

gPAV-based unconditionally energy-stable schemes for the Cahn–Hilliard equation: Stability and error analysis

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Abstract

We present several first-order and second-order numerical schemes for the Cahn–Hilliard equation with unconditional energy stability in terms of a discrete energy. These schemes stem from the generalized Positive Auxiliary Variable (gPAV) idea, and require only the solution of linear algebraic systems with a constant coefficient matrix. More importantly, the computational complexity (operation count per time step) of these schemes is approximately a half of those of the gPAV and the scalar auxiliary variable (SAV) methods in previous works. We investigate the stability properties of the proposed schemes to establish stability bounds for the field function and the auxiliary variable, and also provide their error analyses. Numerical experiments are presented to verify the theoretical analyses and also demonstrate the stability of the schemes at large time step sizes.

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1. Introduction

The Cahn–Hilliard equation [1] plays a key role in the modeling of two-phase and multiphase flows based on the phase field (or diffuse interface) approach [2–5]. Under appropriate boundary conditions, the mass (or volume) of each fluid component described by the Cahn–Hilliard equation is conserved. Indeed, the Cahn–Hilliard equation can be derived from the mass balance equations for individual fluid components in a multicomponent fluid mixture by choosing an appropriate form for the free energy density function; see e.g. [4,6,7]. Developing effective and efficient numerical algorithms for the Cahn–Hilliard equation can have important ramifications on the modeling and simulation of two-phase and multiphase flows. This problem has witnessed a sustained interest from the research community, and we refer to [8–11] for some examples.

The design of numerical schemes for the Cahn–Hilliard equation confronts several challenges. The predominant issue among these is posed by the nonlinear term. The nonlinear term in the Cahn–Hilliard equation stems from the potential energy (double-well) in the free energy density function. The system described by the Cahn–Hilliard equation admits an energy balance equation (energy law) on the continuous level. To achieve discrete energy stability

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in the numerical scheme, i.e. retaining a corresponding discrete energy law, hinges on the numerical treatment of the nonlinear term. Energy-stable schemes allow the use of larger time step sizes, which can potentially accelerate dynamic simulations if its computational cost per time step is manageable. A downside about energy-stable schemes is that their cost is typically markedly higher when compared with semi-implicit type schemes (see e.g. [5,12–16]), which are only conditionally stable. This is because the energy-stable schemes oftentimes entail the solution of nonlinear algebraic equations, or the solution of linear algebraic systems (either coupled linear systems or a linear system for multiple times). To achieve discrete energy stability and a low computational complexity (or operation count) per time step in the numerical scheme is the focus of the current work.

Numerical algorithms for the Cahn–Hilliard equation available in the literature generally consist of two classes: nonlinear schemes and linear schemes. With nonlinear schemes one treats the nonlinear term or a part of the nonlinear term implicitly, and this requires the solution of nonlinear algebraic equations upon discretization; see e.g. [17–24], among others. Among the nonlinear schemes, convex splitting of the potential energy [25,26] and its variants are a widely-used approach for treating the nonlinear term. Other approaches include the midpoint approximation [17,27], Taylor expansion approximation [20], and special quadrature rules [28], among others.

Unlike nonlinear schemes, the linear schemes (see e.g. [16,29–31]) require only the solution of linear algebraic systems upon discretization, due to the explicit treatment of the nonlinear term, while maintaining energy stability. Among the linear schemes, incorporation of a stabilizing zero term, together with a modified potential energy with bounded second derivative, is an often-used method [16,29]. Other researchers have also employed a Lagrange multiplier to enforce energy stability [16,32]. In the past few years, the use of certain auxiliary functions or variables proves to be effective in devising linear energy-stable schemes. The invariant energy quadratization (IEQ) [30] and the scalar auxiliary variable (SAV) [31] are two prominent examples of such methods; see also [11,33–38], among others. The IEQ method introduces an auxiliary field function as an approximation of the square root of the potential energy density function together with a dynamic equation for this field function, and allows one to ensure the energy stability relatively easily. It gives rise to a system of linear algebraic equations involving time-dependent coefficient matrices upon discretization. The SAV method uses an auxiliary variable (a scalar number rather than a field function) to approximate the square root of the potential energy integral. It retains the ease to ensure the energy stability, and moreover leads to linear algebraic systems with a constant coefficient matrix, thus making the implementation considerably simpler [11]. The use of the square root function form in IEQ and SAV, either for a field function and a scalar number, is critical to the proof of energy stability in these methods. A recent further development in this area is the generalized Positive Auxiliary Variable (gPAV) method [39]. The gPAV method also employs a scalar-valued number as the auxiliary variable to ensure the energy stability, and it gives rise to a linear algebraic system with a constant coefficient matrix. This method makes three advances in terms of the methodology: (i) gPAV allows the use of a general class of function forms to define the auxiliary variable, not limited to the square root function as in IEQ and SAV. (ii) gPAV guarantees the positivity of the computed values for the auxiliary variable. (iii) gPAV applies to general types of dissipative or conservative partial differential equations (PDE) for the development of energy-stable schemes, not limited to gradient type systems.

In the current paper we present several unconditionally energy-stable linear schemes with first- and second-order accuracy for solving the Cahn–Hilliard equation, and provide analyses for their stability properties and errors. The unconditional stability properties are with respect to a discrete energy, not the original free energy of the system. These schemes stem from the gPAV idea [39], and inherit the useful properties of guaranteed positivity for the computed auxiliary variable and constant coefficient matrix for the resultant linear algebraic system upon discretization. Two advances have been made algorithm-wise: (i) Stability bounds for both the phase field function and the auxiliary variable can be established with the current schemes. In contrast, with the original gPAV scheme [39] the stability property is only through the auxiliary variable. (ii) The operation counts (or computational cost) per time step of the current schemes are comparable to that of the semi-implicit schemes (see e.g. [14]), and are about a half of those of the gPAV scheme [39] and the SAV scheme [31]. This is because the linear system resulting from the Cahn–Hilliard equation only needs to be solved once within each time step with the current schemes. In contrast, with gPAV [39] and SAV [11,31] the linear system needs to be solved twice for the two copies of the field function therein within each time step. We provide the stability analyses and error estimates for these schemes, and present numerical experiments to verify the theoretical analyses.

The contributions of this work consist of two aspects: (i) the unconditionally energy-stable schemes for the Cahn–Hilliard equation, and (ii) the stability and error analyses for the proposed schemes.

The rest of this paper is organized as follows. In Section 2 we reformulate the Cahn–Hilliard equation using the gPAV idea, and present two first-order and two second-order schemes for numerically solving the reformulated system of equations. We prove the unconditional energy stability properties of these schemes and provide the error estimates. In Section 3 we present numerical examples to verify the convergence rates and the unconditional stability of these schemes. Section 4 then concludes the presentations with some closing remarks. In the Appendix we provide proofs to several theorems from the main text.

2. gPAV-based unconditionally energy-stable schemes

2.1. Cahn–Hilliard equation and gPAV formulation

Let $\Omega \in \mathbb{R}^d (d = 2, 3)$ be a bounded domain with a smooth boundary $\partial\Omega$. We consider the following gradient flows

$$\frac{\partial\phi}{\partial t} = \Delta\mu = \Delta(-\Delta\phi + \lambda\phi + h(\phi)), \quad (2.1)$$

where $\phi(\mathbf{x}, t)$ is the phase field function, $\lambda \geq 0$ is a constant parameter, Δ is the Laplace operator, and \mathbf{x} and t and the spatial coordinate and time. The nonlinear term

$$h(\phi) = H'(\phi) = \phi^3 - \phi, \quad \text{with } H(\phi) = \frac{1}{4}(\phi^2 - 1)^2 \quad (2.2)$$

being the double-well potential function [1,40]. As is well-known, this is the celebrated Cahn–Hilliard equation with $\lambda = 0$.

Eq. (2.1) is supplemented by the initial condition

$$\phi(\mathbf{x}, t = 0) = \phi_{in}(\mathbf{x}) \quad (2.3)$$

where ϕ_{in} denote the initial phase field distribution, and the boundary conditions of either

$$\nabla\phi \cdot \mathbf{n} = \nabla\mu \cdot \mathbf{n} = 0 \quad \text{on } \partial\Omega, \quad (2.4)$$

or the periodic boundary conditions for ϕ . Here \mathbf{n} denotes the outward-pointing unit normal vector of the boundary.

Taking the L^2 inner product between (2.1) and ϕ , using the integration by parts and (2.4), we derive the following free energy functional E_{tot} for this system

$$E_{tot}(t) = \int_{\Omega} \left(\frac{1}{2} |\nabla\phi|^2 + \frac{\lambda}{2} \phi^2 + H(\phi) \right) d\mathbf{x}.$$

To facilitate energy-stable numerical approximations of the system (2.1), we define a shifted energy of the following form

$$E(t) = \mathbf{E}[\phi] = \int_{\Omega} \left(\frac{1}{2} |\nabla\phi|^2 + \frac{\lambda}{2} \phi^2 + H(\phi) \right) d\mathbf{x} + c_0, \quad (2.5)$$

where c_0 is a chosen energy constant to ensure that $E(t) > 0$ for $0 \leq t \leq T$, and T denotes the time interval on which the system to be solved. It is straightforward to verify that the system (2.1)–(2.4) satisfies the energy dissipation law

$$\frac{dE}{dt} = \int_{\Omega} (\nabla\phi \cdot \nabla\phi_t + \lambda\phi\phi_t + h(\phi)\phi_t) d\mathbf{x} = \int_{\Omega} \phi_t \mu d\mathbf{x} = - \int_{\Omega} |\nabla\mu|^2 d\mathbf{x} \leq 0, \quad (2.6)$$

where ϕ_t denotes the time derivative of ϕ .

Following the gPAV idea [39], we introduce a positive scalar variable $R(t)^2 = E(t)$ (or $R(t) = \sqrt{E(t)}$). $R(t)$ satisfies the following evolution equation

$$2R \frac{dR}{dt} = \frac{dE}{dt} = - \int_{\Omega} |\nabla\mu|^2 d\mathbf{x}. \quad (2.7)$$

Noting that $\frac{R}{\sqrt{E}} = 1$, we rewrite (2.7) into

$$\frac{dR}{dt} = - \frac{1}{2R} \int_{\Omega} |\nabla\mu|^2 d\mathbf{x} = - \frac{1}{2\sqrt{E}} \int_{\Omega} |\nabla\mu|^2 d\mathbf{x} = - \frac{1}{2\sqrt{E}} \frac{R}{\sqrt{E}} \int_{\Omega} |\nabla\mu|^2 d\mathbf{x} = - \frac{R}{2E} \int_{\Omega} |\nabla\mu|^2 d\mathbf{x}. \quad (2.8)$$

Then, we rewrite (2.1) into the following equivalent form

$$\phi_t = \Delta\mu, \quad (2.9a)$$

$$\mu = -\Delta\phi + \lambda\phi + \frac{R^2}{E}h(\phi), \quad (2.9b)$$

$$\frac{dR}{dt} = -\frac{R}{2E} \int_{\Omega} |\nabla\mu|^2 dx. \quad (2.9c)$$

In this reformulated system, the dynamic variables are ϕ , μ and R , which are coupled in Eqs. (2.9), together with the boundary conditions (2.4), the initial condition (2.3) for ϕ , and the following initial condition for $R(t)$

$$R(0) = \sqrt{E[\phi_{in}]}, \quad \text{where } E[\phi_{in}] = \int_{\Omega} \left(\frac{\lambda}{2} \phi_{in}^2 + \frac{1}{2} |\nabla\phi_{in}|^2 + H(\phi_{in}) \right) dx + c_0. \quad (2.10)$$

Note that $R(t)$ in this system is determined by solving the coupled system of equations, not by using the relation $R^2(t) = E(\phi)$. Therefore $R^2(t)$ is an approximation of $E(t)$, rather than $E(t)$ itself.

2.2. Preliminaries

We first outline the notation used herein and recall some basic results, including the existence, uniqueness, and regularity results about the H^{-1} gradient flows.

For the non-negative integers p, k and an open Lipschitz subdomain $D \subset \overline{\Omega}$, let $L^p(D)$ denote the standard Banach space with norm $\|v\|_{0,p,D} = (\int_D |v|^p dx)^{1/p}$ and $W^{k,p}(D)$ the standard Sobolev space with the norm $\|v\|_{k,p,D} = (\sum_{|\alpha| \leq k} \int_D |D^\alpha v|^p dx)^{1/p}$. For simplicity, we take the Sobolev space $H^k(D) = W^{k,2}(D)$ with the norm $\|\cdot\|_{k,D}$ and semi-norm $|\cdot|_{k,D}$, and the space $H^0(D) = L^2(D)$ with the usual L^2 -inner product $(\cdot, \cdot)_D$ and L^2 -norm $\|\cdot\|_{0,D}$. If D is chosen as Ω , we abbreviate them by the norms $\|\cdot\|_k$, $\|\cdot\|_0$, the semi-norm $|\cdot|_k$ and the inner product (\cdot, \cdot) , respectively. Therefore, we introduce the space $L^p(0, T; V)$, $L^\infty(0, T; V)$ and $C(0, T; V)$ with the norms

$$\|\varphi\|_{L^p(0,T;V)} = \left[\int_0^T \|\varphi(t)\|_V^p dt \right]^{1/p}, \quad \|\varphi\|_{L^\infty(0,T;V)} = \operatorname{ess\,sup}_{0 \leq t \leq T} \|\varphi(t)\|_V \quad \text{and} \quad \|\varphi\|_{C(0,T;V)} = \max_{0 \leq t \leq T} \|\varphi(t)\|_V.$$

Assume that the nonlinear free energy potential $H(s) \in C^3(\mathbb{R})$. For some cases, in order to ensure the uniqueness, we assume the following condition: there exists a constant $c_1 > 0$ such that

$$H''(s) = h'(s) \geq -c_1. \quad (2.11)$$

Lemma 2.1 (See [41]). (i) For the H^{-1} gradient flow, assume that (2.11) holds, $\phi_{in} \in L^2(\Omega)$ and there exists $p_0 > 0$ such that

$$sh(s) \geq b|s|^{p_0} - c_2, \quad (2.12)$$

where $b > 0$ and c_2 are constants. Then, for any $T > 0$, there exists a unique solution ϕ for (2.1) such that

$$\phi \in C(0, T; L^2(\Omega)) \cap L^2(0, T; H^2(\Omega)) \cap L^{p_0}(0, T; L^{p_0}(\Omega)). \quad (2.13)$$

(ii) For the H^{-1} gradient flow, assume that $\phi_{in} \in H^2(\Omega)$ and

$$|h'(x)| < C(|x|^{p_1} + 1), \quad p_1 > 0 \text{ arbitrary if } d = 1, 2; \quad 0 < p_1 < 4 \text{ if } d = 3, \quad (2.14)$$

$$|h''(x)| < C(|x|^{p_2} + 1), \quad p_2 > 0 \text{ arbitrary if } d = 1, 2; \quad 0 < p_2 < 3 \text{ if } d = 3, \quad (2.15)$$

where d denotes the dimension in space. Then, for any $T > 0$, there exists a unique solution ϕ for (2.1) such that

$$\phi \in C(0, T; H^2(\Omega)) \cap L^2(0, T; H^4(\Omega)). \quad (2.16)$$

Lemma 2.2 (See [34]). Assume that $\|\phi\|_1 \leq M$.

