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UNIQUE SOLVABILITY AND ERROR ANALYSIS OF A SCHEME USING THE LAGRANGE MULTIPLIER APPROACH FOR GRADIENT FLOWS*

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Abstract. The unique solvability and error analysis of a scheme using the original Lagrange multiplier approach proposed in [Q. Cheng, C. Liu, and J. Shen, *Comput. Methods Appl. Mech. Engrg.*, 367 (2020), 13070] for gradient flows is studied in this paper. We identify a necessary and sufficient condition that must be satisfied for the nonlinear algebraic equation arising from the original Lagrange multiplier approach to admit a unique solution in the neighborhood of its exact solution. Then we find that the unique solvability of the original Lagrange multiplier approach depends on the aforementioned condition and may be valid over a finite time period. Afterward, we propose a modified Lagrange multiplier approach to ensure that the computation can continue even if the aforementioned condition was not satisfied. Using the Cahn–Hilliard equation as an example, we prove rigorously the unique solvability and establish optimal error estimates of a second-order Lagrange multiplier scheme assuming this condition and that the time step is sufficiently small. We also present numerical results to demonstrate that the modified Lagrange multiplier approach is much more robust and can use a much larger time step than the original Lagrange multiplier approach.

Key words. gradient flow, unique solvability, Lagrange multiplier approach, energy stable, error analysis

MSC codes. 65M12, 65M22, 65N15, 65N22

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1. Introduction.

We consider in this paper numerical approximations of a general gradient flow given by

$$\partial_t \phi = -\mathcal{G}\frac{\delta E}{\delta \phi}, \tag{1.1}$$

where $E(\phi) = \frac{1}{2}(\mathcal{L}^{1/2}\phi, \mathcal{L}^{1/2}\phi) + (F(\phi), 1)$, with $\mathcal{L}$ and $\mathcal{G}$ being positive definite operators on a suitable Hilbert space with inner product $(\cdot,\cdot)$, and $F(\phi)$ is a nonlinear potential function. An important property of (1.1) is an associated energy dissipation law:

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$$\frac{d}{dt}E = -\left(\mathcal{G}\frac{\delta E}{\delta \phi}, \frac{\delta E}{\delta \phi}\right). \tag{1.2}$$

It is highly desirable to design numerical schemes which can satisfy a discrete version of (1.2).

In recent years, a great deal of effort has been devoted to construct efficient and accurate energy dissipative schemes for various gradient flows in the form of (1.1); we refer the reader to [3, 15, 16, 21, 22, 28] and the references therein for more details. For example, the convex splitting method [2, 5, 12, 13, 14, 17, 18, 32], which treats the convex part implicitly and the concave part explicitly, ensures the unique solvability and unconditional energy stability at a theoretical level. On the other hand, the price of this numerical approach is associated with a nonlinear solver at each time step, due to the fact that the nonlinear terms in the gradient flow usually correspond to a convex energy. Moreover, some higher-order versions of this approach, in both the second and third accuracy orders, have been extensively studied [6, 7, 8, 11, 19, 20, 30], and the stability analysis for a modified energy functional, composed of the original free energy and a few numerical correction terms, has been reported. Again, a nonlinear solver has to be implemented in these higher-order energy stable schemes, which has always been a huge numerical challenge.

To avoid the difficulty associated with a nonlinear solver in the numerical implementation, many linear approach efforts have been made for various gradient flows. In particular, the stabilization method is applied to the Cahn–Hilliard equation [23, 24, 25, 29], in which an artificial regularization term is added to ensure the energy stability, either in terms of the original free energy or a modified energy functional, usually under a global Lipschitz condition on the nonlinear part of the free energy. On the other hand, the invariant energy quadratization approach proposed in [31] gives a linear and unconditionally energy stable (with respect to a modified energy) scheme, but it requires solving a linear system with variable coefficients. The original scalar auxiliary variable (SAV) approach, proposed in [27], leads to a linear, decoupled, and unconditionally energy stable (with respect to a modified energy) scheme, which is very efficient and easy to implement, while it is not energy dissipative with respect to the original energy. In fact, the key idea of the SAV approach is to rewrite the original energy into a modified formula. In turn, this numerical approach could only preserve a discrete modified energy dissipative law. On the other hand, the Lagrange multiplier approach is able to preserve a discrete dissipative law in an original formula. In particular, it preserves the original energy law if the original Crank–Nicolson scheme is used, and it preserves the original energy law with an additional higher-order dissipation term if a modified Crank–Nicolson scheme or second-order Backward Difference Formulas (BDF) is used. In more detail, the original Lagrange multiplier approach, proposed in [10], leads to a linear, decoupled, and unconditionally energy stable (with respect to the original energy) scheme, combined with a nonlinear algebraic equation for the Lagrange multiplier. In comparison with the nonlinearly implicit numerical methods for the PDEs, such as the convex-splitting method, the computational cost of solving one nonlinear algebraic equation is negligible, in which only a few Newton iterations are needed, in terms of a single parameter. In principle, this approach has essentially all the desired attributes for solving gradient flows; however, it is not clear whether the nonlinear algebraic equation admits a unique solution in the desired range.

Although there are ample numerical results indicating that the original Lagrange multiplier approach works well in many applications, there are cases where exceedingly small time steps are needed or one is unable to find a suitable solution of this nonlinear algebraic equation [1, 9]. Therefore, it is very important to identify condition(s) which can ensure the unique solvability, and modify the original Lagrange multiplier approach so that the computation can continue even if theses condition(s) are not satisfied.

We observe from (2.3), which is the last equation in the original Lagrange multiplier scheme (2.1)–(2.3), that the Lagrange multiplier $\eta^{n+1/2}$ cannot be uniquely determined around the exact solution $\eta(t)=1$ if $(F(\phi^{n+1})-F(\phi^n),1)=0$. Therefore, we make the following assumption on the exact solution:

$$|S_n| \geq \gamma \quad \text{with } S_n := \frac{d}{dt}\int_\Omega F(\Phi)\,d\boldsymbol{x}|_{t=t^n}, \tag{1.3}$$

where $0<\gamma\ll 1$ is a prescribed small number. This assumption, of course, cannot be satisfied a priori at every time step. Hence, it is necessary to modify the Lagrange multiplier approach so that the computation can continue even if (1.3) is not satisfied at some time.

The main purpose of this work is to take the Cahn–Hilliard equation as an example of gradient flow to study the unique solvability of the nonlinear algebraic equation in the original Lagrange multiplier approach, and to carry out its error analysis. The main contributions of this work are as follows:

- We propose a modified Lagrange multiplier approach to deal with the case when $|S_n|<\gamma$, and provide numerical results to show that the modified Lagrange multiplier approach is much more robust and can use much larger time steps than the original Lagrange multiplier approach.
- We prove rigorously that if the assumption (1.3) is satisfied and $\Delta t \leq (\frac{S_n}{4})^4$, then the original Lagrange multiplier scheme (3.4)–(3.5) admits a unique solution $\eta^{n+1/2}$ in the interval $[1-S_n^2/16, 1+S_n^2/16]$, and its numerical solution satisfies an optimal error estimate.

The unique solvability of the nonlinear algebraic equation in the Lagrange multiplier approach turns out to be very challenging. First of all, it is observed that the implicit part of the numerical scheme (3.4)–(3.5) does not correspond to a globally monotone functional in terms of the numerical solution at the next time step. To overcome this difficulty, we have to apply certain local analysis technique to obtain the unique solvability, viewed as a perturbation of the exact solution at each time step. To achieve this goal, an a priori assumption has to be made at the previous time step, in terms of the convergence estimate. With the help of this a priori assumption, the unique solvability can then be carefully proved under the assumption (1.3) on the exact solution. Subsequently, to recover the a priori assumption in the unique solvability analysis, we derive an optimal rate convergence analysis at the next time step. By a mathematical induction argument, we are able to complete the proof of unique solvability and error analysis.

The rest of this paper is organized as follows. In section 2, we recall a second-order scheme for the gradient flows using the original Lagrange multiplier approach, and then present a modified Lagrange multiplier approach to deal with the case when (1.3) is not satisfied. A numerical example is given to validate the efficiency of the improved Lagrange multiplier approach. In section 3, we consider the Cahn–Hilliard equation as an example and establish the unique solvability of the nonlinear system of algebraic equations, under an a priori assumption on the previous time step. Afterward, an error analysis is presented in section 4, and the a priori assumption is theoretically recovered. Finally, we provide some concluding remarks in section 5.

2. The Lagrange multiplier approach and a modified version. We denote $\mu = \frac{\delta E}{\delta \phi} = \mathcal{L}\phi + F'(\phi)$. A second-order modified Crank–Nicolson scheme has been proposed for the general gradient flow (1.1), based on the original Lagrange multiplier approach [9]:

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} = -\mathcal{G}\mu^{n+1}, \tag{2.1}$$

$$\mu^{n+1} = \mathcal{L}\left(\frac{3}{4}\phi^{n+1} + \frac{1}{4}\phi^{n-1}\right) + \eta^{n+1/2}F'(\phi^{*,n}), \tag{2.2}$$

$$(F(\phi^{n+1}) - F(\phi^n), 1) = \eta^{n+1/2}(F'(\phi^{*,n}), \phi^{n+1} - \phi^n), \tag{2.3}$$

where $\phi^{*,n} = \frac{3}{2}\phi^n - \frac{1}{2}\phi^{n-1}$, $\eta^{n+1/2} = \frac{\eta^{n+1}+\eta^n}{2}$. The energy stability result for the above scheme (2.1)–(2.3) could be established following an idea similar to that in [9]; see the following theorem.

Theorem 2.1. *The numerical scheme* (2.1)–(2.3) *is unconditionally stable and satisfies the energy dissipative law*

$$\frac{E^{n+1} - E^n}{\delta t} = -(\mathcal{G}\mu^{n+1}, \mu^{n+1}) - (\mathcal{L}(\phi^{n+1} - 2\phi^n + \phi^{n-1}), \phi^{n+1} - 2\phi^n + \phi^{n-1}), \tag{2.4}$$

where the energy E^{n+1} *is defined as*

$$E^{n+1} = \frac{1}{2}(\mathcal{L}\phi^{n+1}, \phi^{n+1}) + \frac{1}{8}(\mathcal{L}(\phi^{n+1} - \phi^n), \phi^{n+1} - \phi^n) + (F(\phi^{n+1}), 1). \tag{2.5}$$

Proof. Taking the inner product of (2.1), (2.2) with μ^{n+1}, $\frac{\phi^{n+1}-\phi^n}{\Delta t}$, respectively, we obtain

$$\left(\frac{\phi^{n+1} - \phi^n}{\Delta t}, \mu^{n+1}\right) = -(\mathcal{G}\mu^{n+1}, \mu^{n+1}) \tag{2.6}$$

and

$$\left(\frac{\phi^{n+1} - \phi^n}{\Delta t}, \mu^{n+1}\right) = \left(\mathcal{L}\left(\frac{3}{4}\phi^{n+1} + \frac{1}{4}\phi^{n-1}\right) + \eta^{n+1/2}F'(\phi^{*,n}), \frac{\phi^{n+1} - \phi^n}{\Delta t}\right). \tag{2.7}$$

Notice the equality

$$\begin{aligned} &\left(\mathcal{L}\left(\frac{3}{4}\phi^{n+1} + \frac{1}{4}\phi^{n-1}\right), \phi^{n+1} - \phi^n\right) \\ &= \frac{1}{8}\{(\mathcal{L}(\phi^{n+1} - \phi^n), \phi^{n+1} - \phi^n) - (\mathcal{L}(\phi^n - \phi^{n-1}), \phi^n - \phi^{n-1}) \\ &\quad + (\mathcal{L}(\phi^{n+1} - 2\phi^n + \phi^{n-1}), \phi^{n+1} - 2\phi^n + \phi^{n-1})\} \\ &\quad + \frac{1}{2}\{(\mathcal{L}\phi^{n+1}, \phi^{n+1}) - (\mathcal{L}\phi^n, \phi^n)\}. \end{aligned} \tag{2.8}$$

Combining (2.6) and (2.7) and using (2.3) and (2.8), we derived the desired energy law. ∎

Note that the energy defined in (2.5) is not exactly the original energy, but is the sum of the original energy and a positive second-order perturbation. However, if we replace the modified Crank–Nicolson scheme by the original Crank–Nicolson scheme, it will be energy stable with respect to the original energy [9]. However, the original Crank–Nicolson scheme is generally not recommended for dealing with dissipative systems, as it does not introduce any additional dissipation which is needed to dump initial errors.

The implementation process of the above scheme can be outlined as follows. First, we define

$$\phi^{n+1} = \phi_1^{n+1} + \eta^{n+\frac{1}{2}}\phi_2^{n+1}, \quad \mu^{n+\frac{1}{2}} = \mu_1^{n+\frac{1}{2}} + \eta^{n+\frac{1}{2}}\mu_2^{n+\frac{1}{2}}. \tag{2.9}$$

Substituting $(\phi^{n+1}, \mu^{n+\frac{1}{2}})$ into (2.1)–(2.3), we are able to obtain ϕ_1^{n+1} and ϕ_2^{n+1} from the following two linear systems:

$$\frac{\phi_1^{n+1} - \phi^n}{\Delta t} = -\mathcal{G}\mu_1^{n+\frac{1}{2}}, \quad \mu_1^{n+\frac{1}{2}} = \mathcal{L}\left(\frac{3}{4}\phi_1^{n+1} + \frac{1}{4}\phi^{n-1}\right) \tag{2.10}$$

and

$$\frac{\phi_2^{n+1}}{\Delta t} = -\mathcal{G}\mu_2^{n+\frac{1}{2}}, \quad \mu_2^{n+\frac{1}{2}} = \mathcal{L}\left(\frac{3}{4}\phi_2^{n+1}\right) + F'(\phi^{*,n}). \tag{2.11}$$

It is obvious that ϕ_1^{n+1} and ϕ_2^{n+1} can be solved uniquely from (2.10)–(2.11). In more detail, the associated implicit operator is given by $\frac{1}{\Delta t}\mathcal{G}^{-1} + \mathcal{L}$, and the unique solvability of this linear system comes from the positive definite feature of both $\mathcal{G}^{-1}$ and $\mathcal{L}$. Moreover, if the operators $\mathcal{G}$ and $\mathcal{L}$ only involve constant coefficients, such as $\mathcal{G} = -\Delta$ and $\mathcal{L} = -\varepsilon^2\Delta$ in the case of a constant-mobility Cahn–Hilliard equation, then the above systems can be efficiently solved by using a Fourier-spectral method if periodic boundary conditions are prescribed, or a fast spectral method if Neumann-type boundary conditions are prescribed [4]. On the other hand, if $\mathcal{G}$ and $\mathcal{L}$ involve nonconstant coefficients, one can use suitable positive definite operators with constant coefficients as preconditioners, and use a preconditioned conjugate gradient iteration (cf. section 4.4 in [26]).

