pi_h u(t)\|_{L^2}^2 + c\left\{\|u_0^h - u_0\|_{L^2}^2 + \int_0^t [\|D_t(u(\tau) - \Pi_h u(\tau))\|_{L^2}^2 + \|u(\tau) - \Pi_h u(\tau)\|_{L^2}^2 + \|p(\tau) - \Pi_h p(\tau)\|_{L^2}^2]\, dt\right\}$$

and

$$\int_0^t \|P^h(\tau) - p(\tau)\|_{L^2}^2\, d\tau \leqq C\left\{\|u_0^h - u_0\|_{L^2}^2 + \int_0^T [\|D_t(u(\tau) - \Pi_h u(\tau))\|_{L^2}^2 + \|u(\tau) - \Pi_h u(\tau)\|_{L^2}^2 + \|p(\tau) - \Pi_h p(\tau)\|_{L^2}^2]\, d\tau\right\}.$$

Proof. Define

$$E^h(t) = U^h(t) - \Pi_h u(t), \qquad 0 \leqq t \leqq T,$$
$$F^h(t) = P^h(t) - \Pi_h p(t), \qquad 0 \leqq t \leqq T.$$

[1] This turns out to be true. Further discussions are made in our subsequent report.

Both E^h and F^h are in S_h^r. From §§ 2 and 3 E^h and F^h satisfy the equations

$$\langle D_t E^h(t), V^h\rangle - \langle D_x F^h(t), D_x V^h\rangle = \langle D_t \xi(t), V^h\rangle \quad \forall V^h \in S_h^r, \tag{4.1}$$

where $\xi(t) = u(t) - \Pi_h u(t)$. Also,

$$\langle F^h(t), w^h\rangle + \langle \sigma D_x E^h(t), D_x w^h\rangle = \langle \phi(U^h(t)) - \phi(u(t)), w^h\rangle + \langle \eta(t), w^h\rangle \qquad \forall w^h \in S_h^r, \tag{4.2}$$

where $\eta(t) = p(t) - \Pi_h p(t)$. Now, taking $V^h = \sigma E^h(t)$ in (4.1) and taking $w^h = F^h(t)$ in (4.2), addition of the resulting relations gives

$$\frac{\sigma}{2}\frac{d}{dt}\|E^h(t)\|_{L^2}^2 + \|F^h(t)\|_{L^2}^2 \leqq \frac{\sigma}{2}\|D_t\xi(t)\|_{L^2}^2 + \frac{\sigma}{2}\|E^h(t)\|_{L^2}^2$$
$$+\|\phi(U^h(t)) - \phi(u(t))\|_{L^2}^2 + \|\eta(t)\|_{L^2}^2 + \frac{1}{2}\|F^h(t)\|_{L^2}^2.$$

Hence, using Lemma 4.2, we get

$$\frac{\sigma}{2}\frac{d}{dt}\|E^h(t)\|_{L^2}^2 + \frac{1}{2}\|F^h(t)\|_{L^2}^2 - \frac{\sigma}{2}\|E^h(t)\|_{L^2}^2$$
$$\leqq \frac{\sigma}{2}\|D_t\xi(t)\|_{L^2}^2 + C\|U^h(t) - u(t)\|_{L^2}^2 + \|\eta(t)\|_{L^2}^2$$
$$\leqq \frac{\sigma}{2}\|D_t\xi(t)\|_{L^2}^2 + C\|\xi(t)\|_{L^2}^2 + \|\eta(t)\|_{L^2}^2 + C\|E^h(t)\|_{L^2}^2,$$

i.e., for some $\lambda > 0$,

$$\frac{d}{dt}\|E^h(t)\|_{0,2}^2 + \frac{1}{\sigma}\|F^h(t)\|_{0,2}^2 - \lambda\|E^h(t)\|_{0,2}^2 \leqq \|D_t\xi(t)\|_{0,2}^2 + C\|\xi(t)\|_{0,2}^2 + \frac{2}{\sigma}\|\eta(t)\|_{0,2}^2.$$

Use of Gronwall's inequality now gives the result. □

As a consequence of this we can show that the error is of optimal order under proper regularity assumptions on the solution u.