(i) Under the conditions of (2.14) and $\phi \in H^3(\Omega)$, there exist $0 < \sigma < 1$ and a constant $C(M)$ such that

$$\|\nabla h(\phi)\|_0^2 \leq C(M)(1 + \|\nabla \Delta\phi\|_0^{2\sigma}). \quad (2.17)$$

(ii) Under the assumptions of (2.14), (2.15) and $\phi \in H^4(\Omega)$, there exist $0 < \sigma < 1$ and a constant $C(M)$ such that

$$\|\Delta h(\phi)\|_0^2 \leq C(M)(1 + \|\Delta^2 \phi\|_0^{2\sigma}). \quad (2.18)$$

Lemma 2.3 (Discrete Gronwall Lemma [42]). Let $a_i, b_i, c_i, d_i, \Delta t$ and C_0 , for integers $i \geq 0$, be non-negative numbers such that

$$a_n + \Delta t \sum_{i=0}^n b_i \leq \Delta t \sum_{i=0}^n d_i a_i + \Delta t \sum_{i=0}^n c_i + C_0, \quad \forall n \geq 0.$$

Then, if $d_i \Delta t < 1$ for all i ,

$$a_n + \Delta t \sum_{i=0}^n b_i \leq \left(C_0 + \Delta t \sum_{i=0}^n c_i \right) \exp \left(\Delta t \sum_{i=0}^n \frac{d_i}{1 - d_i \Delta t} \right), \quad \forall n \geq 0.$$

Lemma 2.4 (Discrete Gronwall Lemma [43,44]). Let $a_i, b_i, c_i, d_i, \Delta t$ and C_0 , for integers $i \geq 0$, be non-negative numbers such that

$$a_n + \Delta t \sum_{i=0}^n b_i \leq \Delta t \sum_{i=0}^{n-1} d_i a_i + \Delta t \sum_{i=0}^{n-1} c_i + C_0, \quad \forall n \geq 0.$$

Then,

$$a_n + \Delta t \sum_{i=0}^n b_i \leq \left(C_0 + \Delta t \sum_{i=0}^{n-1} c_i \right) \exp \left(\Delta t \sum_{i=0}^{n-1} d_i \right), \quad \forall n \geq 0.$$

2.3. First-order schemes

We introduce several unconditionally energy-stable schemes for solving the reformulated Cahn–Hilliard equations (2.9), the boundary conditions (2.4), and the initial conditions (2.3) and (2.10). These schemes stem from the gPAV idea [39], and they inherit some of the attractive properties of gPAV. For example, the auxiliary variable is computed via a well-defined explicit form, and its computed values are guaranteed to be positive. The departure point lies in that all the schemes presented herein require only the computation of a single copy of the field functions per time step. In contrast, the original gPAV method [39] entails the computation of two copies of the field functions within each time step. The amount of operations involved in the current schemes is approximately a half of that in the scheme of [39]. The current schemes have a computational cost roughly the same as the semi-implicit schemes for the Cahn–Hilliard equation (see e.g. [14]).

We provide stability analysis and error estimates for these schemes in what follows. The first-order schemes are discussed in this section, followed by the second-order schemes in the subsequent section.

2.3.1. Scheme 1A

Let $\Delta t > 0$ be the time step size and $n \geq 0$ denote the time step index, and we set $t^n = n\Delta t$ for $0 \leq n \leq N$ with $N = T/\Delta t$. For a generic function $\chi(\mathbf{x}, t)$ continuous in t , let χ^n denote the approximation of $\chi(\mathbf{x}, t^n)$ at time t^n , where χ can be ϕ, μ or ψ (defined below). Similarly, let R^n denote the approximation of $R(t^n)$. Set

$$\begin{cases} \phi^0 = \phi_{in}, \quad \mu^0 = -\Delta \phi^0 + \lambda \phi^0 + h(\phi^0), \\ R^0 = \sqrt{E(0)} = \sqrt{\int_{\Omega} \left(\frac{1}{2} |\nabla \phi^0|^2 + \frac{\lambda}{2} |\phi^0|^2 + H(\phi^0) \right) d\mathbf{x} + c_0}. \end{cases} \quad (2.19)$$

Then given ϕ^n , μ^n and R^n , we compute ϕ^{n+1} , μ^{n+1} and R^{n+1} through the following scheme,

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} = \Delta \mu^{n+1}, \quad (2.20a)$$

$$\mu^{n+1} = -\Delta \phi^{n+1} + \lambda \phi^{n+1} + |\xi_{1A}^{n+1}|^2 h(\phi^n), \quad (2.20b)$$

$$\frac{R^{n+1} - R^n}{\Delta t} = -\frac{\xi_{1A}^{n+1}}{2\sqrt{E[\phi^n]}} \int_{\Omega} |\nabla \mu^n|^2 d\mathbf{x}, \quad (2.20c)$$

with the boundary conditions

$$\nabla \phi^{n+1} \cdot \mathbf{n} = \nabla \mu^{n+1} \cdot \mathbf{n} = 0, \quad \text{on } \partial\Omega, \quad (2.21)$$

where

$$\xi_{1A}^{n+1} = \frac{R^{n+1}}{\sqrt{E[\phi^n]}}. \quad (2.22)$$

Note that here ξ_{1A}^{n+1} is an approximation of the constant $\frac{R(t)}{\sqrt{E(t)}} = 1$.

Remark 2.5. In this scheme we have treated the nonlinear term $h(\phi)$ in (2.20b) and the $|\nabla \mu|^2$ term in (2.20c) explicitly. Consequently, Eq. (2.20c) for R^{n+1} is not coupled with Eqs. (2.20a) and (2.20b) for ϕ^{n+1} and μ^{n+1} on the discrete level.

Substituting the ξ_{1A}^{n+1} expression in (2.22) into Eq. (2.20c), we get

$$\xi_{1A}^{n+1} = \frac{R^n}{\sqrt{E[\phi^n]} + \frac{\Delta t}{2\sqrt{E[\phi^n]}} \int_{\Omega} |\nabla \mu^n|^2 d\mathbf{x}}. \quad (2.23)$$

Since $R^0 > 0$ according to Eq. (2.19), we conclude by induction that $\xi_{1A}^n > 0$ for all n . Then R^{n+1} is given by, in light of (2.22),

$$R^{n+1} = \xi_{1A}^{n+1} \sqrt{E[\phi^n]}. \quad (2.24)$$

We conclude that $R^{n+1} > 0$ for all time steps n .

The time stepping with the current scheme is thus as follows. Within a time step, given ϕ^n , μ^n and R^n , we compute $E[\phi^n]$ by (2.5), ξ_{1A}^{n+1} by (2.23), and R^{n+1} by (2.24). Then with ξ_{1A}^{n+1} known, we compute ϕ^{n+1} and μ^{n+1} by solving Eqs. (2.20a)–(2.20b) together with the boundary conditions (2.21).

It should be emphasized that the Cahn–Hilliard field equation is only solved once per time step with the current scheme. This is very different from the previous gPAV and SAV-type schemes (see e.g. [11,31,39]), which require solving the field equations twice per time step (for two copies of the field variables therein). Therefore, the operation count induced by the current scheme is approximately a half of those with the previous SAV and gPAV schemes, and it is comparable to that of the semi-implicit type schemes (see e.g. [14]). It can further be noted that the auxiliary variables R^{n+1} and ξ_{1A}^{n+1} are computed by well-defined explicit forms, with their values guaranteed to be positive.

Stability properties. The scheme given by Eqs. (2.20)–(2.22) is unconditionally stable. We summarize its stability properties into several lemmas or theorems below.

Lemma 2.6. *The scheme (2.20) is mass conserving in the sense that $(\phi^{n+1}, 1) = (\phi^n, 1)$.*

Proof. In light of the boundary conditions (2.21), the L^2 inner product between (2.20a) and the constant one leads to

$$(\phi^{n+1} - \phi^n, 1) = \Delta t (\Delta \mu^{n+1}, 1) = -\Delta t (\nabla \mu^{n+1}, \nabla 1) = 0.$$

So the solution of (2.20) satisfies $(\phi^n, 1) = (\phi^0, 1)$ for any n . \square

Lemma 2.7. *With the scheme (2.20) for all time step n ,*

$$0 < R^{n+1} \leq R^n. \quad (2.25)$$

Proof. Multiplying $2\Delta t R^{n+1}$ to Eq. (2.20c) and using Eq. (2.22), we get

$$|R^{n+1}|^2 - |R^n|^2 \leq |R^{n+1}|^2 - |R^n|^2 + |R^{n+1} - R^n|^2 = -\frac{\Delta t |R^{n+1}|^2}{E[\phi^n]} \int_{\Omega} |\nabla \mu^n|^2 d\mathbf{x} \leq 0. \quad (2.26)$$

We arrive at (2.26) by further noting that $R^n > 0$ for all n . \square

Lemma 2.7 implies that there exists a constant M , depending only on Ω , ϕ_{in} and c_0 , such that for any n ,

$$R^n \leq M. \quad (2.27)$$

Note that c_0 in (2.5) is a chosen constant to ensure $E(t) > 0$ for $0 \leq t \leq T$. We can choose c_0 such that $E(t) \geq C_0$, for some constant $C_0 > 0$. It then follows from Eq. (2.23) that ξ_{1A}^{n+1} is bounded from above, since

$$\xi_{1A}^{n+1} = \frac{R^n}{\sqrt{E[\phi^n]} + \frac{\Delta t}{2\sqrt{E[\phi^n]}} \int_{\Omega} |\nabla \mu^n|^2 d\mathbf{x}} \leq \frac{R^n}{\sqrt{E[\phi^n]}} \leq \frac{M}{\sqrt{C_0}}. \quad (2.28)$$

Theorem 2.8. Suppose $\phi_{in} \in H^3(\Omega)$ and the condition (2.14) holds. The following inequality holds for all n with the scheme (2.20),

$$\|\nabla \phi^{n+1}\|_0^2 + \frac{\lambda}{2} \|\phi^{n+1}\|_0^2 + \frac{\Delta t}{2} \|\nabla \Delta \phi^{n+1}\|_0^2 + \lambda \Delta t \sum_{k=0}^n \|\Delta \phi^{k+1}\|_0^2 + \frac{\Delta t}{2} \sum_{k=0}^n \|\nabla \mu^{k+1}\|_0^2 \leq \widehat{C}_1,$$

where $\widehat{C}_1 = \exp(C(M)T) (\|\nabla \phi^0\|_0^2 + \frac{\lambda}{2} \|\phi^0\|_0^2 + \frac{\Delta t}{2} \|\nabla \Delta \phi^0\|_0^2)$, and $C(M)$ is a constant depending on M .

Proof. Taking the L^2 inner product between (2.20a) and $\Delta t \mu^{n+1}$ and between (2.20b) and $-(\phi^{n+1} - \phi^n)$, and summing up the two resultant equations, we have

$$\begin{aligned} & \frac{1}{2} (\|\nabla \phi^{n+1}\|_0^2 - \|\nabla \phi^n\|_0^2 + \|\nabla \phi^{n+1} - \nabla \phi^n\|_0^2) + \frac{\lambda}{2} (\|\phi^{n+1}\|_0^2 - \|\phi^n\|_0^2 \\ & + \|\phi^{n+1} - \phi^n\|_0^2) + \Delta t \|\nabla \mu^{n+1}\|_0^2 = -|\xi_{1A}^{n+1}|^2 (h(\phi^n), \phi^{n+1} - \phi^n), \end{aligned} \quad (2.29)$$

where the boundary condition (2.21) has been used. In light of (2.20a), we have

$$\begin{aligned} & -|\xi_{1A}^{n+1}|^2 (h(\phi^n), \phi^{n+1} - \phi^n) = -|\xi_{1A}^{n+1}|^2 \Delta t (h(\phi^n), \Delta \mu^{n+1}) = |\xi_{1A}^{n+1}|^2 \Delta t (\nabla h(\phi^n), \nabla \mu^{n+1}) \\ & \leq \frac{\Delta t}{2} \|\nabla \mu^{n+1}\|_0^2 + \frac{|\xi_{1A}^{n+1}|^4 \Delta t}{2} \|\nabla h(\phi^n)\|_0^2. \end{aligned} \quad (2.30)$$

Taking the L^2 inner product between (2.20a) and $\Delta \phi^{n+1}$ and between (2.20b) and $\Delta^2 \phi^{n+1}$, and summing up the resultant equations, we arrive at

$$\begin{aligned} & \frac{1}{2} (\|\nabla \phi^{n+1}\|_0^2 - \|\nabla \phi^n\|_0^2 + \|\nabla (\phi^{n+1} - \phi^n)\|_0^2) + \Delta t \|\nabla \Delta \phi^{n+1}\|_0^2 + \lambda \Delta t \|\Delta \phi^{n+1}\|_0^2 \\ & = \Delta t |\xi_{1A}^{n+1}|^2 (\nabla h(\phi^n), \nabla \Delta \phi^{n+1}) \leq \frac{\Delta t}{2} \|\nabla \Delta \phi^{n+1}\|_0^2 + \frac{|\xi_{1A}^{n+1}|^4 \Delta t}{2} \|\nabla h(\phi^n)\|_0^2. \end{aligned} \quad (2.31)$$

By incorporating (2.30) into (2.29) and summing up Eqs. (2.29) and (2.31), we get

$$\begin{aligned} & \|\nabla \phi^{n+1}\|_0^2 - \|\nabla \phi^n\|_0^2 + \|\nabla \phi^{n+1} - \nabla \phi^n\|_0^2 + \frac{\lambda}{2} (\|\phi^{n+1}\|_0^2 - \|\phi^n\|_0^2 + \|\phi^{n+1} - \phi^n\|_0^2) \\ & + \frac{\Delta t}{2} \|\nabla \mu^{n+1}\|_0^2 + \frac{\Delta t}{2} \|\nabla \Delta \phi^{n+1}\|_0^2 + \lambda \Delta t \|\Delta \phi^{n+1}\|_0^2 \leq |\xi_{1A}^{n+1}|^4 \Delta t \|\nabla h(\phi^n)\|_0^2. \end{aligned} \quad (2.32)$$

To deal with the term on the right hand side of (2.32), we use an idea from [34,41]. Noting that $\nabla h(\phi^n) = h'(\phi^n) \nabla \phi^n$, Eq. (2.2) and the relation (2.14), we have

$$\|\nabla h(\phi^n)\|_0^2 \leq \|h'(\phi^n)\|_{0,\infty}^2 \|\nabla \phi^n\|_0^2 \leq C (\|\nabla \phi^n\|_0^2 + \|\nabla \phi^n\|_0^2 \|\phi^n\|_{0,\infty}^4). \quad (2.33)$$

Let $\check{\phi}^n = \frac{1}{|\Omega|} \int_{\Omega} \phi^n d\mathbf{x}$. Lemma 2.6 implies that

$$|\check{\phi}^n|^2 = |\check{\phi}^0|^2 \leq \frac{1}{|\Omega|} \|\phi^0\|_0^2 \leq C. \quad (2.34)$$

Using Sobolev embedding theorems $H^1(\Omega) \hookrightarrow L^\infty(\Omega)$ ($d = 1$), $H^{1+2\sigma}(\Omega) \hookrightarrow L^\infty(\Omega)$ for any $\sigma > 0$ ($d = 2$), the Agmon's inequality ($d = 3$, see [34,41] for more details) and the interpolation inequality about the spaces $H^s(\Omega)$, we deduce that

$$\|\phi^n - \check{\phi}^n\|_{0,\infty} \leq \begin{cases} C\|\nabla\phi^n\|_0 & \text{for } d = 1, \\ C\|\nabla\phi^n\|_0^{1-\sigma}\|\nabla\Delta\phi^n\|_0^\sigma & \text{for } d = 2, \\ C\|\nabla\phi^n\|_0^{3/4}\|\nabla\Delta\phi^n\|_0^{1/4} & \text{for } d = 3. \end{cases} \quad (2.35)$$

By the triangle inequality, we have

$$\|\phi^n\|_{0,\infty}^4 \leq 8 \left(\|\phi^n - \check{\phi}^n\|_{0,\infty}^4 + \|\check{\phi}^n\|_{0,\infty}^4 \right).$$

By setting $\sigma = 1/4$ and using $\|\check{\phi}^n\|_{0,\infty}^4 \leq C$, we arrive at the relation

$$\|\nabla\phi^n\|_0^2\|\phi^n\|_{0,\infty}^4 \leq \begin{cases} C\|\nabla\phi^n\|_0^2 + C\|\nabla\phi^n\|_0^6 & \text{for } d = 1, \\ C\|\nabla\phi^n\|_0^2 + C\|\nabla\phi^n\|_0^5\|\nabla\Delta\phi^n\|_0 & \text{for } d = 2, \\ C\|\nabla\phi^n\|_0^2 + C\|\nabla\phi^n\|_0^5\|\nabla\Delta\phi^n\|_0 & \text{for } d = 3. \end{cases}$$