A substitution of (2.9) into (2.3) leads to the following nonlinear algebraic equation for $\eta^{n+1/2}$:

$$g_n(\eta) := \int_\Omega (F(\phi_1^{n+1} + \eta\phi_2^{n+1}) - F(\phi^n))\, d\boldsymbol{x} - \eta\int_\Omega F'(\phi^{*,n})(\phi_1^{n+1} + \eta\phi_2^{n+1} - \phi^n)\, d\boldsymbol{x} = 0. \tag{2.12}$$

As mentioned in the introduction, (2.12) may not be uniquely solvable near $\eta = 1$ if the assumption (1.3) is not satisfied. Hence, we need to modify the Lagrange multiplier approach so that the computation can continue even if (1.3) is not satisfied.

Below we introduce a modified Lagrange multiplier approach for gradient flow (1.1). For a given tolerance $\gamma \ll 1$, we proceed as follows.

We first compute ϕ_1^{n+1} and ϕ_2^{n+1} from (2.10) and (2.11), respectively. Then we set $\tilde{\phi}^{n+1} = \phi_1^{n+1} + \phi_2^{n+1}$. If $e_{n+1} = |\frac{\int_\Omega F(\tilde{\phi}^{n+1}) - F(\phi^n)dx}{\Delta t}| \geq \gamma$, we continue with the original Lagrange multiplier approach; otherwise we set $\eta^{n+1/2} = 1$ and $\phi^{n+1} = \tilde{\phi}^{n+1}$.

Modified Lagrange multiplier approach:

Given numerical solutions at time steps n and $n-1$; the parameter γ, and the preassigned time step δt.

Step 1 Compute ϕ_1^{n+1} and ϕ_2^{n+1} from (2.10) and (2.11), and set $\tilde{\phi}^{n+1} = \phi_1^{n+1} + \phi_2^{n+1}$.

Step 2 Calculate $e_{n+1} = \frac{\int_\Omega F(\tilde{\phi}^{n+1}) - F(\phi^n)dx}{\Delta t}$.

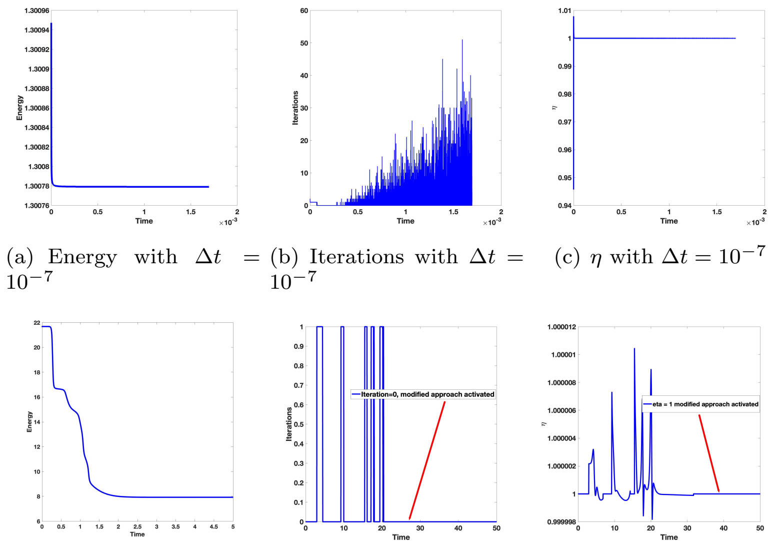
Step 3 if $|e_{n+1}| \geq \gamma$, **then**

Step 4 Determine $\eta^{n+1/2}$ from (2.12).

Step 5 else

Set $\phi^{n+1} = \tilde{\phi}^{n+1}$.

Step 6 endif



(a) Energy with $\Delta t = 10^{-7}$ (b) Iterations with $\Delta t = 10^{-7}$ (c) η with $\Delta t = 10^{-7}$

(d) Energy with $\Delta t = 10^{-3}$ (e) Iterations with $\Delta t = 10^{-3}$ (f) η with $\Delta t = 10^{-3}$

FIG. 1. (a)–(c) *The evolution of energy, iterations and η using the original Lagrange multiplier approach with $\Delta t = 10^{-7}$.* (d)–(f) *The evolution of energy, iterations and η using modified Lagrange multiplier approach with $\gamma = \Delta t = 10^{-3}$.*

More precisely, the modified Lagrange multiplier algorithm is outlined below.

We now provide a numerical example to demonstrate the effectiveness of this modified approach. We consider the Cahn–Hilliard equation

$$\phi_t + \varepsilon^2 \Delta^2 \phi - \Delta((\phi^2 - 1)\phi) = 0, \tag{2.13}$$

with the initial condition

$$u(t=0) = 0.3 + 0.01\,\mathrm{rand}(x,y), \quad \mathrm{rand}(x,y)\text{: uniform random distribution in } [-1,1]. \tag{2.14}$$

The interface width parameter is set to be $\varepsilon^2 = 0.06$.

In Figure 1(a)–(c), we plot the evolution of energy, iterations, and η with respect to time by using the modified Crank–Nicolson scheme based on the original Lagrange multiplier approach. We observe that even with a very small time step $\Delta t = 10^{-7}$, the scheme based on the original Lagrange multiplier approach failed to converge at about $t = 1.65 \times 10^{-3}$. In Figure 1(d)–(f), we plot the evolution of energy, iterations, and η with respect to time by using the scheme based on the modified Lagrange multiplier approach with $\gamma = \Delta t$ and $\Delta t = 10^{-3}$. For the sake of comparison, we also plot the energy evolution by using a second-order SAV scheme with $\Delta t = 10^{-5}$. We observe from Figure 1(d) that the energy curves obtained by both methods overlap and decrease monotonically, indicating that the modified Lagrange multiplier approach leads to correct results even at a relatively large time step $\Delta t = 10^{-3}$. We also observe from Figure 1(e) that the modified approach is activated (i.e., $e_{n+1} \le \gamma$) in a large time interval, while only one iteration is needed for solving the nonlinear algebraic equation (2.12) when $e_{n+1} \ge \gamma$. These results indicate that the modified Lagrange multiplier approach is very effective.

3. The unique solvability of (3.6). In this section, we provide the unique solvability analysis of (3.6). To fix the idea, we consider the Cahn–Hilliard equation, a typical gradient flow. In this physical model, the energy functional is given by

$$E(\phi) := \int_\Omega \left(\frac{1}{4}\phi^4 - \frac{1}{2}\phi^2 + \frac{1}{4} + \frac{\varepsilon^2}{2}|\nabla\phi|^2 \right) \mathrm{d}\boldsymbol{x} \tag{3.1}$$

where the constant $\varepsilon > 0$ stands for the interface width parameter, and $\mathcal{G} = -\Delta$. In turn, the Cahn–Hilliard equation can be written as

$$\partial_t \phi = \Delta\mu = \Delta\left(\phi^3 - \phi - \varepsilon^2\Delta\phi\right), \tag{3.2}$$

in which μ is the chemical potential

$$\mu := \frac{\delta E}{\delta \phi} = \phi^3 - \phi - \varepsilon^2 \Delta\phi. \tag{3.3}$$

To fix the idea, we impose periodic boundary conditions for both the phase variable, ϕ, and the chemical potential, μ. An extension to the case of the homogeneous Neumann boundary condition is possible but not straightforward, so it will not be considered in this paper.

In more detail, the scheme (2.1)–(2.3) could be represented as

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} = \Delta\left(F'(\phi^{*,n})\eta^{n+1/2} - \varepsilon^2\Delta\left(\frac{3}{4}\phi^{n+1} + \frac{1}{4}\phi^{n-1}\right)\right), \tag{3.4}$$

$$\left(F(\phi^{n+1}) - F(\phi^n), 1\right) = \eta^{n+1/2}\left(F'(\phi^{*,n}), \phi^{n+1} - \phi^n\right). \tag{3.5}$$

Meanwhile, the Lagrange multiplier $\eta^{n+1/2}$ is a solution of the nonlinear algebraic equation

$$g_n(\eta) := \int_\Omega \left(F(p^n + \eta\Delta t q^n) - F(\phi^n)\right) d\boldsymbol{x} - \eta\int_\Omega F'(\phi^{*,n})(p^n + \eta\Delta t q^n - \phi^n)\, d\boldsymbol{x} = 0. \tag{3.6}$$

Setting $\phi^{n+1} = p^n + \eta^{n+1/2}\Delta t q^n$ and plugging it into (3.4), we find that

$$p^n = (I + \frac{3}{4}\varepsilon^2\Delta t\Delta^2)^{-1}\left(\phi^n - \frac{1}{4}\varepsilon^2\Delta t\Delta^2\phi^{n-1}\right), \tag{3.7}$$

$$q^n = \left(I + \frac{3}{4}\varepsilon^2\Delta t\Delta^2\right)^{-1}\Delta F'(\phi^{*,n}). \tag{3.8}$$

3.1. The main result. We aim to provide a theoretical analysis for the nonlinear algebraic equation (3.6), by making use of certain localized estimates. The numerical error function is defined as

$$e^k := \Phi^k - \phi^k \quad \forall k \geq 0, \tag{3.9}$$

in which Φ^k is the exact solution to the original PDE (3.2), and ϕ^k is denoted as the numerical solution of (3.4)–(3.5). With an initial data with sufficient regularity, it is assumed that the exact solution Φ has regularity of class $\mathcal{R}$:

$$\Phi \in \mathcal{R} := C^3(0,T;C^2) \cap C^2(0,T;C^6) \cap L^\infty(0,T;H^8). \tag{3.10}$$

In turn, the following functional bounds are available for the exact solution:

$$\|\partial_t^3 \Phi\|_{L^\infty(0,T^*;C^2)} + \|\Phi_{tt}\|_{L^\infty(0,T^*;C^6)} + \|\Phi_t\|_{L^\infty(0,T^*;C^6)} \le A^*, \ \ \|\Phi^k\|_{H^8} \le A^* \quad \forall k \ge 0. \tag{3.11}$$

To proceed with the nonlinear analysis for (3.6), we begin with the following a priori assumption for the numerical error at the previous time steps:

$$\|e^k\|_{H^4} \le \Delta t^{3/2}, \quad \|e^k\|_{H^6} \le \Delta t \quad \forall k \le n. \tag{3.12}$$

In turn, the following H^4 and H^6 bounds are valid for the numerical solution at the previous time steps:

$$\|\phi^k\|_{H^6} \le \|\Phi^k\|_{H^6} + \|e^k\|_{H^4} \le A^* + \Delta t \le A^* + 1 := \tilde{A}_1 \quad \text{for } k = n, n-1. \tag{3.13}$$

In particular, by the fact that $\phi^{*,n} = \frac{3}{2}\phi^n - \frac{1}{2}\phi^{n-1}$, we have the following a priori bounds for $\phi^{*,n}$:

$$\|\phi^{*,n}\|_{H^2},\ \|\phi^{*,n}\|_{H^4},\ \|\phi^{*,n}\|_{H^6} \le 2\tilde{A}_1, \quad \|\phi^{*,n}\|_{L^\infty} \le C\tilde{A}_1. \tag{3.14}$$

The a priori assumption (3.12) will be recovered by the convergence estimate at the next time step, as will be demonstrated in the later analysis.

The following theorem is the main result of this section.

THEOREM 3.1. *Suppose the exact solution Φ for the Cahn–Hilliard equation* (3.2) *is of regularity class $\mathcal{R}$ and satisfies the assumption* (1.3)*. We also make the a priori assumption* (3.12)*, and assume that the time step is sufficiently small such that*

$$\Delta t \le \min\left\{ \frac{1}{A_1}, \frac{1}{A_4}, \frac{S_n^2}{4A_{12}}, \left(\frac{S_n}{4}\right)^4 \right\}, \tag{3.15}$$

with the constants A_1, A_4, and A_{12} only dependent on A^*. Then the nonlinear scalar equation (3.6) *has a unique solution in* $[1-\sqrt{\Delta t}, 1+\sqrt{\Delta t}]$.

We notice that the numerical results presented in the last section indicate that the condition $\Delta t \le (\gamma/4)^4)$ is most likely too pessimistic. In particular, if a lower bound of S_n is of $O(1)$, which corresponds to the short and medium time scales in the numerical simulation, the time step constraint (3.15) turns out to be a mild one. On the other hand, if the large time scale is considered, so that the value of $|S_n|$ may become small, a restart of the numerical solution is needed in the modified Lagrange multiplier approach, as outlined above. In other words, the theoretical analysis presented in this article is more appropriate to the short and medium time scales in the numerical simulation, and a modified approach is suggested in the long time simulation to implement the Lagrange multiplier method.