COROLLARY 4.1. *Assume that u, u_t and $p \in H^{r+1}(0,1)$. Then there exists a constant C', independent of h, such that*

$$\|U^h(t) - u(t)\|_{0,2} \leqq C'h^{r+1} \quad \forall t \in (0, T).$$

Proof. By Lemma 4.1, we have

$$\|u(\tau) - \Pi_h u(\tau)\|_{0,2} \leqq Ch^{r+1} \quad \text{for some } C > 0.$$

Similarly,

$$\|D_t u(t) - \Pi_h D_t u(\tau)\|_{0,2} \leqq Ch^{r+1},$$

and

$$\|p(\tau) - \Pi_h p(\tau)\|_{0,2} \leqq Ch^{r+1}.$$

Combining these estimates with Theorem 4.1, we get the desired optimal order error estimate.

Next, we present the error estimate for the fully discrete scheme which is given in § 3. The derivation of this estimate is similar to the one above. However, Lemma 4.2 will be modified to give a discrete version.

LEMMA 4.3. *Let* $t_{n+(1/2)}=\frac{1}{2}(t_n+t_{n+1})$; *then there exists a constant* $C'>0$ *such that*

$$\|\tilde{\phi}(U^n, U^{n+1})-\phi(u(t_{n+(1/2)}))\|_{0,2}$$
$$\leqq C'\left\{\|U^{n+1}-u(t_{n+1})\|_{0,2}+\|U^n-u(t_n)\|_{0,2}\right.$$
$$\left.+\|u(t_n)-u(t_{n+1})\|_{0,4}^2+\left\|\frac{u(t_n)+u(t_{n+1})}{2}-u(t_{n+(1/2)})\right\|_{0,2}\right\}.$$

Proof. Let $u_{n+(1/2)}=\frac{1}{2}(u(t_n)+u(t_{n+1}))$. By the triangle inequality,

$$\|\tilde{\phi}(U^n, U^{n+1})-\phi(u(t_{n+(1/2)}))\|_{0,2}$$
$$\leqq\|\tilde{\phi}(U^n, U^{n+1})-\tilde{\phi}(U^n, u(t_{n+1}))\|_{0,2}+\|\tilde{\phi}(U^n, u(t_{n+1}))-\tilde{\phi}(u(t_n), u(t_{n+1}))\|_{0,2}$$
$$+\|\tilde{\phi}(u(t_n), u(t_{n+1}))-\phi(u_{n+(1/2)})\|_{0,2}+\|\phi(u_{n+(1/2)})-\phi(u(t_{n+(1/2)}))\|_{0,2}$$
$$=I_1+I_2+I_3+I_4,$$

where $\{I_i\}$ $(i=1,2,3,4)$ denote the terms in the summation in their corresponding order.

Since $\|U^n\|_{0,\infty}$, $\|u(t)\|_{0,\infty}$ are uniformly bounded with respect to $n=1,2,\cdots,N$, and $t\in(0,T)$, it easily follows that

$$I_1\leqq C\|U^{n+1}-u(t_{n+1})\|_{0,2},$$
$$I_2\leqq C\|u(t_n)-U^n\|_{0,2},$$
$$I_4\leqq C\|u_{n+(1/2)}-u(t_{n+(1/2)})\|_{0,2}$$
$$=C\left\|\frac{u(t_n)+u(t_{n+1})}{2}-u(t_{n+(1/2)})\right\|_{0,2}.$$