Applying the following inequality

$$\xi_{1A}^{n+1} = \frac{R^n}{\sqrt{E[\phi^n]} + \frac{\Delta t}{2\sqrt{E[\phi^n]}} \int_{\Omega} |\nabla\mu^n|_0^2 dx} \leq \frac{C(M)}{\|\phi^n\|_1} \quad (2.36)$$

and (2.28), i.e. $\xi_{1A}^{n+1} \leq C(M)$, we obtain

$$|\xi_{1A}^{n+1}|^4 \|\nabla\phi^n\|_0^2\|\phi^n\|_{0,\infty}^4 \leq \begin{cases} C(M)\|\nabla\phi^n\|_0^2 + \frac{C(M)}{\|\phi^n\|_1^4} \|\nabla\phi^n\|_0^6 & \text{for } d = 1, \\ C(M)\|\nabla\phi^n\|_0^2 + \frac{C(M)}{\|\phi^n\|_1^4} \|\nabla\phi^n\|_0^5\|\nabla\Delta\phi^n\|_0 & \text{for } d = 2, \\ C(M)\|\nabla\phi^n\|_0^2 + \frac{C(M)}{\|\phi^n\|_1^4} \|\nabla\phi^n\|_0^5\|\nabla\Delta\phi^n\|_0 & \text{for } d = 3. \end{cases}$$

By using the Cauchy Schwarz inequality, for any $\varepsilon_i > 0$ ($i = 1, 2$), there exist constants $C(\varepsilon_i, M)$ depending on ε_i and M , such that

$$|\xi_{1A}^{n+1}|^4 \|\nabla h(\phi^n)\|_0^2 \leq \begin{cases} C(M)\|\nabla\phi^n\|_0^2 & \text{for } d = 1, \\ C(M)\|\nabla\phi^n\|_0^2 + C(\varepsilon_1, M)\|\nabla\phi^n\|_0^2 + \varepsilon_1\|\nabla\Delta\phi^n\|_0^2 & \text{for } d = 2, \\ C(M)\|\nabla\phi^n\|_0^2 + C(\varepsilon_2, M)\|\nabla\phi^n\|_0^2 + \varepsilon_2\|\nabla\Delta\phi^n\|_0^2 & \text{for } d = 3. \end{cases} \quad (2.37)$$

We set $\varepsilon_1 = \varepsilon_2 = \frac{1}{2}$ and combine the above inequalities with (2.32), and then

$$\begin{aligned} & \|\nabla\phi^{n+1}\|_0^2 - \|\nabla\phi^n\|_0^2 + \frac{\lambda}{2}(\|\phi^{n+1}\|_0^2 - \|\phi^n\|_0^2) + \frac{\Delta t}{2}\|\nabla\mu^{n+1}\|_0^2 \\ & + \frac{\Delta t}{2}(\|\nabla\Delta\phi^{n+1}\|_0^2 - \|\nabla\Delta\phi^n\|_0^2) + \lambda\Delta t\|\Delta\phi^{n+1}\|_0^2 \leq C(M)\Delta t\|\nabla\phi^n\|_0^2. \end{aligned} \quad (2.38)$$

We conclude the proof by summing up the above relation for indices from 0 to n and by using the discrete Gronwall lemma 2.4. \square

Theorem 2.9. Suppose $\phi_{in} \in H^4(\Omega)$, and that the conditions for Lemmas 2.1 and 2.2 hold. The following inequality holds for all n with the scheme (2.20),

$$\|\Delta\phi^{n+1}\|_0^2 + \frac{\Delta t}{2}\|\Delta^2\phi^{n+1}\|_0^2 + \frac{\Delta t}{2} \sum_{k=0}^n \|\Delta^2\phi^{k+1}\|_0^2 + 2\lambda\Delta t \sum_{k=0}^n \|\nabla\Delta\phi^{k+1}\|_0^2 \leq \widehat{C}_2,$$

where $\widehat{C}_2 = \|\Delta\phi^0\|_0^2 + \frac{\Delta t}{2}\|\Delta^2\phi^0\|_0^2 + C(M)T$.

Proof. The proof is similar to that for the SAV scheme in [34], by using Lemmas 2.1 and 2.2. \square

Error estimate. We next examine the errors of the solution to the Cahn–Hilliard equation with the scheme (2.20). Let

$$e_\phi^n = \phi^n - \phi(t^n), \quad e_\mu^n = \mu^n - \mu(t^n) \quad \text{and} \quad e_R^n = R^n - R(t^n). \quad (2.39)$$

Assume that $\phi_{in} \in H^4(\Omega)$ and the solution (ϕ, μ) of Eqs. (2.1)–(2.4) satisfies

$$\begin{aligned} \phi &\in L^\infty(0, T; W^{3,\infty}(\Omega)), & \phi_t &\in L^4(0, T; H^1(\Omega)) \cap L^2(0, T; H^1(\Omega)), \\ \phi_{tt} &\in L^2(0, T; H^{-1}(\Omega)), & \mu &\in L^\infty(0, T; H^1(\Omega)). \end{aligned} \quad (2.40)$$

In light of Lemma 2.1 and Theorems 2.8 and 2.9, we conclude that

$$\|\phi(t)\|_2 \leq C, \quad \|\phi^n\|_2 \leq C, \quad (2.41)$$

where the constant C is dependent on T , ϕ_{in} , and Ω . Since $H^2(\Omega) \hookrightarrow L^\infty(\Omega)$, we conclude that

$$|h(\phi)|, |h'(\phi)|, |h''(\phi)|, |h(\phi^n)|, |h'(\phi^n)|, |h''(\phi^n)| \leq C. \quad (2.42)$$

Based on the relation $R(t) = \sqrt{E[\phi]}$ and Eq. (2.5), we have

$$\begin{aligned} \frac{d^2 R}{dt^2} &= -\frac{1}{4\sqrt{E[\phi]^3}} \left(\int_\Omega (\nabla \phi \cdot \nabla \phi_t + \lambda \phi \phi_t + h(\phi) \phi_t) d\mathbf{x} \right)^2 \\ &\quad + \frac{1}{2\sqrt{E[\phi]}} \int_\Omega (|\nabla \phi_t|^2 + \nabla \phi \cdot \nabla \phi_{tt} + \lambda |\phi_t|^2 + \lambda \phi \phi_{tt} + h'(\phi) |\phi_t|^2 + h(\phi) \phi_{tt}) d\mathbf{x}. \end{aligned} \quad (2.43)$$

Combining (2.4), (2.40), (2.41) and (2.42) with (2.43), we deduce that

$$\int_0^T \left| \frac{d^2 R}{dt^2} \right|^2 dt \leq C \int_0^T (\|\phi_t\|_1^4 + \|\phi_t\|_1^2 + \|\phi_{tt}\|_{-1}^2) dt, \quad (2.44)$$

where ϕ_{tt} denotes the second time derivative of ϕ .

The truncation errors $T_{\phi_{1A}}^{n+1}$ and $T_{R_{1A}}^{n+1}$ are defined by

$$\frac{\phi(t^{n+1}) - \phi(t^n)}{\Delta t} = \Delta \mu(t^{n+1}) + \frac{1}{\Delta t} T_{\phi_{1A}}^{n+1}, \quad (2.45a)$$

$$\mu(t^{n+1}) = -\Delta \phi(t^{n+1}) + \lambda \phi(t^{n+1}) + \frac{R(t^{n+1})^2}{E[\phi(t^{n+1})]} h(\phi(t^{n+1})), \quad (2.45b)$$

$$\frac{R(t^{n+1}) - R(t^n)}{\Delta t} = -\frac{R(t^n)}{2E[\phi(t^n)]} \int_\Omega |\nabla \mu(t^n)|^2 d\mathbf{x} + \frac{1}{\Delta t} T_{R_{1A}}^{n+1}, \quad (2.45c)$$

where

$$T_{\phi_{1A}}^{n+1} = \int_{t^n}^{t^{n+1}} (t^n - t) \phi_{tt}(t) dt \quad \text{and} \quad T_{R_{1A}}^{n+1} = \int_{t^n}^{t^{n+1}} (t^{n+1} - t) \frac{d^2 R(t)}{dt^2} dt. \quad (2.46)$$

With the above definitions and relations, the errors of the scheme (2.20) is summarized by the following result.

Theorem 2.10. Suppose the condition (2.40), and the conditions for Theorems 2.8 and 2.9 hold. The following result holds with sufficiently small Δt ,

$$\frac{1}{2} \|\nabla e_\phi^{n+1}\|_0^2 + \frac{\lambda}{2} \|e_\phi^{n+1}\|_0^2 + \frac{\Delta t}{2} \|\nabla e_\mu^{n+1}\|_0^2 + |e_R^{n+1}|^2 \leq \widehat{C}_3 \Delta t^2, \quad (2.47)$$

where $\widehat{C}_3 = C \exp(\Delta t \sum_{k=0}^n \frac{r^k}{1-r^k \Delta t}) \int_0^{t^{n+1}} (\|\phi_t(s)\|_1^4 + \|\phi_t(s)\|_1^2 + \|\phi_{tt}(s)\|_{-1}^2) ds$, $r^k = 1 + \|\nabla \mu^k\|_0^2$ and the constant C is dependent on T , ϕ_{in} , Ω , $\|\phi\|_{L^\infty(0,T;W^{3,\infty}(\Omega))}$ and $\|\mu\|_{L^\infty(0,T;H^1(\Omega))}$.

Proof. By subtracting (2.45) from (2.20), we have

$$\frac{e_\phi^{n+1} - e_\phi^n}{\Delta t} = \Delta e_\mu^{n+1} - \frac{1}{\Delta t} T_{\phi_{1A}}^{n+1}, \quad (2.48a)$$

$$e_\mu^{n+1} = -\Delta e_\phi^{n+1} + \lambda e_\phi^{n+1} + A_1^{n+1}, \quad (2.48b)$$

$$\frac{e_R^{n+1} - e_R^n}{\Delta t} = -\frac{1}{2} A_2^{n+1} - \frac{1}{\Delta t} T_{R_{1A}}^{n+1}, \quad (2.48c)$$

where

$$\begin{aligned} A_1^{n+1} &= |\xi_{1A}^{n+1}|^2 h(\phi^n) - \frac{R(t^{n+1})^2}{E[\phi(t^{n+1})]} h(\phi(t^{n+1})) \\ &= \frac{e_R^{n+1}(R^{n+1} + R(t^{n+1}))}{E[\phi^n]} h(\phi^n) + R(t^{n+1})^2 \left(\frac{h(\phi^n)}{E[\phi^n]} - \frac{h(\phi(t^n))}{E[\phi(t^n)]} \right) \\ &\quad + R(t^{n+1})^2 \left(\frac{h(\phi(t^n))}{E[\phi(t^n)]} - \frac{h(\phi(t^{n+1}))}{E[\phi(t^{n+1})]} \right), \\ A_2^{n+1} &= \frac{\xi_{1A}^{n+1}}{\sqrt{E[\phi^n]}} \int_\Omega |\nabla \mu^n|^2 dx - \frac{R(t^n)}{E[\phi(t^n)]} \int_\Omega |\nabla \mu(t^n)|^2 dx \\ &= \frac{e_R^{n+1}}{E[\phi^n]} \int_\Omega |\nabla \mu^n|^2 dx + \frac{R(t^{n+1})}{E[\phi^n]} \int_\Omega (|\nabla \mu^n|^2 - |\nabla \mu(t^n)|^2) dx \\ &\quad + R(t^{n+1}) \left(\frac{1}{E[\phi^n]} - \frac{1}{E[\phi(t^n)]} \right) \int_\Omega |\nabla \mu(t^n)|^2 dx + \frac{R(t^{n+1}) - R(t^n)}{E[\phi(t^n)]} \int_\Omega |\nabla \mu(t^n)|^2 dx. \end{aligned}$$

Taking the inner product between (2.48a) and $\Delta t e_\mu^{n+1}$ and between (2.48b) and $e_\phi^{n+1} - e_\phi^n$, multiplying (2.48c) by $2\Delta t e_R^{n+1}$, and combining the resultant equations, we get

$$\begin{aligned} \frac{1}{2} (\|\nabla e_\phi^{n+1}\|_0^2 - \|\nabla e_\phi^n\|_0^2 + \|\nabla e_\phi^{n+1} - \nabla e_\phi^n\|_0^2) + \frac{\lambda}{2} (\|e_\phi^{n+1}\|_0^2 - \|e_\phi^n\|_0^2) \\ + \|e_\phi^{n+1} - e_\phi^n\|_0^2 + \Delta t \|\nabla e_\mu^{n+1}\|_0^2 = -(T_{\phi_{1A}}^{n+1}, e_\mu^{n+1}) - (A_1^{n+1}, e_\phi^{n+1} - e_\phi^n), \end{aligned} \quad (2.49a)$$

$$|e_R^{n+1}|^2 - |e_R^n|^2 + |e_R^{n+1} - e_R^n|^2 = -\Delta t A_2^{n+1} e_R^{n+1} - 2e_R^{n+1} T_{R_{1A}}^{n+1}. \quad (2.49b)$$

By the Taylor expansion theorem, we deal with the truncation errors as follows,

$$\begin{aligned} -(T_{\phi_{1A}}^{n+1}, e_\mu^{n+1}) &\leq \frac{\Delta t}{8} \|\nabla e_\mu^{n+1}\|_0^2 + \frac{2}{\Delta t} \|(-\Delta)^{-1/2} T_{\phi_{1A}}^{n+1}\|_0^2 \\ &\leq \frac{\Delta t}{8} \|\nabla e_\mu^{n+1}\|_0^2 + C \Delta t^2 \int_{t^n}^{t^{n+1}} \|\phi_{tt}(s)\|_{-1}^2 ds, \\ -2e_R^{n+1} T_{R_{1A}}^{n+1} &\leq \Delta t |e_R^{n+1}|^2 + \frac{1}{\Delta t} |T_{R_{1A}}^{n+1}|^2 \leq \Delta t |e_R^{n+1}|^2 + C \Delta t^2 \int_{t^n}^{t^{n+1}} \left| \frac{d^2 R(s)}{dt^2} \right|^2 ds, \end{aligned}$$

where $(-\Delta)^{-1/2}$ denotes the power of $-\Delta$ by the spectral theory of self-adjoint operators. We treat the A_1^{n+1} term on the right-hand side of (2.49a) as follows.

$$\begin{aligned} &-e_R^{n+1}(R^{n+1} + R(t^{n+1})) \left(\frac{h(\phi^n)}{E[\phi^n]}, e_\phi^{n+1} - e_\phi^n \right) \\ &= e_R^{n+1}(R^{n+1} + R(t^{n+1})) \left(\frac{h(\phi^n)}{E[\phi^n]}, \Delta t \Delta e_\mu^{n+1} - T_{\phi_{1A}}^{n+1} \right) \\ &\leq C e_R^{n+1} \left(\Delta t \|\nabla e_\mu^{n+1}\|_0 + \|(-\Delta)^{-1/2} T_{\phi_{1A}}^{n+1}\|_0 \right) \left\| \frac{\nabla h(\phi^n)}{E[\phi^n]} \right\|_0 \\ &= C e_R^{n+1} \left(\Delta t \|\nabla e_\mu^{n+1}\|_0 + \|(-\Delta)^{-1/2} T_{\phi_{1A}}^{n+1}\|_0 \right) \left\| \frac{h'(\phi^n) \nabla \phi^n}{E[\phi^n]} \right\|_0 \\ &\leq \frac{\Delta t}{8} \|\nabla e_\mu^{n+1}\|_0^2 + C \Delta t |e_R^{n+1}|^2 + C \Delta t^2 \int_{t^n}^{t^{n+1}} \|\phi_{tt}(s)\|_{-1}^2 ds. \end{aligned} \quad (2.50)$$

Additionally,

$$\begin{aligned}
& -R(t^{n+1})^2 \left(\frac{h(\phi^n)}{E[\phi^n]} - \frac{h(\phi(t^n))}{E[\phi(t^n)]}, e_\phi^{n+1} - e_\phi^n \right) \\
& \leq \frac{\Delta t}{8} \|\nabla e_\mu^{n+1}\|_0^2 + C \Delta t \left\| \frac{\nabla h(\phi^n)}{E[\phi^n]} - \frac{\nabla h(\phi(t^n))}{E[\phi(t^n)]} \right\|_0^2 + C \Delta t^2 \int_{t^n}^{t^{n+1}} \|\phi_{tt}(s)\|_{-1}^2 ds, \\
& -R(t^{n+1})^2 \left(\frac{h(\phi(t^n))}{E[\phi(t^n)]} - \frac{h(\phi(t^{n+1}))}{E[\phi(t^{n+1})]}, e_\phi^{n+1} - e_\phi^n \right) \\
& \leq \frac{\Delta t}{8} \|\nabla e_\mu^{n+1}\|_0^2 + C \Delta t \left\| \frac{\nabla h(\phi(t^n))}{E[\phi(t^n)]} - \frac{\nabla h(\phi(t^{n+1}))}{E[\phi(t^{n+1})]} \right\|_0^2 + C \Delta t^2 \int_{t^n}^{t^{n+1}} \|\phi_{tt}(s)\|_{-1}^2 ds.
\end{aligned}$$