A few preliminary estimates are needed before we can proceed with the proof of this theorem.

3.2. Some preliminary estimates. For the sake of simplicity, we remove the dependence on n from all constants A_k below.

LEMMA 3.2. *Given ϕ^n, ϕ^{n-1}, under the assumption* (1.3) *and the a priori assumption* (3.12)*, we have the following estimates:*

$$\|p^n - \phi^n\|_{L^\infty} \le A_1 \Delta t, \quad \|p^n\|_{L^\infty} \le A_2, \quad \|q^n\|_{L^\infty} \le A_3, \tag{3.16}$$

$$\|\phi^{*,n} - \phi^n\|_{L^\infty} \le A_4 \Delta t, \quad \|\phi^{*,n}\|_{L^\infty} \le A_5, \quad \|\phi^{*,n} - p^n\|_{L^\infty} \le A_6 \Delta t, \tag{3.17}$$

$$\|\Delta(F'(p^n) - F'(\phi^n))\| \le A_7 \Delta t, \quad \|\Delta(F'(\phi^{*,n}) - F'(\phi^n))\| \le A_8 \Delta t, \tag{3.18}$$

$$\|F'(\phi^{*,n}) - F'(\phi^n)\|_{L^\infty} \le A_9 \Delta t, \quad \|F'(\Phi^n) - F'(\phi^n)\|_{L^\infty} \le A_{10} \Delta t, \tag{3.19}$$

$$\|\Delta(F'(\Phi^n) - F'(\phi^n))\| \le A_{11} \Delta t, \tag{3.20}$$

in which A_j $(1 \le j \le 10)$ only depends on A^*, and the time step size satisfies the requirement $A_1 \Delta t \le 1$, $A_4 \Delta t \le 1$.

Proof. By the representation formula (3.7) for p^n, we see that

$$p^n - \phi^n = -\varepsilon^2 \Delta t \left(I + \frac{3}{4}\varepsilon^2 \Delta t \Delta^2 \right)^{-1} \Delta^2 \left(\frac{3}{4}\phi^n + \frac{1}{4}\phi^{n-1} \right), \tag{3.21}$$

$$\Delta(p^n - \phi^n) = -\varepsilon^2 \Delta t \left(I + \frac{3}{4}\varepsilon^2 \Delta t \Delta^2 \right)^{-1} \Delta^3 \left(\frac{3}{4}\phi^n + \frac{1}{4}\phi^{n-1} \right). \tag{3.22}$$

Meanwhile, by the a priori H^6 estimate (3.13) for the numerical solution ϕ^n, ϕ^{n-1}, we have

$$\left\| \Delta^2 \left(\frac{3}{4}\phi^n + \frac{1}{4}\phi^{n-1} \right) \right\|, \left\| \Delta^3 \left(\frac{3}{4}\phi^n + \frac{1}{4}\phi^{n-1} \right) \right\| \le \left(\frac{3}{4} + \frac{1}{4} \right) \tilde{A}_1 = \tilde{A}_1. \tag{3.23}$$

On the other hand, the following inequality is always available, because all the eigenvalues associated with the operator $(I + \frac{3}{4}\varepsilon^2 \Delta t \Delta^2)^{-1}$ are bounded by 1:

$$\left\| \left(I + \frac{3}{4}\varepsilon^2 \Delta t \Delta^2 \right)^{-1} f \right\| \le \|f\| \quad \forall f \in L^2(\Omega). \tag{3.24}$$

Then we arrive at

$$\|p^n - \phi^n\| \le \varepsilon^2 \Delta t \left\| \Delta^2 \left(\frac{3}{4}\phi^n + \frac{1}{4}\phi^{n-1} \right) \right\| \le \tilde{A}_1 \varepsilon^2 \Delta t, \tag{3.25}$$

$$\|\Delta(p^n - \phi^n)\| \le \varepsilon^2 \Delta t \left\| \Delta^3 \left(\frac{3}{4}\phi^n + \frac{1}{4}\phi^{n-1} \right) \right\| \le \tilde{A}_1 \varepsilon^2 \Delta t. \tag{3.26}$$

Therefore, an application of 3-D Sobolev embedding implies that

$$\|p^n - \phi^n\|_{L^\infty} \le C\|p^n - \phi^n\|_{H^2} \le C(\|p^n - \phi^n\| + \|\Delta(p^n - \phi^n)\|) \le C\tilde{A}_1 \varepsilon^2 \Delta t, \tag{3.27}$$

with the elliptic regularity used in the second step. In turn, the first inequality of (3.16) has been proved by taking $A_1 = C\tilde{A}_1 \varepsilon^2$.

The proof of the second inequality in (3.16) is more straightforward:

$$\begin{aligned} \|p^n\|_{L^\infty} &\le \|\phi^n\|_{L^\infty} + \|p^n - \phi^n\|_{L^\infty} \le C\|\phi^n\|_{H^2} + \|p^n - \phi^n\|_{L^\infty} \\ &\le C\tilde{A}_1 + A_1 \Delta t \le C\tilde{A}_1 + 1, \end{aligned}$$

provided that $A_1 \Delta t \le 1$. Again, the elliptic regularity has been recalled in the second step. As a result, the proof for the second inequality in (3.16) is complete by taking $A_2 = C\tilde{A}_1 + 1$.

For the third inequality in (3.16), we begin with the following expansion, based on the fact that $F'(\phi) = \phi^3 - \phi$:

$$\Delta F'(\phi^{*,n}) = (3(\phi^{*,n})^2 - 1)\Delta(\phi^{*,n}) + 6\phi^{*,n}|\nabla(\phi^{*,n})|^2. \tag{3.28}$$

In turn, a combination of Hölder inequality and Sobolev embedding implies that

$$\begin{aligned}\|\Delta F'(\phi^{*,n})\| &\le (3\|\phi^{*,n}\|_{L^\infty}^2+1)\|\Delta(\phi^{*,n})\| + 6\|\phi^{*,n}\|_{L^\infty}\cdot\|\nabla(\phi^{*,n})\|_{L^4}^2 \\ &\le C(\|\phi^{*,n}\|_{H^2}^2+1)\|\Delta(\phi^{*,n})\| + C\|\phi^{*,n}\|_{H^2}^3 \le C(\|\phi^{*,n}\|_{H^2}^3+\|\phi^{*,n}\|_{H^2}).\end{aligned} \tag{3.29}$$

A similar estimate could also be derived; the details are skipped for the sake of brevity:

$$\|\Delta^2 F'(\phi^{*,n})\| \le C(\|\phi^{*,n}\|_{H^4}^3+\|\phi^{*,n}\|_{H^4}). \tag{3.30}$$

As a consequence, we arrive at

$$\begin{aligned}\|q^n\| &= \left\|\left(I+\frac{3}{4}\varepsilon^2\Delta t\Delta^2\right)^{-1}\Delta F'(\phi^{*,n})\right\| \le \|\Delta F'(\phi^{*,n})\| \le C(\|\phi^{*,n}\|_{H^2}^3+\|\phi^{*,n}\|_{H^2}),\\ \|\Delta q^n\| &= \left\|\left(I+\frac{3}{4}\varepsilon^2\Delta t\Delta^2\right)^{-1}\Delta^2 F'(\phi^{*,n})\right\| \le \|\Delta^2 F'(\phi^{*,n})\| \\ &\le C(\|\phi^{*,n}\|_{H^4}^3+\|\phi^{*,n}\|_{H^4}).\end{aligned}$$

Furthermore, its combination with the a priori bound (3.14) (for $\phi^{*,n}$) results in

$$\|q^n\|,\ \|\Delta q^n\| \le C(\tilde{A}_1^3+\tilde{A}_1),$$

and an application of Sobolev embedding yields

$$\|q^n\|_{L^\infty} \le C\|q^n\|_{H^2} \le C(\|q^n\|+\|\Delta q^n\|) \le C(\tilde{A}_1^3+\tilde{A}_1).$$

This finishes the proof of the third inequality in (3.16) by taking $A_3 = C(\tilde{A}_1^3+\tilde{A}_1)$.

In terms of the inequalities in (3.17), we recall the regularity assumption (3.11) and the a priori assumption (3.12):

$$\|\Phi^n-\phi^n\|_{H^6},\ \|\Phi^{n-1}-\phi^{n-1}\|_{H^6} \le \Delta t,\ \ \|\Phi^n-\Phi^{n-1}\|_{H^6} \le \Delta t\|\partial_t\Phi\|_{H^6} \le A^*\Delta t, \tag{3.31}$$

which in turn leads to the estimate

$$\|\phi^{*,n}-\phi^n\|_{H^6} = \frac{1}{2}\|\phi^n-\phi^{n-1}\|_{H^6} \le \frac{1}{2}(A^*+2)\Delta t. \tag{3.32}$$

Therefore, the first inequality in (3.17) becomes a direct consequence of Sobolev embedding:

$$\|\phi^{*,n}-\phi^n\|_{L^\infty} \le C\|\phi^{*,n}-\phi^n\|_{H^2} \le C\|\phi^{*,n}-\phi^n\|_{H^6} \le A_4\Delta t, \quad A_4 = C(A^*+2). \tag{3.33}$$

The second and third inequalities in (3.17) come from an application of triangular inequality:

$$\|\phi^{*,n}\|_{L^\infty} \le \|\phi^n\|_{L^\infty} + \|\phi^{*,n}-\phi^n\|_{L^\infty} \le C\|\phi^n\|_{H^2} + A_4\Delta t \le A_5 = C\tilde{A}_1+1, \tag{3.34}$$

$$\begin{aligned}&\|\phi^{*,n}-p^n\|_{L^\infty} \le \|p^n-\phi^n\|_{L^\infty} + \|\phi^{*,n}-\phi^n\|_{L^\infty} \le A_1 + A_4\Delta t = A_6\Delta t,\\ &\qquad A_6 = A_1+A_4.\end{aligned} \tag{3.35}$$

In terms of the first inequality in (3.18), we begin with the following expansion identity:

(3.36)
$$\begin{aligned} F'(p^n) - F'(\phi^n) &= (\mathcal{NLD} - 1)(p^n - \phi^n), \ \mathcal{NLD} = (p^n)^2 + p^n\phi^n + (\phi^n)^2, \quad \text{so that} \\ \Delta(F'(p^n) - F'(\phi^n)) &= (\mathcal{NLD} - 1)\Delta(p^n - \phi^n) + (p^n - \phi^n)\Delta\mathcal{NLD} \\ &\quad + 2\nabla\mathcal{NLD}\cdot\nabla(p^n - \phi^n). \end{aligned}$$

Meanwhile, an application of the Sobolev inequality indicates that

(3.37)
$$\|\mathcal{NLD}\|_{L^\infty}, \|\nabla\mathcal{NLD}\|_{L^4}, \|\Delta\mathcal{NLD}\| \le C(\|p^n\|_{H^2}^2 + \|\phi^n\|_{H^2}^2) \le C((\tilde{A}_1+1)^2 + \tilde{A}_1^2),$$

in which the preliminary estimates (3.13) and (3.27) have been recalled. Subsequently, an application of the Hölder and Sobolev inequalities to the expansion (3.36) results in

(3.38)
$$\begin{aligned} \|\Delta(F'(p^n) - F'(\phi^n))\| &\le C(\|\mathcal{NLD}\|_{L^\infty} + \|\nabla\mathcal{NLD}\|_{L^4} + \|\Delta\mathcal{NLD}\|)\cdot\|p^n - \phi^n\|_{H^2} \\ &\le C((\tilde{A}_1+1)^2 + \tilde{A}_1^2 + 1)\tilde{A}_1\varepsilon^2\Delta t = A_7\Delta t. \end{aligned}$$

As a result, the proof of the first inequality in (3.18) has been completed by taking $A_7 = C((\tilde{A}_1+1)^2 + \tilde{A}_1^2 + 1)\tilde{A}_1\varepsilon^2$.

The other inequalities in (3.18)–(3.20) could be similarly derived. The constants A_j ($8 \le j \le 11$) are stated below, and the details are skipped for simplicity of presentation.

(3.39)
$$\begin{aligned} &A_8 = C((\tilde{A}_1+1)^2 + \tilde{A}_1^2 + 1)(A^*+2), \quad A_9 = CA_8, \quad A_{11} = C((A^*)^2 + \tilde{A}_1^2 + 1), \\ &A_{10} = CA_{11}. \end{aligned}$$

Notice that all the constants A_j only depend on A^*. This finishes the proof of Lemma 3.2. ∎

We aim to prove that the nonlinear equation (3.6) has a unique solution in a neighborhood of 1. An estimate of the value for $g_n(1)$ is given by the following lemma.