For the term I_3, recall the algebraic identities

$$\frac{u^2+uv+v^2}{3}-\left(\frac{u+v}{2}\right)^2\equiv\frac{1}{12}(u-v)^2,$$
$$\frac{u^3+u^2v+uv^2+v^3}{4}-\left(\frac{u+v}{2}\right)^3\equiv\frac{1}{8}(u+v)(u-v)^2.$$

Then,

$$\tilde{\phi}(u(t_n), u(t_{n+1}))-\phi(u_{n+(1/2)})=\left(\frac{\gamma_2}{4}u_{n+(1/2)}+\frac{\gamma_1}{12}\right)[u(t_n)-u(t_{n+1})]^2,$$

and thus,

$$I_3\leqq C\|u(t_n)-u(t_{n+1})\|_{0,4}^2.$$

These estimates on $\{I_i, i=1,2,3,4\}$ give the result. □

COROLLARY 4.2. *Let* $u_t\in L^4(0,1)$, $u_{tt}\in L^2(0,1)$. *Then*

$$\|\tilde{\phi}(U^n, U^{n+1})-\phi(u(t_{n+(1/2)}))\|_{0,2}\leqq C\{\|U^{n+1}-u(t_{n+1})\|_{0,2}+\|U^n-u(t_n)\|_{0,2}+(\Delta t)^2\}.$$

We now have the following estimate.

THEOREM 4.2. *There exists a constant $C>0$, independent of Δt and h, such that, for $n=1,2,\cdots,[T/\Delta t]$,*

$$\begin{aligned}\|U^n-u(t_n)\|_{0,2} &\leqq \|u(t_n)-\Pi_h u(t_n)\|_{0,2}\\ &\quad + C\Big\{\|u_0^h-u_0\|_{0,2}+(\Delta t)^2+\sum_{i=1}^{n-1}\Delta t\\ &\qquad \cdot[\|u(t_i)-\Pi_h u(t_i)\|_{0,2}+\|p(t_{i+(1/2)})-\Pi_h p(t_{i+(1/2)})\|_{0,2}\\ &\qquad +\|D_t(u(t_{i+(1/2)})-\Pi_h u(t_{i+(1/2)}))\|_{0,2}+\Delta t\\ &\qquad \cdot\|D_{tt}(u(t_{i+\theta})-\Pi_h u(t_{i+\theta})\|_{0,2}]\Big\},\end{aligned}$$

where $t_{i+\theta}=\theta t_i+(1-\theta)t_{i+1}$ for some constant θ, $0<\theta<1$, and D_t denotes $\partial/\partial t$.

Proof. Define

$$\begin{aligned}E^n &= U^n-\Pi_h u(t_n), \qquad n=0,1,2,\cdots,N,\\ F^{n+(1/2)} &= P^{n+1}-\Pi_h p(t_{n+(1/2)}),\\ E^{n+(1/2)} &= \tfrac{1}{2}(U^n+U^{n+1})-\Pi_h u(t_{n+(1/2)}),\\ \delta_t E^{n+(1/2)} &= \frac{E^{n+1}-E^n}{\Delta t},\end{aligned}$$

and

$$\begin{aligned}\delta_t u(t_{n+(1/2)}) &= \frac{u(t_{n+1})-u(t_n)}{\Delta t},\\ \delta_t \xi(t_{n+(1/2)}) &= \frac{\xi(t_{n+1})-\xi(t_n)}{\Delta t}.\end{aligned}$$

By the definition of the fully discrete scheme we see that the above quantities satisfy the following equations:

$$\begin{aligned}&\langle \delta_t E^{n+(1/2)}, V^h\rangle-\langle D_x F^{n+(1/2)}, D_x V^h\rangle\\ &\quad=\langle \delta_t u(t_{n+(1/2)})-D_t u(t_{n+(1/2)}), V^h\rangle+\langle \delta_t \xi(t_{n+(1/2)})-D_t\xi(t_{n+(1/2)}), V^h\rangle\\ &\qquad+\langle D_t\xi(t_{n+(1/2)}), V^h\rangle,\\ &\langle F^{n+(1/2)}, w^h\rangle+\langle \sigma D_x E^{n+(1/2)}, D_x w^h\rangle\\ &\quad=\langle \eta(t_{n+(1/2)}), w^h\rangle+\langle \tilde{\phi}(U^n, U^{n+1})-\phi(u(t_{n+(1/2)})), w^h\rangle.\end{aligned}$$