Note that $\int_\Omega \phi(t) d\mathbf{x}$ is a constant and $\int_\Omega T_{\phi_1 A}^{n+1} d\mathbf{x} = 0$. Noting the definition of $E[\phi]$ and that $H(s) \in C^3(\mathbb{R})$, we have

$$\begin{aligned}
& E[\phi^n] - E[\phi(t^n)] \\
& = \frac{1}{2} \int_\Omega (\nabla \phi^n + \nabla \phi(t^n)) \nabla e_\phi^n d\mathbf{x} + \frac{\lambda}{2} \int_\Omega (\phi^n + \phi(t^n)) e_\phi^n d\mathbf{x} + \int_\Omega (H(\phi^n) - H(\phi(t^n))) d\mathbf{x} \\
& \leq C \|\nabla e_\phi^n\|_0 + C \|e_\phi^n\|_0 + \int_\Omega H'(\theta \phi^n + (1-\theta)\phi(t^n)) (\phi^n - \phi(t^n)) d\mathbf{x} \\
& \leq C \|\nabla e_\phi^n\|_0 + C \|e_\phi^n\|_0.
\end{aligned} \tag{2.51}$$

We rewrite the term $\frac{\nabla h(\phi^n)}{E[\phi^n]} - \frac{\nabla h(\phi(t^n))}{E[\phi(t^n)]}$ into

$$\frac{\nabla h(\phi^n)}{E[\phi^n]} - \frac{\nabla h(\phi(t^n))}{E[\phi(t^n)]} = \frac{\nabla h(\phi^n) - \nabla h(\phi(t^n))}{E[\phi^n]} + \frac{\nabla h(\phi(t^n))(E[\phi(t^n)] - E[\phi^n])}{E[\phi^n]E[\phi(t^n)]}.$$

It follows from the Hölder's inequality and Sobolev embedding theorem that,

$$\begin{aligned}
\|\nabla h(\phi^n) - \nabla h(\phi(t^n))\|_0 & \leq \|h'(\phi^n) - h'(\phi(t^n))\|_0 \|\nabla \phi(t^n)\|_0 + \|h'(\phi^n) \nabla e_\phi^n\|_0 \\
& \leq C \|\nabla \phi(t^n) e_\phi^n\|_0 + C \|\nabla e_\phi^n\|_0 \leq C(\|\nabla \phi(t^n)\|_{0,3} \|e_\phi^n\|_{0,6} + \|\nabla e_\phi^n\|_0) \\
& \leq C \|\phi(t^n)\|_2 \|e_\phi^n\|_1 + C \|\nabla e_\phi^n\|_0 \leq C(\|\nabla e_\phi^n\|_0 + \|e_\phi^n\|_0).
\end{aligned}$$

Then,

$$\begin{aligned}
& \left\| \frac{\nabla h(\phi^n)}{E[\phi^n]} - \frac{\nabla h(\phi(t^n))}{E[\phi(t^n)]} \right\|_0^2 \\
& = \left\| \frac{\nabla h(\phi^n) - \nabla h(\phi(t^n))}{E[\phi^n]} + \frac{\nabla h(\phi(t^n))(E[\phi(t^n)] - E[\phi^n])}{E[\phi^n]E[\phi(t^n)]} \right\|_0^2 \\
& \leq C \|\nabla h(\phi^n) - \nabla h(\phi(t^n))\|_0^2 + C \|\nabla h(\phi(t^n))\|_0^2 |E[\phi^n] - E[\phi(t^n)]|^2 \\
& \leq C(\|\nabla e_\phi^n\|_0^2 + \|e_\phi^n\|_0^2).
\end{aligned} \tag{2.52}$$

Similarly,

$$\begin{aligned}
& \left\| \frac{\nabla h(\phi(t^n))}{E[\phi(t^n)]} - \frac{\nabla h(\phi(t^{n+1}))}{E[\phi(t^{n+1})]} \right\|_0^2 \\
& \leq C \|\nabla h(\phi(t^n)) - \nabla h(\phi(t^{n+1}))\|_0^2 + C \|\nabla h(\phi(t^{n+1}))\|_0^2 |E[\phi(t^{n+1})] - E[\phi(t^n)]|^2 \\
& \leq C(\|\nabla \phi(t^{n+1}) - \nabla \phi(t^n)\|_0^2 + \|\phi(t^{n+1}) - \phi(t^n)\|_0^2) \\
& \leq C \Delta t \int_{t^n}^{t^{n+1}} \|\phi_t(s)\|_1^2 ds.
\end{aligned} \tag{2.53}$$

Next, we treat the right-hand side of (2.49b) as follows:

$$\left\{ \begin{aligned} & -\frac{\Delta t |e_R^{n+1}|^2}{E[\phi^n]} \int_{\Omega} |\nabla \mu^n|^2 d\mathbf{x} \leq C \Delta t \|\nabla \mu^n\|_0^2 |e_R^{n+1}|^2, \\ & -\frac{\Delta t e_R^{n+1} R(t^{n+1})}{E[\phi^n]} \int_{\Omega} (|\nabla \mu^n|^2 - |\nabla \mu(t^n)|^2) d\mathbf{x} \\ & \quad \leq \frac{\Delta t e_R^{n+1} R(t^{n+1})}{E[\phi^n]} \|\nabla e_{\mu}^n\|_0 \|\nabla \mu^n + \nabla \mu(t^n)\|_0 \\ & \quad \leq C \Delta t (\|\nabla \mu^n\|_0^2 + 1) |e_R^{n+1}|^2 + \frac{\Delta t}{2} \|\nabla e_{\mu}^n\|_0^2, \\ & -\Delta t R(t^{n+1}) e_R^{n+1} \left(\frac{1}{E[\phi^n]} - \frac{1}{E[\phi(t^n)]} \right) \int_{\Omega} |\nabla \mu(t^n)|^2 d\mathbf{x} \\ & \quad \leq C \Delta t \|\nabla \mu(t^n)\|_0^2 (|e_R^{n+1}|^2 + |E[\phi^n] - E[\phi(t^n)]|^2) \\ & \quad \leq C \Delta t (|e_R^{n+1}|^2 + \|\nabla e_{\phi}^n\|_0^2 + \|e_{\phi}^n\|_0^2), \\ & -\Delta t e_R^{n+1} \frac{R(t^{n+1}) - R(t^n)}{E[\phi(t^n)]} \int_{\Omega} |\nabla \mu(t^n)|^2 d\mathbf{x} \\ & \quad \leq C \Delta t \|\nabla \mu(t^n)\|_0^2 (|e_R^{n+1}|^2 + |R(t^{n+1}) - R(t^n)|^2) \\ & \quad \leq C \Delta t |e_R^{n+1}|^2 + C \Delta t^2 \int_{t^n}^{t^{n+1}} \left| \frac{dR(s)}{ds} \right|^2 ds. \end{aligned} \right. \quad (2.54)$$

By combining the above inequalities with (2.49a) and (2.49b), we have

$$\begin{aligned} & \frac{1}{2} (\|\nabla e_{\phi}^{n+1}\|_0^2 - \|\nabla e_{\phi}^n\|_0^2) + \frac{\lambda}{2} (\|e_{\phi}^{n+1}\|_0^2 - \|e_{\phi}^n\|_0^2) + |e_R^{n+1}|^2 - |e_R^n|^2 + \frac{\Delta t}{2} (\|\nabla e_{\mu}^{n+1}\|_0^2 - \|\nabla e_{\mu}^n\|_0^2) \\ & \quad + \frac{1}{2} \|\nabla e_{\phi}^{n+1} - \nabla e_{\phi}^n\|_0^2 + \frac{\lambda}{2} \|e_{\phi}^{n+1} - e_{\phi}^n\|_0^2 + |e_R^{n+1} - e_R^n|^2 \\ & \leq C \Delta t (1 + \|\nabla \mu^n\|_0^2) |e_R^{n+1}|^2 + C \Delta t (\|\nabla e_{\phi}^n\|_0^2 + \|e_{\phi}^n\|_0^2) + C \Delta t^2 \int_{t^n}^{t^{n+1}} \|\phi_t(s)\|_1^2 ds \\ & \quad + C \Delta t^2 \int_{t^n}^{t^{n+1}} \|\phi_{tt}(s)\|_{-1}^2 ds + C \Delta t^2 \int_{t^n}^{t^{n+1}} \left| \frac{d^2 R(s)}{ds^2} \right|^2 ds + C \Delta t^2 \int_{t^n}^{t^{n+1}} \left| \frac{dR(s)}{ds} \right|^2 ds. \end{aligned} \quad (2.55)$$

We sum up the above inequality for the indices from 0 to n and use the discrete Gronwall lemma 2.3 to finish the proof. \square

2.3.2. Scheme 1B

An alternative algorithm, in some sense reciprocal to the scheme presented in the previous section, is as follows. Let ϕ^0 , μ^0 and R^0 be defined by (2.19). Given (ϕ^n, R^n) , we compute $(\phi^{n+1}, \mu^{n+1}, R^{n+1})$ by the following procedure,

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} = \Delta \mu^{n+1}, \quad (2.56a)$$

$$\mu^{n+1} = -\Delta \phi^{n+1} + \lambda \phi^{n+1} + |\xi_{1B}^n|^2 h(\phi^n), \quad (2.56b)$$

$$\frac{R^{n+1} - R^n}{\Delta t} = -\frac{\xi_{1B}^{n+1}}{2\sqrt{E[\phi^{n+1}]}} \int_{\Omega} |\nabla \mu^{n+1}|^2 d\mathbf{x}, \quad (2.56c)$$

with the boundary conditions

$$\nabla \phi^{n+1} \cdot \mathbf{n} = \nabla \mu^{n+1} \cdot \mathbf{n} = 0, \quad \text{on } \partial\Omega, \quad (2.57)$$

where

$$\xi_{1B}^{n+1} = \frac{R^{n+1}}{\sqrt{E[\phi^{n+1}]}}. \quad (2.58)$$

Note that ξ_{1B}^{n+1} is again an approximation of the constant $\frac{R(t)}{\sqrt{E(t)}} = 1$.

Remark 2.11. In this scheme Eqs. (2.56a)–(2.56b) are not coupled with Eqs. (2.56c) and (2.58), because of the explicit treatments of $h(\phi^n)$ and ξ_{1B}^n in (2.56b). Therefore, the computations for (ϕ^{n+1}, μ^{n+1}) and for R^{n+1} are de-coupled with this scheme.

Substituting the ξ_{1B}^{n+1} expression in (2.58) into Eq. (2.56c) leads to

$$\xi_{1B}^{n+1} = \frac{R^n}{\sqrt{E[\phi^{n+1}] + \frac{\Delta t}{2\sqrt{E[\phi^{n+1}]}} \int_{\Omega} |\nabla \mu^{n+1}|^2 dx}}. \quad (2.59)$$

Since $R^0 > 0$, we conclude by induction that $\xi_{1B}^n > 0$ for all n .

Given ϕ^n , ξ_{1B}^n and R^n , we first compute ϕ^{n+1} and μ^{n+1} by solving Eqs. (2.56a)–(2.56b), together with the boundary conditions (2.57). Then, we compute $E[\phi^{n+1}]$ and ξ_{1B}^{n+1} by Eqs. (2.5) and (2.59), respectively. R^{n+1} can then be computed based on Eq. (2.58) as follows,

$$R^{n+1} = \xi_{1B}^{n+1} \sqrt{E[\phi^{n+1}]}. \quad (2.60)$$

We therefore conclude that $R^{n+1} > 0$ for all n with this scheme.

Similar to Scheme 1A from Section 2.3.1, this scheme requires the solution of the Cahn–Hilliard field equation only once per time step. Its operation count per time step is comparable to that of Scheme 1A, and is approximately a half of those of the original gPAV scheme [39] and the SAV scheme [11,31]. Note that in Scheme 1A R^{n+1} is computed first, followed by the fields (ϕ^{n+1}, μ^{n+1}) . In contrast, in the current scheme the fields (ϕ^{n+1}, μ^{n+1}) are computed first, followed by the variables $(\xi_{1B}^{n+1}, R^{n+1})$.

Stability properties. The scheme given by Eqs. (2.56)–(2.58) is unconditionally stable. Its stability properties are summarized by the following results.

Lemma 2.12. The scheme (2.56) is mass conserving in the sense that $(\phi^{n+1}, 1) = (\phi^n, 1)$.

Proof. Integrating equation (2.56a) over Ω and using the boundary condition (2.57) lead to the result. \square

Lemma 2.13. With the scheme (2.56),

$$0 < R^{n+1} \leq R^n \leq M, \quad (2.61)$$

$$0 < \xi_{1B}^{n+1} \leq \frac{M}{\sqrt{C_0}}, \quad (2.62)$$

for some constant $C_0 > 0$, and a constant M that depends only on Ω , ϕ_{in} and c_0 .

Theorem 2.14. Suppose $\phi_{in} \in H^3(\Omega)$ and the condition (2.14) holds. The following inequality holds with the scheme (2.56),

$$\|\nabla \phi^{n+1}\|_0^2 + \frac{\lambda}{2} \|\phi^{n+1}\|_0^2 + \frac{\Delta t}{2} \|\nabla \Delta \phi^{n+1}\|_0^2 + \lambda \Delta t \sum_{k=0}^n \|\Delta \phi^{k+1}\|_0^2 + \frac{\Delta t}{2} \sum_{k=0}^n \|\nabla \mu^{k+1}\|_0^2 \leq \widehat{C}_1,$$

where \widehat{C}_1 is the constant as given in Theorem 2.8.

The proof of this theorem is provided in Appendix.

Theorem 2.15. Suppose $\phi_{in} \in H^4(\Omega)$, and the conditions for [Lemmas 2.1](#) and [2.2](#) hold. The following inequality holds,

$$\|\Delta\phi^{n+1}\|_0^2 + \frac{\Delta t}{2} \|\Delta^2\phi^{n+1}\|_0^2 + \frac{\Delta t}{2} \sum_{k=0}^n \|\Delta^2\phi^{k+1}\|_0^2 + \frac{\lambda\Delta t}{2} \sum_{k=0}^n \|\nabla\Delta\phi^{k+1}\|_0^2 \leq \widehat{C}_2,$$

where the constant \widehat{C}_2 is given in [Theorem 2.9](#).