LEMMA 3.3. *Given ϕ^n, ϕ^{n-1}, under the assumption* (1.3) *and the a priori assumption* (3.12)*, we have $|g_n(1)| \le A_{12}\Delta t^2$, with A_{12} only depending on A^*.*

Proof. We begin with the expansion of $g_n(1)$:

$$g_n(1) = \int_\Omega (F(p^n + \Delta t q^n) - F(\phi^n) - F'(\phi^{*,n})(p^n + \Delta t q^n - \phi^n))\, d\boldsymbol{x}. \tag{3.40}$$

An application of the intermediate value theorem implies that

$$F(p^n + \Delta t q^n) - F(\phi^n) = F'(\xi^{(1)})(p^n + \Delta t q^n - \phi^n), \quad \text{with } \xi^{(1)} \text{ between } p^n + \Delta t q^n \text{ and } \phi^n.$$

As a consequence, we get

(3.41)
$$\begin{aligned} &F(p^n + \Delta t q^n) - F(\phi^n) - F'(\phi^{*,n})(p^n + \Delta t q^n - \phi^n) \\ &\quad = \Big(F'(\xi^{(1)}) - F'(\phi^{*,n})\Big)(p^n + \Delta t q^n - \phi^n) \\ &\quad = F''(\xi^{(2)})(\xi^{(1)} - \phi^{*,n})(p^n + \Delta t q^n - \phi^n), \quad \text{with } \xi^{(2)} \text{ between } \xi^{(1)} \text{ and } \phi^{*,n}. \end{aligned}$$

By inequality (3.16), the following estimate is available:

$$\|p^n + \Delta t q^n - \phi^n\|_{L^\infty} \le \|p^n - \phi^n\|_{L^\infty} + \Delta t\|q^n\|_{L^\infty} \le (A_1 + A_3)\Delta t. \tag{3.42}$$

Moreover, since $\xi^{(1)}$ is between $p^n + \Delta t q^n$ and ϕ^n, we see that

$$\|\xi^{(1)} - \phi^{*,n}\|_{L^\infty} \le \max\Big(\|p^n + \Delta t q^n - \phi^{*,n}\|_{L^\infty}, \|\phi^n - \phi^{*,n}\|_{L^\infty}\Big). \tag{3.43}$$

Meanwhile, the following inequalities are available:

$$\begin{aligned}
\|\phi^n - \phi^{*,n}\|_{L^\infty} &= \frac{1}{2}\|\phi^n - \phi^{n-1}\|_{L^\infty} = \frac{1}{2}\|\Phi^n - \Phi^{n-1}\|_{L^\infty} + \frac{1}{2}\|e^n - e^{n-1}\|_{L^\infty} \\
&\le \frac{1}{2}A^*\Delta t + C\Delta t^{3/2} \le \left(\frac{1}{2}A^* + 1\right)\Delta t, \\
\|p^n + \Delta t q^n - \phi^{*,n}\|_{L^\infty} &\le \|p^n + \Delta t q^n - \phi^n\|_{L^\infty} + \|\phi^n - \phi^{*,n}\|_{L^\infty} \\
&\le (A_1 + A_3)\Delta t + \frac{1}{2}A^*\Delta t + C\Delta t^{3/2} \\
&\le \left(A_1 + A_3 + \frac{1}{2}A^* + 1\right)\Delta t,
\end{aligned}$$

in which the regularity assumption (3.11) and the a priori assumption (3.12) have been applied. This in turn yields

$$\|\xi^{(1)} - \phi^{*,n}\|_{L^\infty} \le \left(A_1 + A_3 + \frac{1}{2}A^* + 1\right)\Delta t. \tag{3.44}$$

To obtain a bound for $F''(\xi^{(2)})$, we observe that

$$\|F''(\xi^{(2)})\|_{L^\infty} \le \max(\|F''(p^n + \Delta t q^n)\|_{L^\infty}, \|F''(\phi^n)\|_{L^\infty}, \|F''(\phi^{*,n})\|_{L^\infty}), \tag{3.45}$$

which comes from the range of $\xi^{(1)}$ and $\xi^{(2)}$. Meanwhile, by the fact that $F''(\phi) = 3\phi^2 - 1$, the following bounds could be derived:

$$\|F''(\phi^n)\|_{L^\infty} \le 3\|\phi^n\|_{L^\infty}^2 + 1 \le C\|\phi^n\|_{H^2}^2 + 1 \le C\tilde{A}_1^2 + 1, \tag{3.46}$$

$$\|F''(\phi^{*,n})\|_{L^\infty} \le 3\|\phi^{*,n}\|_{L^\infty}^2 + 1 \le C\tilde{A}_1^2 + 1, \tag{3.47}$$

$$\|F''(p^n + \Delta t q^n)\|_{L^\infty} \le 3\|p^n + \Delta t q^n\|_{L^\infty}^2 + 1 \le 3(A_2 + 1)^2 + 1, \tag{3.48}$$

in which the a priori bounds (3.13)–(3.14) have been repeatedly applied, and the last step of (3.48) is based on the following estimate:

$$\begin{aligned}
&\|p^n + \Delta t q^n\|_{L^\infty} \le \|p^n\|_{L^\infty} + \Delta t\|q^n\|_{L^\infty} \le A_2 + A_3\Delta t \le A_2 + 1, \\
&\quad \text{provided that } A_3\Delta t \le 1.
\end{aligned}$$

Going back to (3.45), we arrive at

$$\|F''(\xi^{(2)})\|_{L^\infty} \le A_{13} := \max(C\tilde{A}_1^2 + 1, 3(A_2 + 1)^2 + 1). \tag{3.49}$$

As a result, a substitution of (3.42), (3.44), and (3.49) into (3.41) yields

$$\begin{aligned}
&\|F(p^n + \Delta t q^n) - F(\phi^n) - F'(\phi^{*,n})(p^n + \Delta t q^n - \phi^n)\|_{L^\infty} \\
&\quad \le \|F''(\xi^{(2)})\|_{L^\infty} \cdot \|\xi^{(1)} - \phi^{*,n}\|_{L^\infty} \cdot \|p^n + \Delta t q^n - \phi^n\|_{L^\infty} \\
&\quad \le A_{14}\Delta t^2, \quad \text{with } A_{14} = (A_1 + A_3)\left(A_1 + A_3 + \frac{1}{2}A^* + 1\right)A_{13}.
\end{aligned} \tag{3.50}$$

Finally, its combination with (3.40) implies the desired estimate:

$$|g_n(1)| \le \|F(p^n + \Delta t q^n) - F(\phi^n) - F'(\phi^{*,n})(p^n + \Delta t q^n - \phi^n)\|_{L^\infty} \cdot |\Omega| \le A_{14}|\Omega|\Delta t^2.$$

The proof of Lemma 3.3 is complete by taking $A_{12} = A_{14}|\Omega|$. ∎

The derivative of $g_n(\eta)$ for η around the value of 1 is analyzed in the following lemma.

LEMMA 3.4. *Given ϕ^n, ϕ^{n-1}, under the assumption* (1.3)*, the a priori assumption* (3.12)*, and assuming $\Delta t \le (S_n/4)^4$, we then have $|g_n'(\eta)| \ge \frac{|S_n|}{2}\Delta t$ for any $1-\Delta t^{1/2} \le \eta \le 1 + \Delta t^{1/2}$.*

Proof. Without loss of generality, we assume that $S_n < 0$. A careful calculation reveals the following expression for $g_n'(\eta)$ by making use of the fact that $F(\phi) = \frac{1}{4}(\phi^2 - 1)^2$:

(3.51)
$$g_n'(\eta) = \int_\Omega \Big(\Delta t(p^n)^3 q^n + 3\eta\Delta t^2 (p^n)^2 (q^n)^2 + 3\eta^2 \Delta t^3 p^n (q^n)^3 + \eta^3 \Delta t^4 (q^n)^4 - \Delta t p^n q^n$$
$$- \eta\Delta t^2 (q^n)^2 - F'(\phi^{*,n})(p^n - \phi^n) - 2\eta\Delta t F'(\phi^{*,n}) q^n\Big)\, d\boldsymbol{x} := \sum_{j=1}^{6} I_j, \text{with}$$

(3.52)
$$I_1 = \Delta t((p^n)^3 - p^n, q^n),\ \ I_2 = (-F'(\phi^{*,n}), p^n - \phi^n),\ \ I_3 = -2\eta\Delta t(F'(\phi^{*,n}), q^n),$$

(3.53)
$$I_4 = \eta\Delta t^2(3(p^n)^2 - 1, (q^n)^2),\ \ I_5 = 3\eta^2\Delta t^3(p^n, (q^n)^3),\ \ I_6 = \eta^3\Delta t^4((q^n)^4, 1).$$

For the I_4 part, an application of the L^∞ bound (3.16) for p^n and q^n gives the following estimate:

(3.54)
$$|I_4| \le \eta\Delta t^2(3\|p^n\|_{L^\infty}^2 + 1)\cdot \|q^n\|_{L^\infty}^2 |\Omega| \le (3A_2^2 + 1)A_3^2|\Omega|\eta\Delta t^2 \le (4A_2^2 + 2)A_3^2|\Omega|\Delta t^2,$$

in which the last step is based on the fact that $1 - \Delta t^{1/2} \le \eta \le 1 + \Delta t^{1/2}$. Similar bounds could be obtained for I_5 and I_6; the details are skipped for the sake of brevity:

$$|I_5| \le 4A_2A_3^3|\Omega|\Delta t^3, \quad |I_6| \le 2A_4^3|\Omega|\Delta t^4. \tag{3.55}$$

For the I_1 part, we observe the following transformation:

$$I_1 = \Delta t((p^n)^3 - p^n, q^n) = \Delta t\left((p^n)^3 - p^n, \left(I + \frac{3}{4}\varepsilon^2\Delta t\Delta^2\right)^{-1}\Delta F'(\phi^{*,n})\right)$$
$$= \Delta t\left(F'(\phi^{*,n}), \left(I + \frac{3}{4}\varepsilon^2\Delta t\Delta^2\right)^{-1}\Delta((p^n)^3 - p^n)\right), \tag{3.56}$$

in which the last step comes from the fact that $(I + \frac{3}{4}\varepsilon^2\Delta t\Delta^2)^{-1}\Delta$ is a self-adjoint operator. Meanwhile, we introduce an approximate integral value:

$$I_1^* := \Delta t\left(F'(\Phi^n), \left(I + \frac{3}{4}\varepsilon^2\Delta t\Delta^2\right)^{-1}\Delta F'(\Phi^n)\right). \tag{3.57}$$

On the other hand, the following estimates could be derived:

$$
\begin{aligned}
&\|F'(\phi^{*,n}) - F'(\Phi^n)\|_{L^\infty} \le \|F'(\phi^{*,n}) - F'(\phi^n)\|_{L^\infty} + \|F'(\Phi^n) - F'(\phi^n)\|_{L^\infty} \\
&\quad \le (A_9 + A_{10})\Delta t, \\
&\|F'(\phi^{*,n}) - F'(\Phi^n)\| \le \|F'(\phi^{*,n}) - F'(\Phi^n)\|_{L^\infty} \cdot |\Omega|^{1/2} \le (A_9 + A_{10})|\Omega|^{1/2}\Delta t, \\
&\|F'(\phi^{*,n})\|_{L^\infty} \le \|\phi^{*,n}\|^3_{L^\infty} + \|\phi^{*,n}\|_{L^\infty} \le A_5^3 + A_5, \\
&\|F'(\phi^{*,n})\| \le \|F'(\phi^{*,n})\|_{L^\infty} \cdot |\Omega|^{1/2} \le (A_5^3 + A_5)|\Omega|^{1/2}, \\
&\|\Delta(F'(\Phi^n) - F'(p^n))\| \le \|\Delta(F'(p^n) - F'(\phi^n))\| + \|\Delta(F'(\Phi^n) - F'(\phi^n))\| \\
&\quad \le (A_7 + A_{11})\Delta t, \\
&\|\Delta F'(\Phi^n)\| \le C(\|\Phi^n\|^3_{H^2} + \|\Phi^n\|_{H^2}) \le C((A^*)^3 + A^*),
\end{aligned}
$$

in which in the inequalities in (3.17)–(3.20) have been extensively applied. Using the above inequalities, we get

(3.58)
$$
\begin{aligned}
|I_1 - I_1^*| &\le \Delta t\|F'(\phi^{*,n}) - F'(\Phi^n)\| \cdot \|F'(\phi^{*,n})\| + \Delta t\|\Delta(F'(\Phi^n) - F'(p^n))\| \cdot \|\Delta F'(\Phi^n)\| \\
&\le A_{15}\Delta t^2, \text{with } A_{15} := (A_5^3 + A_5)(A_9 + A_{10})|\Omega| + C((A^*)^3 + A^*)(A_7 + A_{11}).
\end{aligned}
$$

A similar analysis could be performed for the I_3 part, which could be transformed as

$$
\begin{aligned}
I_3 = -2\eta\Delta t(F'(\phi^{*,n}, q^n) &= \Delta t \left((\phi^{*,n})^3 - \phi^{*,n}, \left(I + \frac{3}{4}\varepsilon^2\Delta t\Delta^2\right)^{-1} \Delta F'(\phi^{*,n}) \right) \\
&= \Delta t \left(F'(\phi^{*,n}), \left(I + \frac{3}{4}\varepsilon^2\Delta t\Delta^2\right)^{-1} \Delta((\phi^{*,n})^3 - \phi^{*,n}) \right). \qquad (3.59)
\end{aligned}
$$

On the other hand, we introduce an approximate integral value:

$$
I_3^* := -2\eta I_1^* = -2\eta\Delta t \left(F'(\Phi^n), \left(I + \frac{3}{4}\varepsilon^2\Delta t\Delta^2\right)^{-1} \Delta F'(\Phi^n) \right). \qquad (3.60)
$$

The following estimate could be derived in the same manner; the details are left to interested readers:

(3.61)
$$
|I_3 - I_3^*| \le A_{16}\Delta t^2, \; A_{16} := (A_5^3 + A_5)(A_9 + A_{10})|\Omega| + C((A^*)^3 + A^*)(A_9 + A_{11}).
$$

For the I_2 part, we begin with the following expression, which comes from (3.21):

(3.62)
$$
I_2 = (-F'(\phi^{*,n}), p^n - \phi^n) = \varepsilon^2\Delta t \left(F'(\phi^{*,n}), \left(I + \frac{3}{4}\varepsilon^2\Delta t\Delta^2\right)^{-1} \Delta^2 \left(\frac{3}{4}\phi^n + \frac{1}{4}\phi^{n-1}\right)\right).
$$

Similarly, we also introduce an approximate integral value:

$$
I_2^* := \varepsilon^2\Delta t \left(F'(\phi^{*,n}), \left(I + \frac{3}{4}\varepsilon^2\Delta t\Delta^2\right)^{-1} \Delta^2\Phi^n \right). \qquad (3.63)
$$