The rest of the proof is a discrete analogue of the approach used in the proof of Theorem 4.1, except that Lemma 4.3 needs to be used in place of Lemma 4.2. $\square$

Again, we remark that nonuniform timesteps can be used, with an almost identical analysis.

Finally, let us describe a simple difference approximation scheme which is likely to be useful in computations.

Again, let

$$\delta_t U_k^{n+(1/2)}=\frac{1}{\Delta t}(U_k^{n+1}-U_k^n),\ \delta_x U_k^{n+1}=\frac{1}{\Delta x}(U_{k+1}^{n+1}-U_k^{n+1})$$

for given Δt and Δx and define

$$U_k^0=u^0(x_k), \qquad k=0,1,\cdots,n_k.$$

For $n=0,1,2,\cdots,N-1$, $k=0,1,2,\cdots,n_k$, we seek (U_k^{n+1}, P_k^{n+1}) such that

$$\delta_t U_k^{n+(1/2)} + \delta_{-x}\delta_x P_k^{n+1} = 0, \qquad k=1,2,\cdots,n_k-1,$$
$$P_k^{n+1} = \sigma\delta_{-x}\delta_x U_k^{n+1} - \tilde{\phi}(U_k^n, U_k^{n+1}), \qquad k=1,2,\cdots,n_k-1$$
$$U_0^{n+(1/2)} = U_{n_k}^{n+(1/2)} = 0, \qquad P_0^{n+1} = P_{n_k}^{n+1} = 0.$$

We may define a discrete Lyapunov functional

$$\mathscr{F}^h(U^n) = \sum_{k=0}^{n_k-1} \frac{\sigma}{2} |\delta_x U_k^n|^2 + \sum_{k=0}^{n_k} \mathscr{H}(U_k^n).$$

Direct calculation using summation by parts gives

$$\frac{1}{\Delta t}[\mathscr{F}^h(U^{n+1}) - \mathscr{F}^h(U^n)] = -\sum_{k=0}^{K-1} (\delta_x P_k^{n+1})^2 \leqq 0.$$

Thus, a similar analysis to the one presented for the fully discrete scheme can be done for this.

5. Additional comments. We see nothing to prevent the application of our methods to the mass conserving boundary conditions (1.2), so that discrete schemes with Lyapunov functions can be used here, too.

On the other hand, in more than one space dimension new estimates are needed. In particular, Corollary 2.1, which is not valid in higher dimensions must be extended.

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REFERENCES

[EF] C. ELLIOTT AND D. FRENCH, *Numerical studies of the Cahn-Hilliard equation for phase separation*, IMA J. Appl. Math., 38 (1987), pp. 97–128.

[EFM] C. ELLIOTT, D. FRENCH, AND F. MILNER, *A second order splitting method for the Cahn-Hilliard equation*, Numer. Math., submitted.

[EZ] C. ELLIOTT AND ZHENG SONQMU, *On the Cahn-Hilliard equation*, Arch. Rational Mech. Anal., 96 (1986), pp. 339–357.

[BD] W. BOYCE AND R. DIPRIMA, *Elementary Differential Equations and Boundary Value Problems*, Third edition, John Wiley, New York, 1977.

[LM] J. LIONS AND E. MAGENES, *Nonhomogeneous Boundary Value Problems and Applications*, I, Springer-Verlag, New York, 1979.

[C] P. CIARLET, *The Finite Element Method for Elliptic Problems*, North-Holland, Amsterdam, 1978.