Proof. The proof is similar to that for the SAV scheme in [\[34\]](#), by using [Lemmas 2.1](#) and [2.2](#). \square

Error estimate. We define the errors of the variables by [\(2.39\)](#). Suppose that the solution (ϕ, μ) of Eqs. [\(2.1\)–\(2.4\)](#) satisfies [\(2.40\)](#). Based on [Lemma 2.2](#) and [Theorems 2.14](#) and [2.15](#), we have the same results expressed by the inequalities [\(2.41\)](#), [\(2.42\)](#) and [\(2.43\)](#), i.e.

$$\begin{aligned} \|\phi(t^n)\|_2 &\leq C, \quad \|\phi^n\|_2 \leq C, \\ |h(\phi)|, |h'(\phi)|, |h''(\phi)|, |h(\phi^n)|, |h'(\phi^n)|, |h''(\phi^n)| &\leq C, \\ \int_0^T \left| \frac{d^2 R}{dt^2} \right|^2 dt &\leq C \int_0^T (\|\phi_t\|_1^4 + \|\phi_t\|_1^2 + \|\phi_{tt}\|_{-1}^2) dt. \end{aligned}$$

The truncation errors $T_{\phi_{1B}}^{n+1}$ and $T_{R_{1B}}^{n+1}$ are given by

$$\frac{\phi(t^{n+1}) - \phi(t^n)}{\Delta t} = \Delta\mu(t^{n+1}) + \frac{1}{\Delta t} T_{\phi_{1B}}^{n+1}, \quad (2.63a)$$

$$\mu(t^{n+1}) = -\Delta\phi(t^{n+1}) + \lambda\phi(t^{n+1}) + \frac{R(t^{n+1})^2}{E[\phi(t^{n+1})]} h(\phi(t^{n+1})), \quad (2.63b)$$

$$\frac{R(t^{n+1}) - R(t^n)}{\Delta t} = -\frac{R(t^{n+1})}{2E[\phi(t^{n+1})]} \int_{\Omega} |\nabla\mu(t^{n+1})|^2 dx + \frac{1}{\Delta t} T_{R_{1B}}^{n+1}, \quad (2.63c)$$

where

$$T_{\phi_{1B}}^{n+1} = \int_{t^n}^{t^{n+1}} (t^n - t)\phi_{tt}(t)dt \quad \text{and} \quad T_{R_{1B}}^{n+1} = \int_{t^n}^{t^{n+1}} (t^n - t)\frac{d^2 R(t)}{dt^2} dt. \quad (2.64)$$

Theorem 2.16. Suppose the condition [\(2.40\)](#) and the conditions for [Theorems 2.14](#) and [2.15](#) hold. We have the following result with sufficiently small Δt ,

$$\frac{1}{2} \|\nabla e_{\phi}^{n+1}\|_0^2 + \frac{\lambda}{2} \|e_{\phi}^{n+1}\|_0^2 + |e_R^{n+1}|^2 + \frac{\Delta t}{2} \sum_{k=0}^n \|\nabla e_{\mu}^{k+1}\|_0^2 \leq \widehat{C}_4 \Delta t^2,$$

where $\widehat{C}_4 = C \exp(\Delta t \sum_{k=0}^n \frac{r^{k+1}}{1-r^{k+1}\Delta t}) \int_0^{t^{n+1}} (\|\phi_t(s)\|_1^4 + \|\phi_t(s)\|_1^2 + \|\phi_{tt}(s)\|_{-1}^2) ds$, $r^k = 1 + \|\nabla\mu^k\|_0^2$ and the constant C depends on T , ϕ_{in} , Ω , $\|\phi\|_{L^\infty(0,T;W^{3,\infty}(\Omega))}$ and $\|\mu\|_{L^\infty(0,T;H^1(\Omega))}$.

The proof of this theorem is provided in [Appendix](#).

2.4. Second-order schemes

We next present two second-order schemes for solving the reformulated system of equations, both of which are unconditionally energy stable. Similar to their first-order counterparts from [Section 2.3](#), these schemes solve the Cahn–Hilliard field equation only once per time step. A prominent feature of these schemes lies in that the Cahn–Hilliard field equation and the dynamic equation for the auxiliary variable are discretized in time by different methods, the former by the backward differentiation formula (BDF2) and the latter by the Crank–Nicolson scheme (CN2). This allows the computation of the auxiliary variable, and ensures the positivity of its computed values, in a very straightforward way. We provide stability analyses for both schemes, as well as the error estimate for the second scheme. Due to a technical difficulty caused by its multi-step nature, the error estimate for the first scheme (Scheme 2A) is not available at this time.

2.4.1. Scheme 2A

Suppose (ϕ^0, μ^0, R^0) is given by (2.19). Define

$$\phi^{n-1}|_{n=0} = \phi^0, \quad \mu^0 = -\Delta\phi^0 + \lambda\phi^0 + h(\phi^0), \quad \mu^{n-1}|_{n=0} = \mu^0.$$

Given ϕ^n, R^n, ϕ^{n-1} and μ^{n-1} for $n \geq 0$, we compute ϕ^{n+1}, μ^{n+1} and R^{n+1} as follows,

$$\frac{3\phi^{n+1} - 4\phi^n + \phi^{n-1}}{2\Delta t} = \Delta\mu^{n+1}, \quad (2.65a)$$

$$\mu^{n+1} = -\Delta\phi^{n+1} + \lambda\phi^{n+1} + |\xi_{2A}^{n+1}|^2 h(\bar{\phi}^n), \quad (2.65b)$$

$$\frac{R^{n+1} - R^n}{\Delta t} = -\frac{\xi_{2A}^{n+1}}{2\sqrt{E[\bar{\phi}^{n+1/2}]}} \int_{\Omega} |\nabla \tilde{\mu}^{n+1/2}|^2 dx, \quad (2.65c)$$

$$\mathbf{n} \cdot \nabla \phi^{n+1} = \mathbf{n} \cdot \nabla \mu^{n+1} = 0, \quad \text{on } \partial\Omega, \quad (2.65d)$$

where

$$\xi_{2A}^{n+1} = \frac{R^{n+1}}{\sqrt{E[\bar{\phi}^n]}}. \quad (2.66)$$

The symbols in the above equations are defined by

$$\bar{\phi}^n = 2\phi^n - \phi^{n-1}, \quad \tilde{\phi}^{n+1/2} = \frac{3}{2}\phi^n - \frac{1}{2}\phi^{n-1}, \quad \tilde{\mu}^{n+1/2} = \frac{3}{2}\mu^n - \frac{1}{2}\mu^{n-1}.$$

Obviously, $\bar{\phi}^n$ is a second-order explicit approximation of ϕ^{n+1} , and $\tilde{\mu}^{n+1/2}$ is a second-order explicit approximation of μ at step $(n+1/2)$, both by extrapolations. It follows that ξ_{2A}^{n+1} in (2.66) is a second-order approximation of the constant $\frac{R(t)}{\sqrt{E(t)}} = 1$ at step $(n+1)$.

Notice that we have used BDF2 to approximate $\frac{\partial\phi}{\partial t}$ in (2.65a) and enforced this equation at step $(n+1)$. On the other hand, we approximate $\frac{dR}{dt}$ by the Crank–Nicolson form, and enforce all terms in Eq. (2.65c), except for the variable ξ_{2A}^{n+1} , at the time step $(n+1/2)$. Note that the ξ_{2A}^{n+1} variable in (2.65c) is approximated at the time step $(n+1)$ according to (2.66). This is a crucial point, and it allows R^{n+1} to be computed by a well-defined formula and ensures the positivity of its values. It should be appreciated that this approximation of ξ_{2A}^{n+1} does not spoil the second-order accuracy of the overall scheme, because ξ_{2A}^{n+1} is an approximation of the constant $\frac{R(t)}{\sqrt{E(t)}} = 1$.

Thanks to the explicit nature of $\tilde{\mu}^{n+1/2}$ in (2.65c), the computation for R^{n+1} from (2.65c) and (2.66) is uncoupled with the computations for ϕ^{n+1} and μ^{n+1} from (2.65a)–(2.65b). Substituting the ξ_{2A}^{n+1} expression in (2.66) into Eq. (2.65c), one finds

$$\xi_{2A}^{n+1} = \frac{R^n}{\sqrt{E[\bar{\phi}^n] + \frac{\Delta t}{2\sqrt{E[\bar{\phi}^{n+1/2}]}} \int_{\Omega} |\nabla \tilde{\mu}^{n+1/2}|^2 dx}}. \quad (2.67)$$

Since $R^0 > 0$, we conclude by induction that $\xi_{2A}^n > 0$ for all $n \geq 0$. It then follows that $R^n > 0$ for all $n \geq 0$.

To implement this scheme, we first compute ξ_{2A}^{n+1} from Eq. (2.67) and R^{n+1} from (2.66). Then we solve Eqs. (2.65a)–(2.65b) for ϕ^{n+1} and μ^{n+1} . It can be noted that the Cahn–Hilliard field equation (2.65a)–(2.65b) is solved only once per time step with this scheme.

Stability properties. The scheme given by Eqs. (2.65a)–(2.66) is unconditionally stable. The following lemmas and theorems summarize its stability properties.

Lemma 2.17. *The scheme (2.65) is mass conserving in the sense that $(\phi^{n+1}, 1) = (\phi^0, 1)$.*

Proof. Taking the L^2 inner product between equation (2.65a) and the constant 1 leads to $(\phi^{n+1}, 1) = \frac{4}{3}(\phi^n, 1) - \frac{1}{3}(\phi^{n-1}, 1)$ for all $n \geq 0$. Since $\phi^{n-1}|_{n=0} = \phi^0$ by definition, we conclude by induction that $(\phi^n, 1) = (\phi^0, 1)$ for all $n \geq 0$. \square

Lemma 2.18. With the scheme (2.65),

$$0 < R^{n+1} \leq R^n \leq M, \quad (2.68)$$

$$0 < \xi_{2A}^{n+1} \leq \frac{M}{\sqrt{C_0}}, \quad (2.69)$$

for some constant $C_0 > 0$, and a constant M that depends on Ω , ϕ_{in} and c_0 .

Theorem 2.19. Suppose $\phi_{in} \in H^3(\Omega)$ and the condition (2.14) holds. The following inequality holds for all n with the scheme (2.65),

$$\begin{aligned} & \|\nabla \phi^{n+1}\|_0^2 + \|\nabla(2\phi^{n+1} - \phi^n)\|_0^2 + \frac{1}{2}\|\nabla(\phi^{n+1} - \phi^n)\|_0^2 + \frac{\lambda}{2}(\|\phi^{n+1}\|_0^2 + \|2\phi^{n+1} - \phi^n\|_0^2) \\ & + \lambda \Delta t \|\Delta \phi^{n+1}\|_0^2 + \frac{3\Delta t}{2}\|\nabla \Delta \phi^{n+1}\|_0^2 + \frac{\Delta t}{2}\|\nabla \Delta(\phi^{n+1} - \phi^n)\|_0^2 + \Delta t \sum_{k=0}^n \|\nabla \mu^{k+1}\|_0^2 \leq \widehat{C}_5, \end{aligned}$$

where $\widehat{C}_5 = (2\|\nabla \phi^0\|_0^2 + \lambda\|\phi^0\|_0^2 + \lambda \Delta t \|\Delta \phi^0\|_0^2 + \frac{3\Delta t}{2}\|\nabla \Delta \phi^0\|_0^2) \exp(C(M)T)$.

The proof of this theorem is provided in [Appendix](#).

Theorem 2.20. Suppose $\phi_{in} \in H^4(\Omega)$, and that the conditions for [Lemmas 2.1](#) and [2.2](#) hold. The following inequality holds for all n with the scheme (2.65),

$$\begin{aligned} & \frac{1}{2}\|\Delta \phi^{n+1}\|_0^2 + \frac{1}{2}\|\Delta(2\phi^{n+1} - \phi^n)\|_0^2 + \frac{1}{2}\|\Delta(\phi^{n+1} - \phi^n)\|_0^2 + \lambda \Delta t \|\nabla \Delta \phi^{n+1}\|_0^2 \\ & + \frac{3\Delta t}{2}\|\Delta^2 \phi^{n+1}\|_0^2 + \frac{\Delta t}{2}\|\Delta^2(\phi^{n+1} - \phi^n)\|_0^2 + \lambda \Delta t \sum_{k=0}^n \|\nabla \Delta \phi^{k+1}\|_0^2 \leq \widehat{C}_6, \end{aligned}$$

where $\widehat{C}_6 = \|\Delta \phi^0\|_0^2 + \frac{3\Delta t}{2}\|\Delta^2 \phi^0\|_0^2 + \lambda \Delta t \|\nabla \Delta \phi^0\|_0^2 + C(M)T$.

The proof of this theorem is provided in [Appendix](#).

2.4.2. Scheme 2B

Suppose (ϕ^0, μ^0, R^0) are given by (2.19), and let $\phi^{n-1}|_{n=0} = \phi^0$ and $R^{n-1}|_{n=0} = R^0$. Given $(\phi^n, \phi^{n-1}, R^n, R^{n-1})$ for $n \geq 0$, we compute $(\phi^{n+1}, \mu^{n+1}, R^{n+1})$ as follows,

$$\frac{3\phi^{n+1} - 4\phi^n + \phi^{n-1}}{2\Delta t} = \Delta \mu^{n+1}, \quad (2.70a)$$

$$\mu^{n+1} = -\Delta \phi^{n+1} + \lambda \phi^{n+1} + |\widehat{\xi}_{2B}^n|^2 h(\overline{\phi}^n), \quad (2.70b)$$

$$\frac{R^{n+1} - R^n}{\Delta t} = -\frac{\widehat{\xi}_{2B}^{n+1}}{2\sqrt{E[\widehat{\phi}^{n+1/2}]}} \int_{\Omega} |\nabla \mu^{n+1/2}|^2 dx, \quad (2.70c)$$

$$\mathbf{n} \cdot \nabla \phi^{n+1} = \mathbf{n} \cdot \nabla \mu^{n+1} = 0, \quad \text{on } \partial \Omega, \quad (2.70d)$$

where

$$\xi_{2B}^{n+1} = \frac{R^{n+1}}{\sqrt{E[\phi^{n+1}]}}. \quad (2.71)$$

The symbols in the above equations are defined by

$$\begin{aligned} \overline{R}^n &= 2R^n - R^{n-1}, \quad \overline{\phi}^n = 2\phi^n - \phi^{n-1}, \quad \widehat{\xi}_{2B}^n = \frac{\overline{R}^n}{\sqrt{E[\overline{\phi}^n]}}, \\ \widehat{\phi}^{n+1/2} &= \frac{3}{2}\phi^n - \frac{1}{2}\phi^{n-1}, \quad \mu^{n+1/2} = \frac{1}{2}(\mu^{n+1} + \mu^n). \end{aligned}$$

It can be noted that \overline{R}^n and $\overline{\phi}^n$ are second-order explicit approximations of R^{n+1} and ϕ^{n+1} , respectively. So $\widehat{\xi}_{2B}^n$ is a second-order explicit approximation of the constant $\frac{R(t)}{\sqrt{E(t)}} = 1$ at the time step $(n+1)$.

It should be noted that Eqs. (2.70a)–(2.70b) are enforced at the time step $(n+1)$, while Eq. (2.70c) is enforced at the step $(n+1/2)$, except for the term ξ_{2B}^{n+1} , which is approximated at the time step $(n+1)$. Similar to Scheme

2A in the previous subsection, this treatment of ξ_{2B}^{n+1} here does not spoil the second-order accuracy of the scheme and ensures the positivity of the computed values for R^{n+1} and ξ_{2B}^{n+1} .

Substitution of the ξ_{2B}^{n+1} expression in (2.71) into Eq. (2.70c) leads to

$$\xi_{2B}^{n+1} = \frac{R^n}{\sqrt{E[\phi^{n+1}]} + \frac{\Delta t}{2\sqrt{E[\phi^{n+1/2}]}} \int_{\Omega} |\nabla \mu^{n+1/2}|^2 dx}. \quad (2.72)$$

Since $R^0 > 0$, we conclude by induction that $\xi_{2B}^{n+1} > 0$ and $R^{n+1} > 0$ for all $n \geq 0$ with the current scheme.

Thanks to the explicit nature of $\hat{\xi}_{2B}^n$, the field Eqs. (2.70a)–(2.70b) are de-coupled from Eq. (2.70c). To compute $(\phi^{n+1}, \mu^{n+1}, R^{n+1})$, we can first solve (2.70a)–(2.70b) and (2.70d) for ϕ^{n+1} and μ^{n+1} . Then we compute ξ_{2B}^{n+1} by (2.72), and compute R^{n+1} by Eq. (2.71).

Stability properties. This scheme is also unconditionally energy stable. Its stability properties are summarized by the following results.

Lemma 2.21. The scheme (2.70) is mass conserving in the sense that $(\phi^{n+1}, 1) = (\phi^0, 1)$.

Lemma 2.22. The scheme (2.70) satisfies, for all n ,

$$0 < R^{n+1} \leq R^n \leq M, \quad (2.73)$$

$$0 < \xi_{2B}^{n+1} \leq \frac{M}{\sqrt{C_0}}, \quad (2.74)$$

$$|\hat{\xi}_{2B}^n| \leq \frac{3M}{\sqrt{C_0}}, \quad (2.75)$$

for some constant $C_0 > 0$, and a constant M that depends on Ω , ϕ_{in} and c_0 .

Theorem 2.23. Suppose $\phi_{in} \in H^3(\Omega)$ and the condition (2.14) holds. The following inequality holds for all n with the scheme (2.70),

$$\begin{aligned} & \|\nabla \phi^{n+1}\|_0^2 + \|\nabla(2\phi^{n+1} - \phi^n)\|_0^2 + \frac{1}{2}\|\nabla(\phi^{n+1} - \phi^n)\|_0^2 + \frac{\lambda}{2}(\|\phi^{n+1}\|_0^2 + \|2\phi^{n+1} - \phi^n\|_0^2) \\ & + \lambda \Delta t \|\Delta \phi^{n+1}\|_0^2 + \frac{3\Delta t}{2}\|\nabla \Delta \phi^{n+1}\|_0^2 + \frac{\Delta t}{2}\|\nabla \Delta(\phi^{n+1} - \phi^n)\|_0^2 + \Delta t \sum_{k=0}^n \|\nabla \mu^{k+1}\|_0^2 \leq \hat{C}_5, \end{aligned}$$

where \hat{C}_5 is given in Theorem 2.19.