To estimate the difference between I_1 and I_2^*, we have the following observations:

$$\left\|\Delta^2\left(\frac{3}{4}\phi^n+\frac{1}{4}\phi^{n-1}\right)-\Delta^2\left(\frac{3}{4}\Phi^n+\frac{1}{4}\Phi^{n-1}\right)\right\|=\left\|\Delta^2\left(\frac{3}{4}e^n+\frac{1}{4}e^{n-1}\right)\right\| \le \Delta t^{3/2} \text{ (by (3.12))},$$

$$\left\|\Delta^2\left(\frac{3}{4}\Phi^n+\frac{1}{4}\Phi^{n-1}\right)-\Delta^2\Phi^n\right\|=\frac{1}{4}\|\Delta^2(\Phi^n-\Phi^{n-1})\|\le A^*\Delta t \text{ (by (3.11))},$$

so that

$$\left\|\Delta^2\left(\frac{3}{4}\phi^n+\frac{1}{4}\phi^{n-1}\right)-\Delta^2\Phi^n\right\|\le\left\|\Delta^2\left(\frac{3}{4}\phi^n+\frac{1}{4}\phi^{n-1}\right)-\Delta^2\left(\frac{3}{4}\Phi^n+\frac{1}{4}\Phi^{n-1}\right)\right\|+\left\|\Delta^2\left(\frac{3}{4}\Phi^n+\frac{1}{4}\Phi^{n-1}\right)-\Delta^2\Phi^n\right\|\le(A^*+1)\Delta t. \tag{3.64}$$

Moreover, because of the fact that all the eigenvalues associated with the operator $(I+\frac{3}{4}\varepsilon^2\Delta t\Delta^2)^{-1}$ are bounded by 1, we see that

$$\left\|\left(I+\frac{3}{4}\varepsilon^2\Delta t\Delta^2\right)^{-1}\Delta^2\left(\frac{3}{4}\phi^n+\frac{1}{4}\phi^{n-1}\right)-\left(I+\frac{3}{4}\varepsilon^2\Delta t\Delta^2\right)^{-1}\Delta^2\Phi^n\right\|\le(A^*+1)\Delta t. \tag{3.65}$$

In addition, the fact that $\|\Delta^2\Phi^n\|\le A^*$ gives

$$\left\|\left(I+\frac{3}{4}\varepsilon^2\Delta t\Delta^2\right)^{-1}\Delta^2\Phi^n\right\|\le\|\Delta^2\Phi^n\|\le A^*.$$

Then we arrive at the following estimate:

$$\begin{aligned}|I_2-I_2^*|&\le\Delta t\|F'(\phi^{*,n})-F'(\Phi^n)\|\cdot\|F'(\phi^{*,n})\|\\&\quad+\Delta t\left\|\left(I+\frac{3}{4}\varepsilon^2\Delta t\Delta^2\right)^{-1}\Delta^2\left(\frac{3}{4}\phi^n+\frac{1}{4}\phi^{n-1}-\Phi^n\right)\right\|\\&\quad\cdot\left\|\left(I+\frac{3}{4}\varepsilon^2\Delta t\Delta^2\right)^{-1}\Delta^2\Phi^n\right\|\\&\le A_{17}\Delta t^2,\quad\text{with } A_{17}:=(A_5^3+A_5)(A_9+A_{10})|\Omega|+A^*(A^*+1).\end{aligned} \tag{3.66}$$

As a consequence, a substitution of (3.54), (3.55), (3.58), (3.61), and (3.66) into (3.51)–(3.52) indicates that

$$g_n'(\eta)=I_1^*+I_2^*+I_3^*+\mathcal{R}_1,\qquad|\mathcal{R}_1|\le((4A_2^2+2)A_3^2|\Omega|+A_{15}+A_{16}+A_{17}+1)\Delta t^2, \tag{3.67}$$

provided that $4A_2A_3^3|\Omega|\Delta t\le\frac{1}{2}$, $2A_4^3|\Omega|\Delta t^2\le\frac{1}{2}$. In addition, a careful calculation reveals that

$$I_1^*+I_2^*+I_3^*=\Delta t\left(F'(\Phi^n),\left(I+\frac{3}{4}\varepsilon^2\Delta t\Delta^2\right)^{-1}((1-2\eta)\Delta F'(\Phi^n)+\varepsilon^2\Phi^n)\right). \tag{3.68}$$

A further decomposition is made to facilitate the later analysis:

$$\begin{aligned} &I_1^* + I_2^* + I_3^* = I_7^* + I_8^*, \\ &\quad \text{with } I_7^* = \Delta t \left(F'(\Phi^n), \left(I + \frac{3}{4}\varepsilon^2 \Delta t \Delta^2 \right)^{-1} (-\Delta F'(\Phi^n) + \varepsilon^2 \Delta^2 \Phi^n) \right), \\ &\quad I_8^* = 2(1-\eta)\Delta t \left(F'(\Phi^n), \left(I + \frac{3}{4}\varepsilon^2 \Delta t \Delta^2 \right)^{-1} \Delta F'(\Phi^n) \right). \end{aligned} \tag{3.69}$$

An estimate for I_8^* is straightforward:

$$\begin{aligned} &\|F'(\Phi^n)\|,\ \|\Delta F'(\Phi^n)\| \le C(\|\Phi^n\|_{H^2}^3 + \|\Phi^n\|_{H^2}) \le C((A^*)^3 + A^*), \\ &\left\| \left(I + \frac{3}{4}\varepsilon^2 \Delta t \Delta^2 \right)^{-1} \Delta F'(\Phi^n) \right\| \le \|\Delta F'(\Phi^n)\| \le C((A^*)^3 + A^*), \end{aligned}$$

so that

$$\begin{aligned} |I_8^*| &\le 2|1-\eta|\Delta t \cdot \|F'(\Phi^n)\| \cdot \left\| \left(I + \frac{3}{4}\varepsilon^2 \Delta t \Delta^2 \right)^{-1} \Delta F'(\Phi^n) \right\| \\ &\le C((A^*)^3 + A^*)^2 \Delta t^{3/2}, \end{aligned} \tag{3.70}$$

in which the fact that $|1-\eta| \le \Delta t^{1/2}$ has been applied in the last step. For the part I_7^*, we observe that $-\Delta F'(\Phi^n) + \varepsilon^2 \Delta^2 \Phi^n = -(\Phi_t)^n$ (satisfied by the original PDE), so that a further decomposition is available:

$$\begin{aligned} &I_7^* = -\Delta t \left(F'(\Phi^n), \left(I + \frac{3}{4}\varepsilon^2 \Delta t \Delta^2 \right)^{-1} (\Phi_t)^n \right) := I_9^* + I_{10}^*, \quad \text{with} \\ &I_9^* = -\Delta t (F'(\Phi^n), (\Phi_t)^n), \quad I_{10}^* = \frac{3}{4}\varepsilon^2 \Delta t^2 \left(F'(\Phi^n), \left(I + \frac{3}{4}\varepsilon^2 \Delta t \Delta^2 \right)^{-1} \Delta^2 (\Phi_t)^n \right). \end{aligned} \tag{3.71}$$

By (1.3), an exact value is available for I_9^*:

$$I_9^* = -S_n \Delta t. \tag{3.72}$$

The estimate for I_{10}^* could be carried out as follows

$$\begin{aligned} &\|F'(\Phi^n)\| \le C((A^*)^3 + A^*), \quad \|\Delta^2 (\Phi_t)^n\| \le C A^* \quad \text{by (3.11)}, \\ &\left\| \left(I + \frac{3}{4}\varepsilon^2 \Delta t \Delta^2 \right)^{-1} \Delta^2 (\Phi_t)^n \right\| \le \|F'(\Phi^n)\| \le C A^*, \end{aligned}$$

so that

$$|I_{10}^*| \le \frac{3}{4}\varepsilon^2 \Delta t^2 \|F'(\Phi^n)\| \cdot \left\| \left(I + \frac{3}{4}\varepsilon^2 \Delta t \Delta^2 \right)^{-1} \Delta^2 (\Phi_t)^n \right\| \le C((A^*)^4 + A^2)\varepsilon^2 \Delta t^2. \tag{3.73}$$

Therefore, a substitution of (3.70), (3.71), (3.72), (3.73) into (3.69) results in

$$\begin{aligned} &I_1^* + I_2^* + I_3^* = -S_n \Delta t + \mathcal{R}_2, \\ &\text{with } |\mathcal{R}_2| \le C((A^*)^4 + A^2)\varepsilon^2 \Delta t^2 + C((A^*)^3 + A^*)^2 \Delta t^{3/2} \le \Delta t^{5/4}, \end{aligned} \tag{3.74}$$

provided that Δt is sufficiently small. Its combination with (3.67) leads to

$$g_n'(\eta) = -S_n\Delta t + \mathcal{R}, \quad \text{with } \mathcal{R} = \mathcal{R}_1 + \mathcal{R}_2, \ |\mathcal{R}| \le 2\Delta t^{5/4},$$

for any $1-\Delta t^{1/2} \le \eta \le 1+\Delta t^{1/2}$. Under the assumption $\Delta t \le (S_n/4)^4$ and $|S_n| \ge \gamma$, we have $2\Delta t^{1/4} \le \frac{|S_n|}{2}$. Hence, the following estimate is valid:

$$\frac{|S_n|}{2}\Delta t \le g_n'(\eta) \le \frac{3|S_n|}{2}\Delta t, \ \text{so that } |g_n'(\eta)| \ge \frac{|S_n|}{2}\Delta t, \\ \text{for } 1-\Delta t^{1/2} \le \eta \le 1+\Delta t^{1/2}.$$

This finishes the proof of Lemma 3.4. ∎

3.3. Proof of Theorem 3.1. We can now proceed to the proof of Theorem 3.1. Without loss of generality, we assume that $S_n < 0$ and $g_n(1) > 0$, as the other cases could be analyzed in the same way. By Lemmas 3.3 and 3.4, we have

$$0 \le g_n(1) \le A_{12}\Delta t^2, \quad g_n'(\eta) \ge -\frac{S_n}{2}\Delta t \ \text{for } 1-\Delta t^{1/2} \le \eta \le 1+\Delta t^{1/2}. \tag{3.75}$$

Then we conclude that $g_n(\eta)$ is monotone and increasing over the interval $(1-\delta^*, 1)$, with $\delta^* = -\frac{2A_{12}}{S_n}\Delta t$, so that

$$g_n(1) \ge 0, \ g_n(1-\delta^*) \le g_n(1) + \frac{S_n}{2}\Delta t \cdot \delta^* \le A_{12}\Delta t^2 - A_{12}\Delta t^2 = 0. \tag{3.76}$$

Therefore, there is a unique solution for $g_n(\eta) = 0$ over the interval $(1-\delta^*, 1)$. In addition, we have $\delta^* \le \Delta t^{1/2}$ if $\Delta t \le \frac{S_n^2}{4A_{12}}$ is satisfied. Since $g_n(\eta)$ is increasing over $[1-\Delta t^{1/2}, 1+\Delta t^{1/2}]$, such a solution is unique in the interval $[1-\Delta t^{1/2}, 1+\Delta t^{1/2}]$. The proof is complete.

4. Error analysis. To carry out an error analysis, we shall assume

$$\left|\frac{d}{dt}\int_\Omega F(\Phi)\,d\boldsymbol{x}\right| = \left|\int_\Omega F'(\Phi)\Phi_t\,d\boldsymbol{x}\right| \ge \gamma \ \text{ for } 0 \le t \le T_0, \tag{4.1}$$

which is the continuous version of (1.3) and implies in particular the assumption (1.3) up to $n \le T_0/\Delta t$. We note that if the assumption (4.1) is satisfied initially, it will hold for certain interval $[]0, T_0]$ (where $T_0 \le T$) since the solution depends continuously on the initial data.

For the sake of brevity, we shall only carry out an error analysis for the scheme (3.4)–(3.5) under the above assumption in the time interval $[0, T_0]$. For time intervals where (4.1) is not satisfied, we use the modified Lagrange multiplier approach by setting $\eta^{n+1/2} = 1$ and computing ϕ^{n+1} by (3.4). Note that (3.4) with $\eta^{n+1/2} = 1$ is a linear equation so that its error analysis is much easier than (3.4)–(3.5). In fact, by setting $\eta^{n+1/2} = 1$, the following error analysis is also valid for (3.4) with $\eta^{n+1/2} = 1$. Therefore, the error analysis below can essentially be extended to the whole interval $[0, T]$ with the modified Lagrange multiplier approach.

The main result of this section is stated in the following theorem.

THEOREM 4.1. *Given initial data $\Phi^0 \in H^8_{per}(\Omega)$, suppose the exact solution for the Cahn–Hilliard equation* (3.2) *is of regularity class $\mathcal{R}$ and satisfies the assumption* (4.1). *Then, provided that $\Delta t \le C\min((\hat{C})^{-2}, \hat{C}^2\varepsilon^2, \frac{\gamma^4}{4})$, we have*

$$\|\Delta^2 e^m\| + \left(\varepsilon^2\Delta t\sum_{k=1}^m \|\Delta^3 e^k\|^2\right)^{1/2} \le \hat{C}\Delta t^2 \tag{4.2}$$

for all positive integers m, such that $t^m = m\Delta t \le T_0$, where $\hat{C}, C > 0$ are some positive constants independent of n and Δt.

The proof of this theorem will be carried out through a series of intermediate estimates which we describe below.

4.1. Energy stability and the H^1 estimate. The following result could be proved in a straightforward way.

LEMMA 4.2. *If the numerical system (3.4)–(3.5) is solvable, it is energy stable with respect to the modified energy functional $\tilde{E}(\phi^{n+1},\phi^n) := E(\phi^{n+1}) + \frac{1}{8}\varepsilon^2\|\nabla(\phi^{n+1} - \phi^n)\|^2$; i.e., the following energy inequality holds:*

$$\tilde{E}(\phi^{n+1},\phi^n) \le \tilde{E}(\phi^n,\phi^{n-1}) \quad \forall n \ge 0. \tag{4.3}$$

Proof. Taking an inner product with (3.4) by $(-\Delta)^{-1}(\phi^{n+1} - \phi^n)$ gives

$$\begin{aligned} &(F'(\phi^{*,n})\eta^{n+1/2}, \phi^{n+1} - \phi^n) - \varepsilon^2 \left(\Delta\left(\frac{3}{4}\phi^{n+1} + \frac{1}{4}\phi^{n-1}\right), \phi^{n+1} - \phi^n\right) \\ &\quad = -\frac{1}{\Delta t}\|\phi^{n+1} - \phi^n\|^2_{H^{-1}}. \end{aligned} \tag{4.4}$$

Meanwhile, the following estimates are available:

$$\begin{aligned} &(F'(\phi^{*,n})\eta^{n+1/2}, \phi^{n+1} - \phi^n) = (F(\phi^{n+1}) - F(\phi^n), 1) \quad \text{(by (3.5))}, \\ &\quad -\left(\Delta\left(\frac{3}{4}\phi^{n+1} + \frac{1}{4}\phi^{n-1}\right), \phi^{n+1} - \phi^n\right) = \left(\nabla\left(\frac{3}{4}\phi^{n+1} + \frac{1}{4}\phi^{n-1}\right), \nabla(\phi^{n+1} - \phi^n)\right) \\ &\ge \frac{1}{2}(\|\nabla\phi^{n+1}\|^2 - \|\nabla\phi^n\|^2) + \frac{1}{8}(\|\nabla(\phi^{n+1} - \phi^n)\|^2 - \|\nabla(\phi^n - \phi^{n-1})\|^2). \end{aligned}$$

Going back to (4.4), we arrive at the desired inequality (4.3). ∎

As a result of this result, we obtain a uniform bound of the original energy functional $E(\phi^n)$ for any $n \ge 1$:

$$E(\phi^n) \le \tilde{E}(\phi^n,\phi^{n-1}) \le \cdots \le \tilde{E}(\phi^0,\phi^{-1}) = E(\phi^0) := C_0 \quad \text{by taking } \phi^{-1} = \phi^0.$$

Meanwhile, since $E(\phi^n) \ge \frac{\varepsilon^2}{2}\|\nabla\phi^n\|^2$, we get

$$\frac{\varepsilon^2}{2}\|\nabla\phi^n\|^2 \le E(\phi^n) \le C_0, \quad \text{so that } \|\nabla\phi^n\| \le (2C_0)^{1/2}\varepsilon^{-1}.$$

Also, the numerical solution (3.4)–(3.5) is mass conservative, so that

$$\overline{\phi^n} = \overline{\phi^{n-1}} = \cdots = \overline{\phi^0} := \beta_0 \quad \forall n \ge 0.$$

In turn, an application of the Poincaré inequality yields a uniform-in-time H^1 bound for the numerical solution

$$\|\phi^n\|_{H^1} \le C\Big(|\overline{\phi^n}| + \|\nabla\phi^n\|\Big) \le C_1 := C(|\beta_0| + (2C_0)^{1/2}\varepsilon^{-1}) \quad \forall n \ge 0. \tag{4.5}$$

We notice that C_1 is uniform in time, while it depends on ε^{-1} in a polynomial pattern.

4.2. The $\ell^\infty(0,T;H^2)$ estimate for the numerical solution.

LEMMA 4.3. *Under the assumption* (1.3) *with* $\gamma \geq 4\Delta t^{\frac{1}{4}}$ *and the a priori assumption* (3.12), *we have*

$$\|\phi^n\|_{H^2} \leq C_2 \quad \forall n \geq 1, \tag{4.6}$$

in which C_2 depends on ε^{-1} in a polynomial pattern, while it is independent of Δt and T.

Proof. First, it is noticed that, by the assumptions and Theorem 3.1, the scheme (3.4)–(3.5) has a unique solution in $1-\Delta t^{1/2} \leq \eta \leq 1+\Delta t^{1/2}$. Taking an inner product with (3.4) by $2\Delta^2(\phi^{n+1}-\phi^n)$, we obtain

$$\begin{aligned}&\|\Delta\phi^{n+1}\|^2 - \|\Delta\phi^n\|^2 + \|\Delta(\phi^{n+1}-\phi^n)\|^2 + \varepsilon^2\Delta t\left(\Delta^2\phi^{n+1}, \Delta^2\left(\frac{3}{2}\phi^{n+1}+\frac{1}{2}\phi^{n-1}\right)\right)\\ &= 2\eta^{n+1/2}\Delta t(\Delta F'(\phi^{*,n}), \Delta^2\phi^{n+1}).\end{aligned} \tag{4.7}$$

The inner product associated surface diffusion could be analyzed as follows:

$$\begin{aligned}\left(\Delta^2\phi^{n+1}, \Delta^2\left(\frac{3}{2}\phi^{n+1}+\frac{1}{2}\phi^{n-1}\right)\right) &= \frac{3}{2}\|\Delta^2\phi^{n+1}\|^2 + \frac{1}{2}(\Delta^2\phi^{n+1}, \Delta^2\phi^{n-1})\\ &\geq \frac{3}{2}\|\Delta^2\phi^{n+1}\|^2 - \frac{1}{2}\left(\frac{1}{2}\|\Delta^2\phi^{n+1}\|^2 + \frac{1}{2}\|\Delta^2\phi^{n-1}\|^2\right)\\ &\geq \frac{5}{4}\|\Delta^2\phi^{n+1}\|^2 - \frac{1}{4}\|\Delta^2\phi^{n-1}\|^2.\end{aligned}$$

For the right-hand side in (4.7), we recall the expansion (3.28) and apply the Hölder inequality:

$$\|\Delta F'(\phi^{*,n})\| \leq (3\|\phi^{*,n}\|_{L^\infty}^2 + 1)\|\Delta\phi^{*,n}\| + 6\|\phi^{*,n}\|_{L^\infty} \cdot \|\nabla\phi^{*,n}\|_{L^4}^2. \tag{4.8}$$

Meanwhile, the following estimates are available, based on Sobolev embedding and weighted inequalities, as well as the uniform-in-time estimate (4.5):

$$\begin{aligned}\|\phi^{*,n}\|_{L^\infty} &\leq C\|\phi^{*,n}\|_{H^1}^{5/6} \cdot \|\phi^{*,n}\|_{H^4}^{1/6} \leq C\|\phi^{*,n}\|_{H^1}^{5/6} \cdot (\|\phi^{*,n}\|_{H^1} + \|\Delta^2\phi^{*,n}\|)^{1/6}\\ &\leq CC_1^{5/6} \cdot (C_1 + \|\Delta^2\phi^{*,n}\|)^{1/6},\end{aligned} \tag{4.9}$$

$$\|\Delta\phi^{*,n}\| \leq \|\nabla\phi^{*,n}\|^{2/3} \cdot \|\Delta^2\phi^{*,n}\|^{1/3} \leq CC_1^{2/3} \cdot \|\Delta^2\phi^{*,n}\|^{1/3}, \tag{4.10}$$

$$\|\nabla\phi^{*,n}\|_{L^4} \leq C\|\nabla\phi^{*,n}\|_{H^{3/4}} \leq C\|\nabla\phi^{*,n}\|^{3/4} \cdot \|\Delta\phi^{*,n}\|_{H^4}^{1/4} \leq CC_1^{3/4} \cdot \|\Delta^2\phi^{*,n}\|^{1/4}. \tag{4.11}$$

Going back to (4.8), we get

$$\|\Delta F'(\phi^{*,n})\| \leq CC_1^3 + CC_1^{7/3} \cdot \|\Delta^2\phi^{*,n}\|^{2/3} + CC_1^{2/3} \cdot \|\Delta^2\phi^{*,n}\|^{1/3}. \tag{4.12}$$

In turn, an application of the Cauchy inequality implies that

$$\begin{aligned}
&2\eta^{n+1/2}(\Delta F'(\phi^{*,n}), \Delta^2\phi^{n+1}) \le 3\|\Delta F'(\phi^{*,n})\| \cdot \|\Delta^2\phi^{n+1}\| \\
&\le 9\varepsilon^{-2}\|\Delta F'(\phi^{*,n})\|^2 + \frac{1}{4}\varepsilon^2\|\Delta^2\phi^{n+1}\|^2 \\
&\le C\varepsilon^{-2}(C_1^6 + C_1^{14/3}\cdot\|\Delta^2\phi^{*,n}\|^{4/3} + C_1^{4/3}\cdot\|\Delta^2\phi^{*,n}\|^{2/3}) + \frac{1}{4}\varepsilon^2\|\Delta^2\phi^{n+1}\|^2 \\
&\le C_\varepsilon^{(1)} + \frac{\varepsilon^2}{10}\|\Delta^2\phi^{*,n}\|^2 + \frac{1}{4}\varepsilon^2\|\Delta^2\phi^{n+1}\|^2 \\
&\le C_\varepsilon^{(1)} + \frac{9\varepsilon^2}{20}\|\Delta^2\phi^n\|^2 + \frac{\varepsilon^2}{20}\|\Delta^2\phi^{n-1}\|^2 + \frac{1}{4}\varepsilon^2\|\Delta^2\phi^{n+1}\|^2, \qquad (4.13)
\end{aligned}$$

in which the Young's inequality has been extensively applied in the fourth step, and the last step is based on the fact that $\|\Delta^2\phi^{*,n}\|^2 \le \frac{9}{2}\|\Delta^2\phi^n\|^2 + \frac{1}{2}\|\Delta^2\phi^{n-1}\|^2$. We also notice that $C_\varepsilon^{(1)}$ depends on C_1 and ε^{-1} in a polynomial pattern.

Subsequently, a substitution of (4.8) and (4.13) into (4.7) leads to

$$\|\Delta\phi^{n+1}\|^2 - \|\Delta\phi^n\|^2 + \varepsilon^2\Delta t\|\Delta^2\phi^{n+1}\|^2 \le C_\varepsilon^{(1)}\Delta t + \frac{9\varepsilon^2}{20}\Delta t\|\Delta^2\phi^n\|^2 + \frac{3\varepsilon^2}{10}\Delta t\|\Delta^2\phi^{n-1}\|^2.$$

In fact, this inequality could be rewritten as

$$\begin{aligned}
&\|\Delta\phi^{n+1}\|^2 + \frac{4}{5}\varepsilon^2\Delta t\|\Delta^2\phi^{n+1}\|^2 + \frac{3}{10}\varepsilon^2\Delta t\|\Delta^2\phi^n\|^2 \\
&\quad + \frac{1}{5}\varepsilon^2\Delta t\|\Delta^2\phi^{n+1}\|^2 + \frac{1}{20}\varepsilon^2\Delta t\|\Delta^2\phi^n\|^2 \\
&\le \|\Delta\phi^n\|^2 + \frac{4}{5}\varepsilon^2\Delta t\|\Delta^2\phi^n\|^2 + \frac{3}{10}\varepsilon^2\Delta t\|\Delta^2\phi^{n-1}\|^2 + C_\varepsilon^{(1)}\Delta t.
\end{aligned}$$

With an introduction of a modified H^2 energy

$$G^n := \|\Delta\phi^n\|^2 + \frac{4}{5}\varepsilon^2\Delta t\|\Delta^2\phi^n\|^2 + \frac{3}{10}\varepsilon^2\Delta t\|\Delta^2\phi^{n-1}\|^2,$$

we get

$$G^{n+1} + B_0\varepsilon^2\Delta t G^{n+1} \le G^n + C_\varepsilon^{(1)}\Delta t,$$

in which the following elliptic regularity has been used:

$$B_1\|\Delta f\|^2 \le \|\Delta^2 f\|^2 \quad \text{and} \quad B_0 = \min\left(\frac{B_1}{10}, \frac{1}{8}\right).$$

An application of the induction argument implies that

$$G^{n+1} \le (1 + B_0\varepsilon^2\Delta t)^{-(n+1)}G^0 + \frac{C_\varepsilon^{(1)}}{B_0\varepsilon^2}.$$

Of course, we could introduce a uniform-in-time quantity $B_2^* := G^0 + \frac{C_\varepsilon^{(1)}}{B_0\varepsilon^2}$, so that $\|\Delta\phi^n\|^2 \le G^n \le B_2^*$ for any $n \ge 0$. In turn, an application of the elliptic regularity reveals that

$$\|\phi^n\|_{H^2} \le C(|\overline{\phi^k}| + \|\Delta\phi^k\|) \le C(|\beta_0| + (B_2^*)^{1/2}) := C_2 \quad \forall n \ge 0.$$

in which the uniform-in-time constant C_2 depends on ε^{-1} in a polynomial pattern. This finishes the proof of Lemma 4.3. ∎

Using similar tools, a uniform-in-time H^k bound for the numerical solution could be established, for any $k \ge 3$, by taking the inner product with (3.4) by $2(-\Delta)^k\phi^{n+1}$, and performing the associated estimates. Details are left to interested readers.

LEMMA 4.4. *Under the assumptions of Lemma* 4.3, *we have, for any* $k \geq 3$,

$$\|\phi^n\|_{H^k} \leq C_k \quad \forall n \geq 1, \tag{4.14}$$

in which C_k *depends on* ε^{-1} *in a polynomial power, while it is independent of* Δt *and* T_0.