The proof of this theorem is provided in Appendix.

Theorem 2.24. Suppose $\phi^0 \in H^4(\Omega)$, and that the conditions for Lemmas 2.1 and 2.2 hold. Then the following inequality holds with the scheme (2.70),

$$\begin{aligned} & \frac{1}{2}\|\Delta \phi^{n+1}\|_0^2 + \frac{1}{2}\|\Delta(2\phi^{n+1} - \phi^n)\|_0^2 + \frac{1}{2}\|\Delta(\phi^{n+1} - \phi^n)\|_0^2 + \lambda \Delta t \|\nabla \Delta \phi^{n+1}\|_0^2 \\ & + \frac{3\Delta t}{2}\|\Delta^2 \phi^{n+1}\|_0^2 + \frac{\Delta t}{2}\|\Delta^2(\phi^{n+1} - \phi^n)\|_0^2 + \lambda \Delta t \sum_{k=0}^n \|\nabla \Delta \phi^{k+1}\|_0^2 \leq \hat{C}_6, \end{aligned}$$

where \hat{C}_6 is given in Theorem 2.20.

The proof of this theorem is provided in Appendix.

Error estimate. Assume that

$$\begin{aligned} \phi & \in L^\infty(0, T; W^{3,\infty}(\Omega)), \quad \phi_t \in L^\infty(0, T; L^2(\Omega)) \cap L^4(0, T; H^1(\Omega)) \cap L^2(0, T; H^1(\Omega)), \\ \phi_{tt} & \in L^2(0, T; H^1(\Omega)), \quad \phi_{ttt} \in L^\infty(0, T; H^{-1}(\Omega)), \quad \mu \in L^\infty(0, T; H^1(\Omega)). \end{aligned} \quad (2.76)$$

By Lemma 2.2 and Theorems 2.23 and 2.24, we can also arrive at the boundedness properties in (2.41) and (2.42). In light of the relation $R(t) = \sqrt{E[\phi]}$, we have

$$\frac{d^3 R}{dt^3} = \frac{3}{8\sqrt{E[\phi]^5}} \left(\frac{dE}{dt} \right)^3 - \frac{3}{4\sqrt{E[\phi]^3}} \frac{dE}{dt} \frac{d^2 E}{dt^2} + \frac{1}{2\sqrt{E[\phi]}} \frac{d^3 E}{dt^3}, \quad (2.77)$$

where

$$\begin{aligned}\frac{d^2 E}{dt^2} &= \int_{\Omega} (|\nabla \phi_t|^2 + \nabla \phi \cdot \nabla \phi_{tt} + \lambda |\phi_t|^2 + \lambda \phi \phi_{tt} + h'(\phi) |\phi_t|^2 + h(\phi) \phi_{tt}) d\mathbf{x}, \\ \frac{d^3 E}{dt^3} &= \int_{\Omega} (3 \nabla \phi_t \cdot \nabla \phi_{tt} + \nabla \phi \cdot \nabla \phi_{ttt} + 3 \lambda \phi_t \phi_{tt} + \lambda \phi \phi_{ttt} + h''(\phi) \phi_t^3 + 3 h'(\phi) \phi_t \phi_{tt} + h(\phi) \phi_{ttt}) d\mathbf{x}.\end{aligned}$$

It follows that

$$\int_0^T \left| \frac{d^3 R}{dt^3} \right|^2 dt \leq C \int_0^T (\|\phi_t\|_1^4 + \|\phi_t\|_1^2 + \|\phi_{tt}\|_1^2 + \|\phi_{ttt}\|_{-1}^2) dt. \quad (2.78)$$

Based on the Taylor expansion theorem, we arrive at

$$\frac{3\phi(t^{n+1}) - 4\phi(t^n) + \phi(t^{n-1}))}{2\Delta t} = \Delta \mu(t^{n+1}) + \frac{1}{\Delta t} T_{\phi_{2B}}^{n+1}, \quad (2.79a)$$

$$\mu(t^{n+1}) = -\Delta \phi(t^{n+1}) + \lambda \phi(t^{n+1}) + \frac{R(t^{n+1})}{E[\phi(t^{n+1})]} h(\phi(t^{n+1})), \quad (2.79b)$$

$$\frac{R(t^{n+1}) - R(t^n)}{\Delta t} = -\frac{R(t^{n+1})}{\sqrt{E[\phi(t^{n+1})]}} \frac{1}{2\sqrt{E[\phi(t^{n+1/2})]}} \int_{\Omega} |\nabla \mu(t^{n+1/2})|^2 d\mathbf{x} + \frac{1}{\Delta t} T_{R_{2B}}^{n+1}, \quad (2.79c)$$

where

$$\begin{cases} T_{\phi_{2B}}^{n+1} = \int_{t^n}^{t^{n+1}} (t - t^n)^2 \phi_{ttt}(t) dt - \frac{1}{4} \int_{t^{n-1}}^{t^{n+1}} (t - t^{n-1})^2 \phi_{ttt}(t) dt, \\ T_{R_{2B}}^{n+1} = \frac{1}{2} \int_{t^{n+1/2}}^{t^{n+1}} (t^{n+1} - t)^2 \frac{d^3 R}{dt^3}(t) dt - \frac{1}{2} \int_{t^n}^{t^{n+1/2}} (t^n - t)^2 \frac{d^3 R}{dt^3}(t) dt. \end{cases} \quad (2.80)$$

Theorem 2.25. Suppose the condition (2.76), and the conditions for Theorems 2.23 and 2.24 hold. The following inequality holds for sufficiently small Δt ,

$$\frac{1}{2} (\|\nabla e_{\phi}^{n+1}\|_0^2 + \|\nabla(2e_{\phi}^{n+1} - e_{\phi}^n)\|_0^2) + \frac{\lambda}{2} (\|e_{\phi}^{n+1}\|_0^2 + \|2e_{\phi}^{n+1} - e_{\phi}^n\|_0^2) + \frac{\Delta t}{2} \|\nabla e_{\mu}^{n+1}\|_0^2 + |e_R^{n+1}|^2 \leq \widehat{C}_7 \Delta t^4,$$

where $\widehat{C}_7 = C \exp(\Delta t \sum_{k=0}^{n+1} \frac{r^{k+1/2}}{1-r^{k+1/2}\Delta t}) \int_0^{t^{n+1}} (\|\phi_t(s)\|_1^4 + \|\phi_t(s)\|_1^2 + \|\phi_{tt}(s)\|_1^2 + \|\phi_{ttt}(s)\|_{-1}^2) ds$, $r^{k+1/2} = 1 + \|\nabla \mu^{k+1/2}\|_0^2$, and the constant C depends on T , ϕ_{in} , Ω , $\|\phi\|_{L^\infty(0,T;W^{3,\infty}(\Omega))}$, $\|\phi_t\|_{L^\infty(0,T;L^2(\Omega))}$ and $\|\mu\|_{L^\infty(0,T;H^1(\Omega))}$.

The proof of this theorem is provided in Appendix.

Remark 2.26. The four schemes presented in this section share several common characteristics: (i) They are all unconditionally energy stable. (ii) The Cahn–Hilliard field equation only needs to be computed once per time step, by solving linear algebraic systems with a constant coefficient matrix. (iii) The auxiliary variable is given by a well-defined explicit form, and its computed values are guaranteed to be positive.

Remark 2.27. In the analysis of these schemes (Schemes 1A/1B and 2A/2B) we have focused on the boundary conditions given by (2.4). We would like to point out that the stability properties about these schemes proved in this section equally hold with periodic boundary conditions for the domain.

3. Numerical examples

In this section we provide numerical results to verify the stability and error analysis of the proposed numerical schemes from the previous section. The convergence rates of these schemes are first demonstrated using a manufactured analytic solution. We then look into the coalescence of an array of drops and show that the proposed schemes produce stable and accurate numerical results.

In the forthcoming numerical experiments, we add the mobility coefficient and the interfacial thickness parameter to the Cahn–Hilliard equation as follows so that it resembles the applications (e.g. in two-phase flows) more closely,

$$\phi_t = m_0 \Delta \mu + f(\mathbf{x}, t), \quad \mu = -\beta \Delta \phi + h(\phi), \quad (3.1)$$

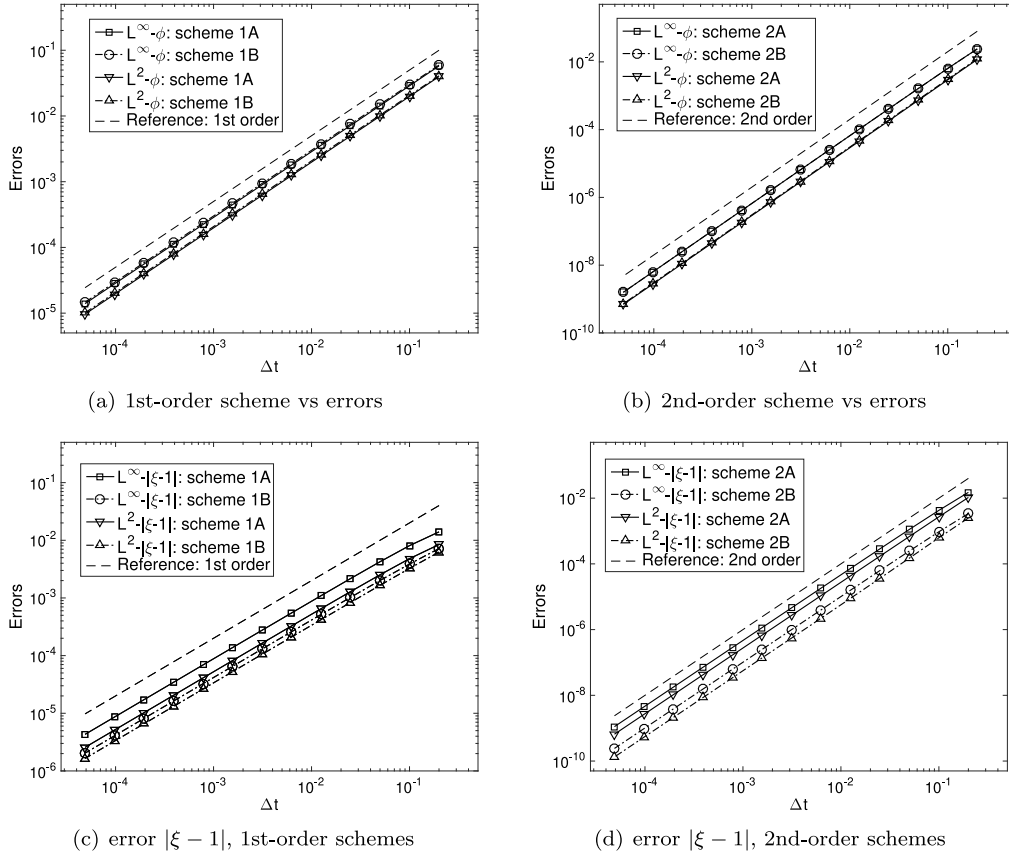


Fig. 3.1. Temporal convergence rates: L^∞ and L^2 errors of ϕ at $t = t_f$ versus Δt for the (a) first-order, and (b) second-order schemes. L^∞ and L^2 errors of the auxiliary variable $\xi(t)$ (for $t \in [t_0, t_f]$) versus Δt for the (c) first-order and (d) second-order schemes. The parameters are $t_0 = 0.1$, $t_f = 1.1$, $(N_x, N_y) = (20, 20)$ and $c_0 = 1$.

where $h(\phi) = H'(\phi)$ with $H(\phi) = \frac{\beta}{4\eta^2}(\phi^2 - 1)^2$. Here, the constant m_0 ($m_0 > 0$) is the mobility of the interface, η is a characteristic scale of the interfacial thickness, β is the mixing energy density coefficient and is related to the surface tension by $\beta = \frac{3}{2\sqrt{2}}\sigma\eta$, where the constant σ is the interface surface tension. $f(\mathbf{x}, t)$ is a prescribed source term for testing the convergence rate only, and will be set to $f = 0$ in practical simulations. For simplicity and efficiency, we will consider periodic boundary conditions in the following tests. These algorithms are employed to numerically integrate the governing equation (3.1) in time from $t = t_0$ to $t = t_f$ (t_0 and t_f to be specified below).

3.1. Convergence rates

We first test the convergence rates of the proposed methods using a manufactured analytic solution. Consider Eq. (3.1) in the domain $\Omega = [0, 2] \times [0, 2]$ with a manufactured solution

$$\phi(\mathbf{x}, t) = \cos(\pi x) \cos(\pi y) \sin(t). \quad (3.2)$$

The external source term $f(\mathbf{x}, t)$ in (3.1) is chosen such that this equation is satisfied by the analytic expression given in (3.2). Periodic conditions are assumed for the boundaries in the x and y directions. We employ the Fourier spectral method for spatial discretization throughout this section. Let N_x and N_y denote the number of Fourier collocation points along x and y directions, respectively. In the simulations, we set $(N_x, N_y) = (20, 20)$, with which the spatial discretization error is negligible compared with the temporal discretization error. Other parameters are $t_0 = 0.1$, $t_f = 1.1$, $m_0 = 0.01$, $\beta = 0.01$, $\eta = 0.1$ and $c_0 = 1$. The L^∞ and L^2 errors of the field function ϕ (against the analytic solution (3.2)) at $t = t_f = 1.1$ are plotted respectively for the Schemes 1A/1B and 2A/2B in Fig. 3.1(a) and (b). In Fig. 3.1(c) and (d) we plot the L^∞ and L^2 errors of the auxiliary variable ξ (against the

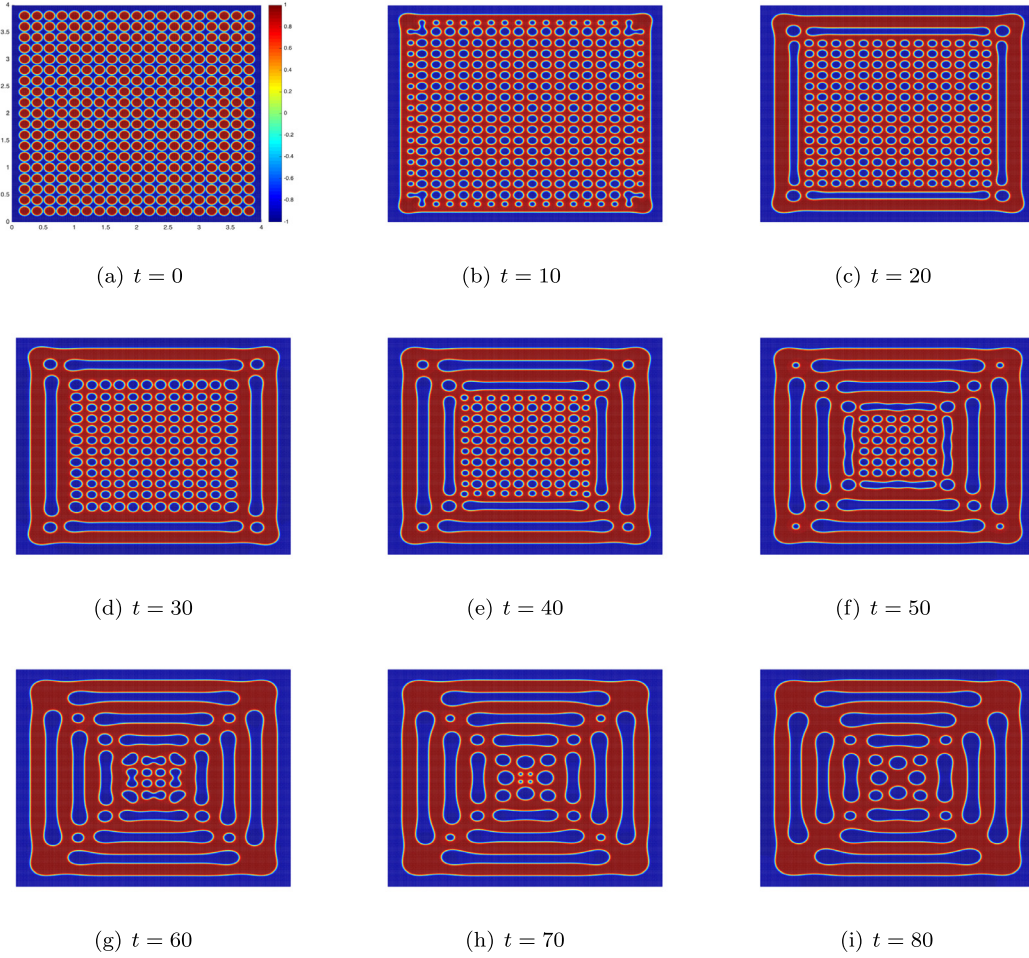


Fig. 3.2. Temporal sequence of snapshots showing the evolution of an array of 361 drops governed by the Cahn-Hilliard equation. Simulation results are obtained using Scheme 2A with $\Delta t = 10^{-3}$. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

constant 1) as a function of Δt corresponding to different schemes. Here the L^∞ and L^2 errors are computed based on the $\xi(t)$ data on the interval $t \in [t_0, t_f]$. We can observe the expected convergence rate for all cases. The error curves of ϕ corresponding to Schemes 1A and 1B, and also for Schemes 2A and 2B, essentially overlap with each other, indicating a negligible difference in the error levels. On the other hand, the error values of ξ corresponding to Scheme 1B appear to be slightly and consistently lower than those of Scheme 1A. Similarly, the error values of ξ corresponding to Scheme 2B appear slightly and consistently lower than those of Scheme 2A.