4.3. Estimate for $\|\phi^{m+1} - \phi^m\|_{H^\ell}$. The following estimate is needed in the later analysis.

LEMMA 4.5. *Under the assumptions of Lemma* 4.3, *for any* $\ell \geq 2$ *we have*

$$\max_{0 \leq m \leq M-1} \|\phi^{m+1} - \phi^m\|_{H^\ell} \leq D_\ell \Delta t, \tag{4.15}$$

where $D_\ell > 0$ *is a constant independent of* Δt *and* T_0, *dependent on* ε^{-1} *in a polynomial style.*

Proof. For any $\ell \geq 2$, the numerical scheme (3.4) implies that

$$\begin{aligned} &\|\phi^{m+1} - \phi^m\|_{H^\ell} = \Delta t \|\Delta \mu^{m+1/2}\|_{H^\ell}, \\ &\qquad \mu^{m+1/2} = F'(\phi^{*,m})\eta^{m+1/2} - \varepsilon^2 \Delta \left(\frac{3}{4}\phi^{m+1} + \frac{1}{4}\phi^{m-1}\right). \end{aligned} \tag{4.16}$$

By the expansion for $\mu^{m+1/2}$, the following estimates could be derived, helped by repeated applications of the Hölder inequality and Sobolev embedding:

$$\begin{aligned} \|\Delta F'(\phi^{*,m})\|_{H^\ell} &\leq C \|F'(\phi^{*,m})\|_{H^{\ell+2}} \leq C \|\phi^{*,m}\|^3_{H^{\ell+2}} \\ &\leq C(\|\phi^m\|^3_{H^{\ell+2}} + \left\|\phi^{m-1}\right\|^3_{H^{\ell+2}}) \leq C C^3_{\ell+2}, \end{aligned} \tag{4.17}$$

$$\left\|\Delta^2 \left(\frac{3}{4}\phi^{m+1} + \frac{1}{4}\phi^{m-1}\right)\right\|_{H^\ell} \leq C(\|\phi^{m+1}\|_{H^{\ell+4}} + \|\phi^{m-1}\|_{H^{\ell+4}}) \leq C C_{\ell+4}, \tag{4.18}$$

with the uniform-in-time estimates (4.14) used. For any $\ell \geq 2$, consequently, a substitution of (4.17)–(4.18) into (4.16) yields

$$\left\|\phi^{m+1} - \phi^m\right\|_{H^\ell} \leq D_\ell \Delta t, \quad D_\ell := C\left(C^3_{\ell+2} + \varepsilon^2 C_{\ell+4}\right).$$

Note that D_ℓ depends on ε^{-1} in a polynomial form, since both $C_{\ell+2}$ and $C_{\ell+4}$ do as well. This completes the proof of Lemma 4.4. ∎

4.4. A refined estimate for $\eta^{n+1/2}$. An $O(\Delta t^{1/2})$ estimate has been derived for $|\eta^{n+1/2}|$ in Theorem 3.1. In fact, by the estimate (3.75), we see that

$$|\eta^{n+1/2} - 1| \leq \frac{A_{12}\Delta t^2}{\frac{|S_n|}{2}\Delta t} = \frac{2A_{12}\Delta t}{|S_n|} \leq \frac{2A_{12}\Delta t}{\gamma}. \tag{4.19}$$

Again, this rough estimate is not sufficient for an optimal rate of convergence. We aim to improve this estimate so that $\eta^{n+1/2} - 1 = O(\Delta t^2)$. The following preliminary lemma is needed.

LEMMA 4.6. *Under the assumptions of Lemma* 4.3, *we have*

$$\left\|\frac{p^n + \Delta t q^n + \phi^n}{2} - \phi^{*,n}\right\| \leq Q_0 \Delta t^2, \tag{4.20}$$

where Q_0 *is a constant independent of* Δt, *dependent on the exact solution* Φ *and* ε^{-1}.

Proof. A careful calculation reveals that

(4.21)
$$\begin{aligned}
\frac{p^n+\Delta t q^n+\phi^n}{2}-\phi^{*,n} &= \frac{p^n-\phi^n+\Delta t q^n}{2}-\frac{1}{2}(\phi^n-\phi^{n-1})\\
&=\frac{1}{2}\Delta t\left(I+\frac{3}{4}\varepsilon^2\Delta t\Delta^2\right)^{-1}\left(-\varepsilon^2\Delta^2\left(\frac{3}{4}\phi^n+\frac{1}{4}\phi^{n-1}\right)+\Delta F'(\phi^{*,n})\right)-\frac{1}{2}(\phi^n-\phi^{n-1})\\
&=\frac{1}{2}\Delta t\left(\left(I+\frac{3}{4}\varepsilon^2\Delta t\Delta^2\right)^{-1}-I\right)r^n+\frac{1}{2}(\Delta t r^n-(\phi^n-\phi^{n-1})),
\end{aligned}$$
with $r^n=-\varepsilon^2\Delta^2\left(\frac{3}{4}\phi^n+\frac{1}{4}\phi^{n-1}\right)+\Delta F'(\phi^{*,n})$,

in which the representation formulas (3.8), (3.21) have been applied.

For the first part of (4.21), we see that $\Delta^2 r^n=-\varepsilon^2\Delta^4(\frac{3}{4}\phi^n+\frac{1}{4}\phi^{n-1})+\Delta^3F'(\phi^{*,n})$, and the following estimates could be derived by (4.14):

$$\|\Delta^4\phi^n\|,\ \|\Delta^4\phi^{n-1}\|\le C_8, \tag{4.22}$$
$$\|\Delta^3F'(\phi^{*,n})\|\le\|F'(\phi^{*,n})\|_{H^6}\le C(\|\phi^{*,n}\|_{H^6}^3+\|\phi^{*,n}\|_{H^6})\le C(C_6^3+C_6), \tag{4.23}$$

in which the 3-D Sobolev embedding and Hölder inequality have been extensively applied, as well as the fact that $F'(\phi)=\phi^3-\phi$. Then we arrive at

(4.24)
$$\|\Delta^2 r^n\|=\|-\varepsilon^2\Delta^4\left(\frac{3}{4}\phi^n+\frac{1}{4}\phi^{n-1}\right)+\Delta^3F'(\phi^{*,n})\|\le Q_1:=\varepsilon^2C_8+C(C_6^3+C_6).$$

This in turn leads to

$$\left\|\left(\left(I+\frac{3}{4}\varepsilon^2\Delta t\Delta^2\right)^{-1}-I\right)r^n\right\|=\frac{3}{4}\varepsilon^2\Delta t\left\|\left(I+\frac{3}{4}\varepsilon^2\Delta t\Delta^2\right)^{-1}\Delta^2r^n\right\|\le\frac{3}{4}Q_1\varepsilon^2\Delta t.$$

For the second part of (4.21), we make use of the following expression of $\phi^n-\phi^{n-1}$ (which comes from the numerical scheme (3.4)):

$$\phi^n-\phi^{n-1}=\eta^{n-1/2}\Delta t\Delta F'(\phi^{*,n-1})-\varepsilon^2\Delta t\Delta^2\left(\frac{3}{4}\phi^n+\frac{1}{4}\phi^{n-2}\right),\quad\text{so that}$$
$$\begin{aligned}\Delta t r^n-(\phi^n-\phi^{n-1})&=(\eta^{n-1/2}-1)\Delta t\Delta F'(\phi^{*,n-1})+\Delta t\Delta(F'(\phi^{*,n})-F'(\phi^{*,n-1}))\\
&\quad+\frac{1}{4}\varepsilon^2\Delta t\Delta^2(\phi^{n-1}-\phi^{n-2}).\end{aligned}\tag{4.25}$$

For the first part of the expansion (4.25), from (4.6) we have

(4.26)
$$\|\Delta F'(\phi^{*,n-1})\|\le\|F'(\phi^{*,n-1})\|_{H^2}\le C(\|\phi^{*,n-1}\|_{H^2}^3+\|\phi^{*,n-1}\|_{H^2})\le C(C_2^3+C_2).$$

Its combination with the preliminary rough estimate (4.19) implies that

$$\|(\eta^{n-1/2}-1)\Delta t\Delta F'(\phi^{*,n-1})\|\le\frac{CA_{12}\Delta t^2}{|S_n^*|}(C_2^3+C_2). \tag{4.27}$$

For the second part of the expansion (4.25), we begin with the following identify:

$$\begin{aligned}&F'(\phi^{*,n})-F'(\phi^{*,n-1})=F''(\xi^{(3)})(\phi^{*,n}-\phi^{*,n-1}),\\
&\quad\text{with } F''(\xi^{(3)})=(\phi^{*,n})^2+\phi^{*,n}\phi^{*,n-1}+(\phi^{*,n-1})^2-1.\end{aligned}\tag{4.28}$$

In turn, extensive applications of the Hölder and Sobolev inequalities indicate that

$$\begin{aligned}\|\Delta(F'(\phi^{*,n})-F'(\phi^{*,n-1}))\| &\le C\|F''(\xi^{(3)})\|_{H^2}^2\|\phi^{*,n}-\phi^{*,n-1}\|_{H^2}\\ &\le C\|F''(\xi^{(3)})\|_{H^2}^2(\|\phi^n-\phi^{n-1}\|_{H^2}+\|\phi^{n-1}-\phi^{n-2}\|_{H^2})\\ &\le C(C_2^2+1)\cdot D_2\Delta t, \end{aligned}\tag{4.29}$$

in which the H^2 estimate (4.6) and the discrete temporal derivative estimate (4.15) have been applied in the last step. For the third part of the expansion (4.25), we make use of (4.15) again and get

$$\left\|\frac{1}{4}\varepsilon^2\Delta t\Delta^2(\phi^{n-1}-\phi^{n-2})\right\| \le \frac{1}{4}\varepsilon^2\Delta t\cdot D_4\Delta t = \frac{1}{4}D_4\varepsilon^2\Delta t^2.\tag{4.30}$$

Therefore, a substitution of (4.27), (4.29), and (4.30) into (4.25) leads to the following estimate:

$$\|\Delta tr^n-(\phi^n-\phi^{n-1})\|\le Q_2\Delta t^2,\quad \text{with } Q_2=\frac{CA_{12}}{|S_n^*|}(C_2^3+C_2)+C(C_2^2+1)D_2+\frac{1}{4}D_4\varepsilon^2.\tag{4.31}$$

Finally, a combination of (4.21), (4.23), and (4.31) yields the desired result (4.20) by taking $Q_0=\frac{3}{8}Q_1\varepsilon^2+\frac{1}{2}Q_2$. This finishes the proof of Lemma 4.6. ∎

As a consequence, we are able to obtain a sharper estimate for $g(1)$, in comparison with Lemma 3.3.

LEMMA 4.7. *Under the assumptions of Lemma 4.3, we have $|g_n(1)|\le A_{18}\Delta t^3$, with Q_3 a constant independent of Δt, but dependent on the exact solution Φ.*

Proof. The expansion formula (3.40) of $g(1)$ indicates that

$$\begin{aligned} &g_n(1)=J_1+J_2,\\ &J_1=\int_\Omega\left(F(p^n+\Delta tq^n)-F(\phi^n)-F'\left(\frac{p^n+\Delta tq^n+\phi^n}{2}\right)(p^n+\Delta tq^n-\phi^n)\right)d\boldsymbol{x},\\ &J_2=\int_\Omega\left(\left(F'\left(\frac{p^n+\Delta tq^n+\phi^n}{2}\right)-F'(\phi^{*,n})\right)(p^n+\Delta tq^n-\phi^n)\right)d\boldsymbol{x}. \end{aligned}\tag{4.32}$$

For the J_1 part, we make use of the following identity:

$$\begin{aligned} &F(x)-F(y)-F'\left(\frac{x+y}{2}\right)(x-y)\\ &\quad=\frac{x+y}{8}(x-y)^3,\quad \forall x,y\in\mathrm{R},\quad \text{so that}\\ &F(p^n+\Delta tq^n)-F(\phi^n)-F'\left(\frac{p^n+\Delta tq^n+\phi^n}{2}\right)(p^n+\Delta tq^n-\phi^n)\\ &\quad=\frac{1}{8}(p^n+\Delta tq^n+\phi^n)\cdot(p^n-\phi^n+\Delta tq^n)^3. \end{aligned}$$

In turn, with an application of the Hölder inequality, combined with inequalities (3.16), (3.42), we obtain

$$\begin{aligned}|J_1| &\le \frac{1}{8}\|p^n+\Delta tq^n+\phi^n\|_{L^\infty}\cdot\|p^n-\phi^n+\Delta tq^n\|_{L^\infty}^3\cdot|\Omega|\\ &\le \frac{1}{8}(A_2+CC_2+1)(A_1+A_3)^3|\Omega|\Delta t^3. \end{aligned}\tag{4.33}$$

For the J_2 part, we begin with the following application of the intermediate value theorem:

$$F'\left(\frac{p^n+\Delta t q^n+\phi^n}{2}\right)-F'(\phi^{*,n})=F''(\xi^{(4)})\cdot\left(\frac{p^n+\Delta t q^n+\phi^n}{2}-\phi^{*,n}\right),$$

with $\xi^{(4)}$ between $\frac{p^n+\Delta t q^n+\phi^n}{2}$ and $\phi^{*,n}$. By the fact that $F''(\phi)=3\phi^2-1$ and the L^∞ bounds for $\frac{p^n+\Delta t q^n+\phi^n}{2}$ and $\phi^{*,n}$, we get

$$\|F''(\xi^{(4)})\|_{L^\infty}\le C\left(\left\|\frac{p^n+\Delta t q^n+\phi^n}{2}\right\|_{L^\infty}^2+\|\phi^{*,n}\|_{L^\infty}^2+1\right)\le C(A_2^2+C_2^2+1).$$

Then we arrive at

$$\begin{aligned}|J_2|&\le\|F''(\xi^{(4)})\|_{L^\infty}\cdot\left\|\frac{p^n+\Delta t q^n+\phi^n}{2}-\phi^{*,n}\right\|\cdot\|p^n+\Delta t q^n-\phi^n\|_{L^\infty}\cdot|\Omega|^{1/2}\\&\le C(A_2^2+C_2^2+1)\cdot Q_0\Delta t^2\cdot(A_1+A_3)\Delta t\cdot|\Omega|^{1/2}\\&=CQ_0|\Omega|(A_2^2+C_2^2+1)(A_1+A_3)\Delta t^3,\end{aligned}\tag{4.34}$$

in which the estimate (4.20) (in Lemma 4.6) has been applied in the second step. Therefore, a combination of (4.32), (4.33), and (4.34) yields the desired result by taking $A_{18}=\frac{1}{8}(A_2+CC_2+1)(A_1+A_3)^3|\Omega|+CQ_0|\Omega|(A_2^2+C_2^2+1)(A_1+A_3)$. This finishes the proof of Lemma 4.7. ∎

Next, we have to obtain a refined estimate for $|\eta^{n+1/2}-1|$.