3.2. Coalescence of an array of drops

Another test problem we would like to consider is the evolution and interaction of 361 circular drops of one material, with their centers arranged on a 19×19 grid (see Fig. 3.2(a)), which are immersed in another material. We assume that the evolution of the material regions is described by the Cahn-Hilliard equation. The computational domain is taken to be $[0, 4] \times [0, 4]$, and the initial phase field distribution is given by

$$\phi_0(\mathbf{x}, t = 0) = 360 - \sum_{i=1}^{19} \sum_{j=1}^{19} \frac{\tanh(\sqrt{(x - x_i)^2 + (y - y_j)^2} - R_0)}{\sqrt{2}\eta}, \quad (3.3)$$

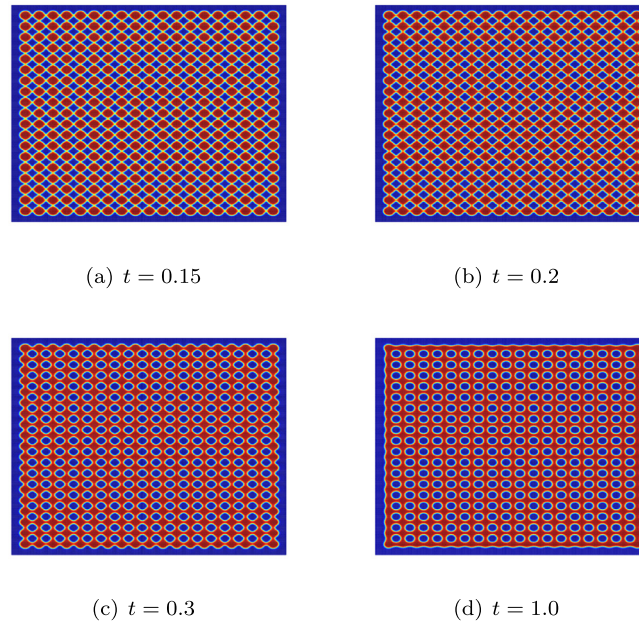


Fig. 3.3. Early evolution of the two material regions: (a) $t = 0.15$, (b) $t = 0.2$, (c) $t = 0.3$, and (d) $t = 1.0$. The initial drops of material one (red) merge to form the new background material. The space between the initial drops filled with material two (blue) form a new 18×18 array of blue drops in the new background material (red). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

where R_0 is the initial drop radius with $R_0 = 0.085$, and $x_i = 0.2 \times i$ and $y_j = 0.2 \times j$ for $i, j = 1, 2, \dots, 19$. We employ 512 grid points in both x and y directions in the Fourier spectral discretization. The other simulation parameters are $m_0 = 10^{-6}$, $\sigma = 151.15$, $\eta = 0.01$, $\beta = \frac{3}{2\sqrt{2}}\sigma\eta$ and $c_0 = 1$. We set $f(\mathbf{x}, t) = 0$ in (3.1) and periodic boundary conditions are prescribed on the domain boundaries in both directions.

The regions for the two materials (circular drops, and the background) are observed to evolve and coalesce to form coarser regions. This process is visualized in Fig. 3.2 with a long temporal sequence of snapshots of the phase field distributions obtained using Scheme 2A with $\Delta t = 10^{-3}$. The first material is marked by red and the other material is marked by blue. Increasingly coarser regions can be observed to form over time. Comparison between Fig. 3.2(a) and (b) indicates that the roles (foreground/background) of the two materials seem to have reversed early in the evolution. The first material (initial red drops) evolves into a new background material, while the second material (initial blue background) form blue drops in the red background; see Fig. 3.2(b). This process is illustrated in Fig. 3.3 with four snapshots at the early stage of the evolution. We can observe that the initial 19×19 array of red drops coalesce to form a new background material, while the second material in the spaces between the red drops evolves into a new 18×18 array of blue drops immersed in the red background material.

The distribution of the material interface at $t = 100$ obtained with several time step sizes, ranging from $\Delta t = 10^{-4}$ to $\Delta t = 10^{-2}$, computed using Scheme 2A are shown in Fig. 3.4. It is observed that the results obtained with $\Delta t = 10^{-4}$ and $\Delta t = 10^{-3}$ are essentially the same. With the larger time step size $\Delta t = 10^{-2}$, we can observe some differences in the material distribution from those obtained using smaller Δt values, indicating that the simulation starts to lose accuracy with this step size.

Note that the quantity $\xi = \frac{R(t)}{\sqrt{E(t)}}$ is an approximation of the unit value. This ξ can serve as an indicator of the accuracy of the simulations. If the deviation of ξ from the unit value is small, then the simulation tends to be more accurate. In Fig. 3.5(a), we depict the time histories of ξ , computed using Scheme 2B with various time step sizes ranging from $\Delta t = 1$ to 10^{-4} . It can be observed that ξ remains close to 1 for small time steps $10^{-3} \sim 10^{-4}$. While for relatively larger time step sizes $1 \sim 10^{-2}$, ξ exhibits an obvious deviation from 1, suggesting that the simulation results are no longer accurate. In Fig. 3.5(b), we compare the time histories of ξ , obtained using the four schemes (1A/1B and 2A/2B) with $\Delta t = 10^{-3}$. The schemes 1A, 2A and 2B all produce quite accurate simulation results

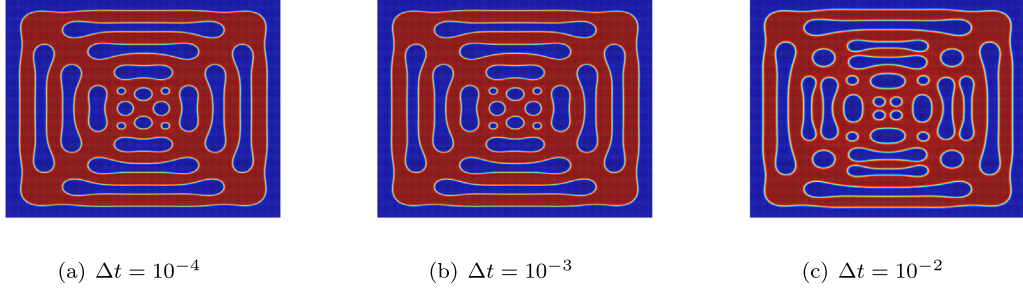


Fig. 3.4. Coalescence of arrays of 361 circles: snapshots of the phase field function at $t = 100$ computed using Scheme 2A with (a) $\Delta t = 10^{-4}$, (b) $\Delta t = 10^{-3}$, (c) $\Delta t = 10^{-2}$.

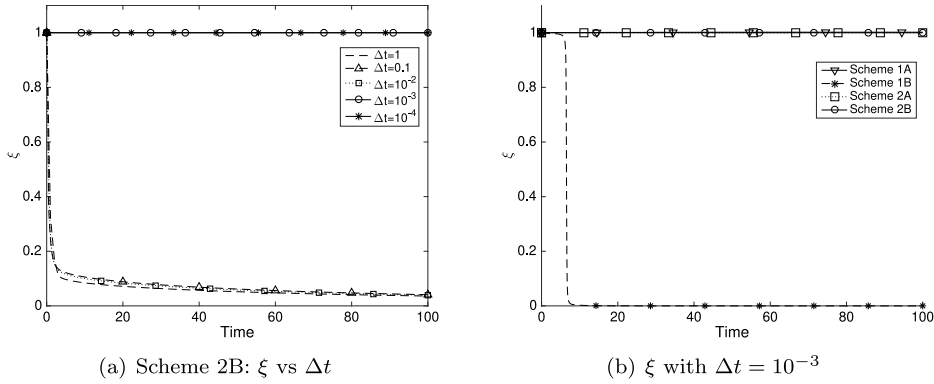


Fig. 3.5. Coalescence of an array of drops: time histories of $\xi(t) = R(t)/\sqrt{E(t)}$ corresponding to (a) a range of time step sizes $\Delta t = 1, 10^{-1}, 10^{-2}, 10^{-3}, 10^{-4}$, computed using Scheme 2B, and (b) computed using different schemes (Schemes 1A/1B, 2A/2B) with a fixed $\Delta t = 10^{-3}$.

with this time step size, with the computed ξ taking essentially the unit value. On the other hand, the ξ computed by Scheme 1B has the unit value initially, and at about $t = 10$ it decreases sharply to a small positive value (on the order 10^{-6}) and remains at that level for the rest of the simulation. As a result, the simulation with Scheme 1B loses accuracy completely from that point onward. It should be noted that this occurs not at the beginning, but after a quite long time (around 10,000 time steps) into the simulation. Since the system is very dynamic, it is hard to pin-point what interactions in the evolution of the drops cause the method to lose accuracy. We can observe from the convergence-rate tests in Fig. 3.1(c) that the Scheme 1B appears to produce more accurate values for the auxiliary variable ξ than Scheme 1A in short-term simulations (The convergence tests cover a unit value in time). The test results here suggest that this is apparently not the case in longer-time simulations. Overall, these results indicate that among the four schemes developed here the Scheme 1B might be somewhat inferior to the other schemes under the same conditions in long-time simulations.

To validate the stability analysis of the schemes in the previous section, we look into the time histories of the H^2 norm of the phase field function ϕ in Fig. 3.6. Fig. 3.6(a) shows the time histories of the H^2 -norm of the phase field function ϕ corresponding to a number of time step sizes, ranging from $\Delta t = 10^{-4}$ to $\Delta t = 1$, obtained using Scheme 2A. It is observed that with smaller Δt values the H^2 norm decreases over time, and for larger Δt values it remains approximately at some constant level over time (except for an initial dip at the early stage of the simulation). These characteristics signify the stability of the computations. In Fig. 3.6(b), we fix $\Delta t = 1$ and depict the time histories of the H^2 -norm of ϕ obtained using the different schemes developed herein. Since the Δt is quite large, we do not expect these simulations to be accurate. Nonetheless, it can be observed that the H^2 -norms are all bounded, indicating the stability of the proposed schemes.

Finally, we compare the performance of the current schemes with the SAV method [11,31] and the semi-implicit scheme [14] for the drop evolution problem. In the SAV method, the auxiliary variable is defined based on the

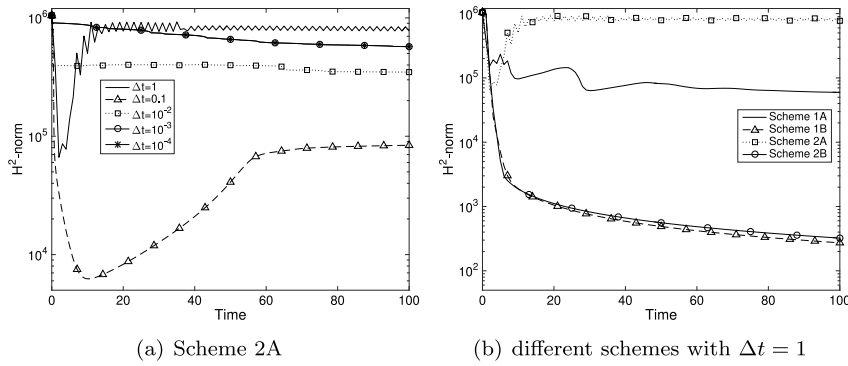


Fig. 3.6. Coalescence of an array of drops: time histories of $\|\phi\|_{H^2(\Omega)}$ corresponding to (a) a range of time step sizes $\Delta t = 1, 10^{-1}, 10^{-2}, 10^{-3}, 10^{-4}$, computed using Scheme 2A, and (b) computed using different schemes with a fixed $\Delta t = 1$.

potential energy only, $R_1(t) = \sqrt{\int_{\Omega} H(\phi) d\Omega + c_0}$. Here we use $R_1(t)$ to denote the auxiliary variable in SAV, in order to distinguish the auxiliary variable $R(t)$ employed here based on the total energy ($R(t) = \sqrt{E(t)}$). In the semi-implicit scheme [14], the nonlinear term $h(\phi)$ is simply treated explicitly and the linear terms are treated implicitly. Note that in the SAV method, the linear system resulting from the Cahn–Hilliard equation needs to be solved twice within a time step [11,31]. On the other hand, with the schemes proposed here we only need to solve the linear system once per time step. So the operation counts of the current schemes are comparable to that of the semi-implicit scheme, and are about a half of that of the SAV method.

Fig. 3.7(a) shows the time histories of the total energy $E[\phi]$ obtained using the current Scheme 2A and the SAV method with several time step sizes (ranging from $\Delta t = 10^{-4}$ to $\Delta t = 10^{-1}$), together with the semi-implicit scheme with a time step size $\Delta t = 5 \times 10^{-3}$. We note that the history curves corresponding to the relatively small time step sizes $\Delta t = 10^{-4}$ and $\Delta t = 10^{-3}$ all overlap with one another for both the current scheme and SAV, while some difference between them can be discerned in the history curves corresponding to $\Delta t = 10^{-2}$, suggesting that both the current scheme and SAV exhibit similar accuracy with relatively small time step sizes. With the larger step size $\Delta t = 10^{-1}$, the simulation result is no longer accurate for both the current scheme and SAV, and indeed we can notice significant differences when compared with the curves obtained with smaller time step sizes; see also Fig. 3.8 for a snapshot of the field distributions at $t = 100$ obtained using these two methods with $\Delta t = 10^{-1}$, which shows a marked difference. Nevertheless, the stability in the computations with the current scheme and SAV is evident. This, however, is not the case with the semi-implicit scheme. Simulation using the semi-implicit scheme blows up after a while into the computation with a relatively small $\Delta t = 5 \times 10^{-3}$, with the energy suddenly growing exponentially. These comparisons indicate that the current methods share some characteristics with SAV in terms of the accuracy and stability. Note that the current methods require the solution of the linear system only once within a time step. So their computational cost is about half of the SAV method.

The schemes proposed here guarantee the unconditional positivity of the computed $R(t)$ values, irrespective of the time step size. In Fig. 3.7(b) and (c), we show the time history of the auxiliary variable $R(t)$ computed using the current Scheme 2A and the history of the auxiliary variable $R_1(t)$ obtained by the SAV method, both with $\Delta t = 0.4$. Note that in the current schemes $R(t)$ is computed by a dynamic equation stemming from the relation $R(t) = \sqrt{E(t)}$, while in the SAV method the auxiliary variable $R_1(t)$ is computed by a dynamic equation stemming from the relation $R_1(t) = \sqrt{\int_{\Omega} H(\phi) d\Omega + c_0}$. So both auxiliary variables should be positive physically. The current schemes indeed guarantee the positivity of $R(t)$. In contrast, SAV lacks such a property and the auxiliary variable computed using SAV can take negative (unphysical) values, which is evident from Fig. 3.7(c).