LEMMA 4.8. *Under the assumptions of Lemma* 4.3*, we have* $|\eta^{n+1/2}-1|\le\frac{2A_{18}}{\gamma}\Delta t^2$ *with* A_{18} *dependent on the exact solution* Φ.

Proof. Again, it is assumed that $g_n(1)>0$ without loss of generality. Following the proof of Theorem 3.1, we see that

$$0\le g_n(1)\le A_{18}\Delta t^3,\quad g_n'(\eta)\ge\frac{\gamma}{2}\Delta t\ \text{ for } 1-\Delta t^{1/2}\le\eta\le 1+\Delta t^{1/2}.$$

Then we conclude that $g_n(\eta)$ is monotone and increasing over the interval $(1-\delta^{**},1)$, with $\delta^{**}=\frac{2A_{18}}{\gamma}\Delta t^2$, so that

$$g_n(1)\ge 0,\ \ g_n(1-\delta^{**})\le g_n(1)-\frac{\gamma}{2}\Delta t\cdot\delta^{**}\le A_{18}\Delta t^3-A_{18}\Delta t^3=0.$$

Therefore, there is a unique solution for $g_n(\eta)=0$ over the interval $(1-\delta^{**},1)$. This finishes the proof of Theorem 4.8. ∎

4.5. Proof of Theorem 4.1. First of all, it is clear that both the exact solution $\Phi(\cdot,t)$ and the numerical solution $\{\phi^k\}$ are mass conservative:

$$\overline{\Phi^k}=\overline{\Phi^0},\quad\overline{\phi^k}=\overline{\phi^0}\quad\forall k\ge 0,\tag{4.35}$$

in which Φ^k is the exact solution evaluated at the time instant t^k. Then we conclude that the numerical error function must have zero-average at each time step:

$$\overline{e^k}=0,\ \ \forall k\ge 0\quad\text{by taking } \phi^0=\Phi^0.\tag{4.36}$$

In turn, the following elliptic regularity estimates are available:

$$\|e^k\|_{H^{2m}}\le C\|\Delta^m e^k\|\quad\text{for } m=1,2,3,\quad\forall k\ge 0.\tag{4.37}$$

First, the a priori assumption (3.12) is made. As a result, the unique solvability for $\eta^{n+1/2}$ (in the range of $1-\Delta t^{1/2} \le \eta^{n+1/2} \le 1+\Delta t^{1/2}$) is assured by Theorem 3.1, and a refined estimate in Lemma 4.8 becomes available.

The following truncation error analysis for the exact solution can be obtained by using a straightforward Taylor expansion:

$$\frac{\Phi^{n+1}-\Phi^n}{\Delta t} = \Delta\left(F'(\Phi^{*,n}) - \varepsilon^2\Delta\left(\frac{3}{4}\Phi^{n+1}+\frac{1}{4}\Phi^{n-1}\right)\right)+\tau^n, \quad \Phi^{*,n}=\frac{3}{2}\Phi^n-\frac{1}{2}\Phi^{n-1}, \tag{4.38}$$

with $\|\Delta\tau^n\| \le C\Delta t^2$.

In turn, subtracting the numerical scheme (3.4) from the consistency estimate (4.38) yields

$$\begin{aligned}\frac{e^{n+1}-e^n}{\Delta t} &= (1-\eta^{n+1/2})\Delta F'(\Phi^{*,n})\\ &\quad + \Delta\left(\eta^{n+1/2}(F'(\Phi^{*,n})-F'(\phi^{*,n})) - \varepsilon^2\Delta\left(\frac{3}{4}e^{n+1}+\frac{1}{4}e^{n-1}\right)\right)+\tau^n.\end{aligned} \tag{4.39}$$

Taking an inner product with (4.39) by $2\Delta^4 e^{n+1}$ gives

$$\begin{aligned}&\|\Delta^2 e^{n+1}\|^2 - \|\Delta^2 e^n\|^2 + \|\Delta^2(e^{n+1}-e^n)\|^2 + \varepsilon^2\Delta t\left(\Delta^3\left(\frac{3}{2}e^{n+1}+\frac{1}{2}e^{n-1}\right),\Delta^3 e^{n+1}\right)\\ &\quad = 2(1-\eta^{n+1/2})\Delta t(\Delta^2 F'(\Phi^{*,n}),\Delta^3 e^{n+1}) + 2\eta^{n+1/2}\Delta t(\Delta^2(F'(\Phi^{*,n})\\ &\qquad - F'(\phi^{*,n})),\Delta^3 e^{n+1}) + 2\Delta t(\Delta\tau^n,\Delta^3 e^{n+1}),\end{aligned} \tag{4.40}$$

in which integration by parts has been extensively applied in the derivation. The surface diffusion term could be analyzed similarly as in (4.8):

$$\begin{aligned}\left(\Delta^3 e^{n+1},\Delta^3\left(\frac{3}{2}e^{n+1}+\frac{1}{2}e^{n-1}\right)\right) &= \frac{3}{2}\|\Delta^3 e^{n+1}\|^2 + \frac{1}{2}(\Delta^3 e^{n+1},\Delta^3 e^{n-1})\\ &\ge \frac{3}{2}\|\Delta^3 e^{n+1}\|^2 - \frac{1}{2}\left(\frac{1}{2}\|\Delta^3 e^{n+1}\|^2+\frac{1}{2}\|\Delta^3 e^{n-1}\|^2\right)\\ &\ge \frac{5}{4}\|\Delta^3 e^{n+1}\|^2 - \frac{1}{4}\|\Delta^3 e^{n-1}\|^2.\end{aligned}$$

The local truncation error term could be bounded by the Cauchy inequality:

$$2(\Delta\tau^n,\Delta^3 e^{n+1}) \le 2\|\Delta\tau^n\|\cdot\|\Delta^3 e^{n+1}\| \le \varepsilon^{-2}\|\Delta\tau^n\|^2 + \frac{1}{4}\varepsilon^2\|\Delta^3 e^{n+1}\|^2. \tag{4.41}$$

For the first nonlinear inner product, we recall the refined estimate $|\eta^{n+1/2}-1| \le Q_3\Delta t^2$, as established in Lemma 4.8. In addition, the following estimate could be derived:

$$\Delta^2 F'(\Phi^{*,n}) \le C(\|\Phi^{*,n}\|_{H^4}^3 + \|\Phi^{*,n}\|_{H^4}) \le C((A^*)^3+A^*), \tag{4.42}$$

based on the fact that $F'(\phi)=\phi^3-\phi$, and the bound (3.11) for the exact solution. Then we arrive at

$$\begin{aligned}2(1-\eta^{n+1/2})(\Delta^2 F'(\Phi^{*,n}),\Delta^3 e^{n+1}) &\le 3Q_3\Delta t^2\cdot\|\Delta^2 F'(\Phi^{*,n})\|\cdot\|\Delta^3 e^{n+1}\|\\ &\le C((A^*)^3+A^*)Q_3\Delta t^2\|\Delta^3 e^{n+1}\|\\ &\le C((A^*)^3+A^*)^2 Q_3^2\varepsilon^{-2}\Delta t^4 + \frac{1}{4}\varepsilon^2\|\Delta^3 e^{n+1}\|^2.\end{aligned} \tag{4.43}$$

For the other nonlinear error term, we begin with the following application of the intermediate value theorem:

$$F'(\Phi^{*,n}) - F'(\phi^{*,n}) = F''(\xi^{(5)})e^{*,n}, \text{ with } F''(\xi^{(5)}) = (\Phi^{*,n})^2 + \Phi^{*,n}\phi^{*,n} + (\phi^{*,n})^2 - 1,$$
$$e^{*,n} = \frac{3}{2}e^n - \frac{1}{2}e^{n-1}.$$

This in turn leads to the following estimate:

$$\begin{aligned}&\|\Delta^2(F'(\Phi^{*,n}) - F'(\phi^{*,n}))\|\\ &\quad = \|\Delta^2(F''(\xi^{(5)})e^{*,n})\| \le C(\|\Phi^{*,n}\|_{H^4}^2 + \|\phi^{*,n}\|_{H^4}^2 + 1) \cdot \|e^{*,n}\|_{H^4}\\ &\quad \le C((A^*)^2 + C_4^2 + 1) \cdot \|\Delta^2 e^{*,n}\|.\end{aligned}$$

Consequently, the following inequality is available:

$$\begin{aligned}&2\eta^{n+1/2}(\Delta^2(F'(\Phi^{*,n}) - F'(\phi^{*,n})), \Delta^3 e^{n+1})\\ &\quad \le C((A^*)^2 + C_4^2 + 1)\|\Delta^2 e^{*,n}\| \cdot \|\Delta^3 e^{n+1}\|\\ &\quad \le C((A^*)^2 + C_4^2 + 1)^2 \varepsilon^{-2}\|\Delta^2 e^{*,n}\|^2 + \frac{1}{4}\varepsilon^2\|\Delta^3 e^{n+1}\|^2\\ &\quad \le C((A^*)^2 + C_4^2 + 1)^2 \varepsilon^{-2}(\|\Delta^2 e^n\|^2 + \|\Delta^2 e^{n-1}\|^2) + \frac{1}{4}\varepsilon^2\|\Delta^3 e^{n+1}\|^2. \qquad (4.44)\end{aligned}$$

Subsequently, a substitution of (4.41), (4.43), and (4.44) into (4.40) leads to

$$\begin{aligned}&\|\Delta^2 e^{n+1}\|^2 - \|\Delta^2 e^n\|^2 + \frac{1}{2}\varepsilon^2\Delta t\|\Delta^3 e^{n+1}\|^2 - \frac{1}{4}\varepsilon^2\Delta t\|\Delta^3 e^{n-1}\|^2\\ &\quad \le C((A^*)^3 + A^*)^2 Q_3^2 \varepsilon^{-2}\Delta t^5 + Q_4\varepsilon^{-2}(\|\Delta^2 e^n\|^2 + \|\Delta^2 e^{n-1}\|^2) + \varepsilon^{-2}\Delta t\|\Delta\tau^n\|^2,\end{aligned}$$

with $Q_4 = C((A^*)^2 + C_4^2 + 1)^2$. Therefore, an application of the discrete Gronwall inequality yields the desired convergence estimate (4.2).

Finally, we have to recover the a priori assumption (3.12) at time step t^{n+1} to close the induction argument. By the convergence estimate (4.2), we get

$$\|\Delta^2 e^{n+1}\| \le \hat{C}\Delta t^2, \quad \varepsilon^2\Delta t\|\Delta^3 e^{n+1}\|^2 \le \hat{C}^2\Delta t^4, \text{ so that } \|\Delta^3 e^{n+1}\| \le \hat{C}\varepsilon^{-1}\Delta t^{3/2}.$$

Making use of the elliptic regularity estimate (4.37), we have

$$\|e^{n+1}\|_{H^4} \le C\|\Delta^2 e^{n+1}\| \le Q_5\hat{C}\Delta t^2, \quad \|e^{n+1}\|_{H^6} \le C\|\Delta^3 e^{n+1}\| \le Q_6\hat{C}\varepsilon^{-1}\Delta t^{3/2}.$$

Therefore, the a priori assumption (3.12) is valid at time step t^{n+1}, provided that

$$\Delta t \le \min\left((Q_5\hat{C})^{-2}, Q_6^2\hat{C}^2\varepsilon^2, \frac{\gamma^4}{4}\right).$$

This finishes the complete induction argument for both the solvability analysis and the convergence estimate.

5. Concluding remarks. In this paper, we investigated the unique solvability and carried out an error analysis for a scheme using the original Lagrange multiplier approach proposed in [9] for gradient flows. We first identified a sufficient condition to ensure the unique solvability, in the neighborhood of its exact solution, of the nonlinear algebraic system arising from the original Lagrange multiplier approach. Then we find that the unique solvability of the original Lagrange multiplier approach depends on a class of initial conditions and is valid over a finite time period. Afterward, we proposed a modified Lagrange multiplier approach to ensure that the computation can continue even if the aforementioned condition was not satisfied.

Using the Cahn–Hilliard equation and a second-order modified Crank–Nicholson scheme with a Lagrange multiplier as an example, we provided a unique solvability analysis using localized estimates in the neighborhood of its exact solution under an a priori assumption, and then carried out a rigorous error analysis, which in turn recovered the a priori assumption using an inductive argument.

The results presented in this paper are the first unique solvability and error analysis for a scheme using the original Lagrange multiplier approach. In a future work, we shall consider a more general Lagrange multiplier approach for gradient flows with global constraints proposed in [10]. Due to the multiple Lagrange multipliers involved in the latter approach, the analysis would be much more challenging, while the analytical techniques introduced in this paper may be helpful.

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