4. Concluding remarks

In this paper we have presented two first-order and two second-order unconditionally energy-stable schemes, in terms of a discrete energy, for numerically solving the Cahn–Hilliard equation. The stability properties of these schemes have been investigated in relative detail, and their error analyses are provided. Besides the discrete

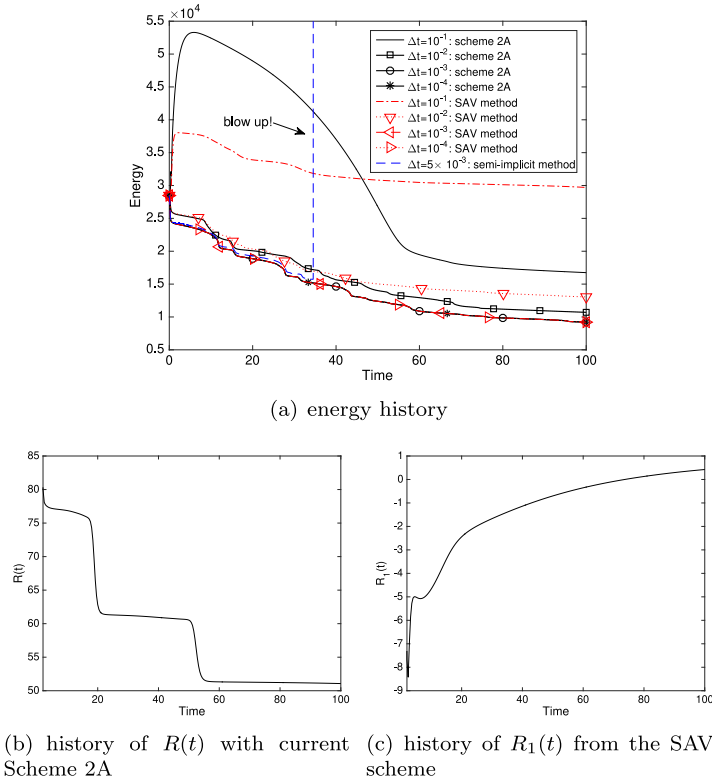


Fig. 3.7. Comparison of current gPAV method with other methods (SAV scheme and the semi-implicit scheme). (a) Time histories of the total energy $E(t)$ obtained by the current Scheme 2A and the SAV scheme with $\Delta t = 10^{-1} - 10^{-4}$, and by the semi-implicit scheme from [14] with $\Delta t = 5 \times 10^{-3}$. (b) Time history of the auxiliary variable $R(t)$ obtained by the current Scheme 2A. (c) Time history of the auxiliary variable (denoted by $R_1(t)$) obtained by the SAV method.

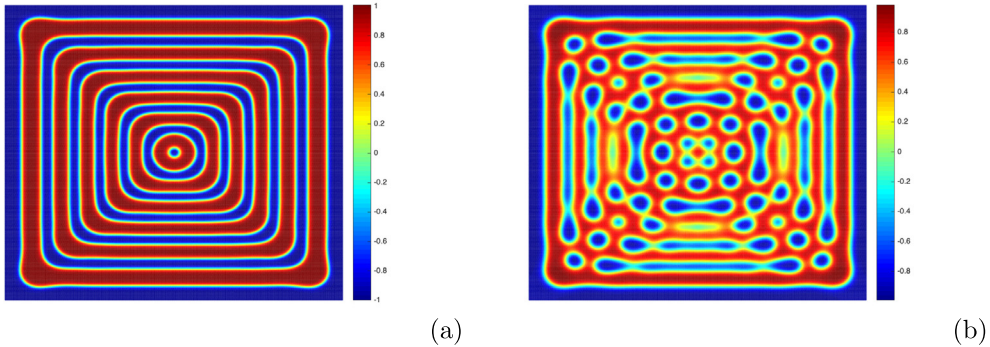


Fig. 3.8. Snapshot of the field function ϕ at $t = 100$ computed with $\Delta t = 0.1$ using the (a) Scheme 2A and (b) SAV method.

unconditional stability, these schemes have several other attractive properties: (i) These are linear schemes, and only linear algebraic systems with a constant coefficient matrix need to be solved. (ii) The auxiliary variable (scalar-valued number) involved in each of these schemes is computed by a well-defined explicit form, and its value is guaranteed to be positive. (iii) The computational complexity (operation count or computational cost per time step) of these schemes is comparable to that of the semi-implicit schemes, and is about a half of the gPAV and SAV schemes.

The proposed schemes allow the use of fairly large time step sizes in dynamic problems and stable computations can be attained. These have been demonstrated by numerical examples. Thanks to the aforementioned properties,

these schemes are computationally efficient and simple to implement. They can be a useful tool for two-phase and multiphase problems and materials applications.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgments

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Appendix. Proofs of several theorems

Theorem 2.14. Suppose $\phi_{in} \in H^3(\Omega)$ and the condition (2.14) holds. The following inequality holds with the scheme (2.56),

$$\|\nabla\phi^{n+1}\|_0^2 + \frac{\lambda}{2}\|\phi^{n+1}\|_0^2 + \frac{\Delta t}{2}\|\nabla\Delta\phi^{n+1}\|_0^2 + \lambda\Delta t \sum_{k=0}^n \|\Delta\phi^{k+1}\|_0^2 + \frac{\Delta t}{2} \sum_{k=0}^n \|\nabla\mu^{k+1}\|_0^2 \leq \widehat{C}_1,$$

where \widehat{C}_1 is the constant as given in Theorem 2.8.

Proof. Taking the inner product of (2.56a) and (2.56b) with $\Delta t\mu^{n+1}$ and $\phi^{n+1} - \phi^n$, respectively, we have

$$\begin{aligned} & \frac{1}{2}(\|\nabla\phi^{n+1}\|_0^2 - \|\nabla\phi^n\|_0^2 + \|\nabla\phi^{n+1} - \nabla\phi^n\|_0^2) + \frac{\lambda}{2}(\|\phi^{n+1}\|_0^2 - \|\phi^n\|_0^2 + \|\phi^{n+1} - \phi^n\|_0^2) \\ & + \Delta t\|\nabla\mu^{n+1}\|_0^2 = -|\xi_{1B}^n|^2(h(\phi^n), \phi^{n+1} - \phi^n) \leq \frac{\Delta t}{2}\|\nabla\mu^{n+1}\|_0^2 + \frac{|\xi_{1B}^n|^4\Delta t}{2}\|\nabla h(\phi^n)\|_0^2. \end{aligned} \quad (\text{A.1})$$

Take the inner product of (2.56a) and (2.56b) with $\Delta\phi^{n+1}$ and $\Delta^2\phi^{n+1}$, respectively. Applying the boundary condition (2.57), we arrive at

$$\begin{aligned} & \frac{1}{2}(\|\nabla\phi^{n+1}\|_0^2 - \|\nabla\phi^n\|_0^2 + \|\nabla(\phi^{n+1} - \phi^n)\|_0^2) + \Delta t\|\nabla\Delta\phi^{n+1}\|_0^2 + \lambda\Delta t\|\Delta\phi^{n+1}\|_0^2 \\ & = |\xi_{1B}^n|^2\Delta t(\nabla h(\phi^n), \nabla\Delta\phi^{n+1}) \leq \frac{\Delta t}{2}\|\nabla\Delta\phi^{n+1}\|_0^2 + \frac{|\xi_{1B}^n|^4\Delta t}{2}\|\nabla h(\phi^n)\|_0^2. \end{aligned} \quad (\text{A.2})$$

Summing up (A.1) and (A.2), we have

$$\begin{aligned} & \|\nabla\phi^{n+1}\|_0^2 - \|\nabla\phi^n\|_0^2 + \|\nabla\phi^{n+1} - \nabla\phi^n\|_0^2 + \frac{\lambda}{2}(\|\phi^{n+1}\|_0^2 - \|\phi^n\|_0^2 + \|\phi^{n+1} - \phi^n\|_0^2) \\ & + \frac{\Delta t}{2}\|\nabla\mu^{n+1}\|_0^2 + \frac{\Delta t}{2}\|\nabla\Delta\phi^{n+1}\|_0^2 + \lambda\Delta t\|\Delta\phi^{n+1}\|_0^2 \leq |\xi_{1B}^n|^4\Delta t\|\nabla h(\phi^n)\|_0^2. \end{aligned} \quad (\text{A.3})$$

As is shown in the proof of Theorem 2.8, the nonlinear term $\|\nabla h(\phi^n)\|_0^2$ can be estimated by using the positive auxiliary variable ξ_{1A}^{n+1} , which satisfies the properties (2.36) and (2.28). Notice that ξ_{1B}^n satisfies similar properties, i.e. $\xi_{1B}^n \leq C(M)$ and

$$\xi_{1B}^n = \frac{R^n}{\sqrt{\mathbf{E}[\phi^n]}} \leq \frac{C(M)}{\|\phi^n\|_1}.$$

The rest of the proof parallel those steps in the proof of Theorem 2.8. \square

Theorem 2.16. Suppose the condition (2.40), and the conditions of Theorems 2.14 and 2.15 hold. We have the following result with sufficiently small Δt ,

$$\frac{1}{2}\|\nabla e_\phi^{n+1}\|_0^2 + \frac{\lambda}{2}\|e_\phi^{n+1}\|_0^2 + |e_R^{n+1}|^2 + \frac{\Delta t}{2} \sum_{k=0}^n \|\nabla e_\mu^{k+1}\|_0^2 \leq \widehat{C}_4\Delta t^2,$$

where $\widehat{C}_4 = C \exp(\Delta t \sum_{k=0}^n \frac{r^{k+1}}{1-r^{k+1}\Delta t}) \int_0^{t^{n+1}} (\|\phi_t(s)\|_1^4 + \|\phi_t(s)\|_1^2 + \|\phi_{tt}(s)\|_1^2) ds$, $r^k = 1 + \|\nabla \mu^k\|_0^2$ and the constant C depends on T , ϕ_{in} , Ω , $\|\phi\|_{L^\infty(0,T;W^{3,\infty}(\Omega))}$ and $\|\mu\|_{L^\infty(0,T;H^1(\Omega))}$.

Proof. By subtracting (2.63) from (2.56), we have

$$\frac{e_\phi^{n+1} - e_\phi^n}{\Delta t} = \Delta e_\mu^{n+1} - \frac{1}{\Delta t} T_{\phi_{1B}}^{n+1}, \quad (\text{A.4a})$$

$$e_\mu^{n+1} = -\Delta e_\phi^{n+1} + \lambda e_\phi^{n+1} + A_3^{n+1}, \quad (\text{A.4b})$$

$$\frac{e_R^{n+1} - e_R^n}{\Delta t} = -\frac{1}{2} A_4^{n+1} - \frac{1}{\Delta t} T_{R_{1B}}^{n+1}, \quad (\text{A.4c})$$

where

$$\begin{aligned} A_3^{n+1} &= |\xi_{1B}^n|^2 h(\phi^n) - \frac{R(t^{n+1})^2}{E[\phi(t^{n+1})]} h(\phi(t^{n+1})) \\ &= \frac{e_R^n (R^n + R(t^n))}{E[\phi^n]} h(\phi^n) + \frac{R(t^n)^2 - R(t^{n+1})^2}{E[\phi^n]} h(\phi^n) + R(t^{n+1})^2 \left(\frac{h(\phi^n)}{E[\phi^n]} - \frac{h(\phi(t^n))}{E[\phi(t^n)]} \right) \\ &\quad + R(t^{n+1})^2 \left(\frac{h(\phi(t^n))}{E[\phi(t^n)]} - \frac{h(\phi(t^{n+1}))}{E[\phi(t^{n+1})]} \right), \\ A_4^{n+1} &= \frac{\xi_{1B}^{n+1}}{\sqrt{E[\phi^{n+1}]}} \int_\Omega |\nabla \mu^{n+1}|^2 dx - \frac{R(t^{n+1})}{E[\phi(t^{n+1})]} \int_\Omega |\nabla \mu(t^{n+1})|^2 dx \\ &= \frac{e_R^{n+1}}{E[\phi^{n+1}]} \int_\Omega |\nabla \mu^{n+1}|^2 dx + \frac{R(t^{n+1})}{E[\phi^{n+1}]} \int_\Omega (|\nabla \mu^{n+1}|^2 - |\nabla \mu(t^{n+1})|^2) dx \\ &\quad + R(t^{n+1}) \left(\frac{1}{E[\phi^{n+1}]} - \frac{1}{E[\phi(t^{n+1})]} \right) \int_\Omega |\nabla \mu(t^{n+1})|^2 dx. \end{aligned}$$

Taking the inner product of (A.4a) with $\Delta t e_\mu^{n+1}$ and (A.4b) with $e_\phi^{n+1} - e_\phi^n$, and multiplying (A.4c) with $2\Delta t e_R^{n+1}$, we get the following:

$$\begin{aligned} \frac{1}{2} (\|\nabla e_\phi^{n+1}\|_0^2 - \|\nabla e_\phi^n\|_0^2 + \|\nabla e_\phi^{n+1} - \nabla e_\phi^n\|_0^2) + \frac{\lambda}{2} (\|e_\phi^{n+1}\|_0^2 - \|e_\phi^n\|_0^2) \\ + \|e_\phi^{n+1} - e_\phi^n\|_0^2 + \Delta t \|\nabla e_\mu^{n+1}\|_0^2 = -(T_{\phi_{1B}}^{n+1}, e_\mu^{n+1}) - (A_3^{n+1}, e_\phi^{n+1} - e_\phi^n), \end{aligned} \quad (\text{A.5a})$$

$$|e_R^{n+1}|^2 - |e_R^n|^2 + |e_R^{n+1} - e_R^n|^2 = -\Delta t A_4^{n+1} e_R^{n+1} - 2e_R^{n+1} T_{R_{1B}}^{n+1}. \quad (\text{A.5b})$$

Now, the right-hand side terms of (A.5a) can be treated as follows.

$$\begin{aligned} -(T_{\phi_{1B}}^{n+1}, e_\mu^{n+1}) &\leq \frac{\Delta t}{12} \|\nabla e_\mu^{n+1}\|_0^2 + \frac{3}{\Delta t} \|(-\Delta)^{-1/2} T_{\phi_{1B}}^{n+1}\|_0^2 \\ &\leq \frac{\Delta t}{12} \|\nabla e_\mu^{n+1}\|_0^2 + C \Delta t^2 \int_0^{t^{n+1}} \|\phi_{tt}(s)\|_1^2 ds, \\ -e_R^n (R^n + R(t^n)) \left(\frac{h(\phi^n)}{E[\phi^n]}, e_\phi^{n+1} - e_\phi^n \right) &= e_R^n (R^n + R(t^n)) \left(\frac{h(\phi^n)}{E[\phi^n]}, \Delta t \Delta e_\mu^{n+1} - T_{\phi_{1B}}^{n+1} \right) \\ &\leq C e_R^n \left(\Delta t \|\nabla e_\mu^{n+1}\|_0 + \|(-\Delta)^{-1/2} T_{\phi_{1B}}^{n+1}\|_0 \right) \left\| \frac{\nabla h(\phi^n)}{E[\phi^n]} \right\|_0 \\ &= C e_R^n \left(\Delta t \|\nabla e_\mu^{n+1}\|_0 + \|(-\Delta)^{-1/2} T_{\phi_{1B}}^{n+1}\|_0 \right) \left\| \frac{h'(\phi^n) \nabla \phi^n}{E[\phi^n]} \right\|_0 \\ &\leq \frac{\Delta t}{12} \|\nabla e_\mu^{n+1}\|_0^2 + C \Delta t |e_R^n|^2 + C \Delta t^2 \int_0^{t^{n+1}} \|\phi_{tt}(s)\|_1^2 ds, \\ -(R(t^n)^2 - R(t^{n+1})^2) \left(\frac{h(\phi^n)}{E[\phi^n]}, e_\phi^{n+1} - e_\phi^n \right) &= (R(t^n)^2 - R(t^{n+1})^2) \left(\frac{h(\phi^n)}{E[\phi^n]}, \Delta t \Delta e_\mu^{n+1} - T_{\phi_{1B}}^{n+1} \right) \\ &\leq \frac{\Delta t}{12} \|\nabla e_\mu^{n+1}\|_0^2 + C \Delta t |R(t^n) - R(t^{n+1})|^2 \\ &\quad + C \Delta t^2 \int_0^{t^{n+1}} \|\phi_{tt}(s)\|_1^2 ds, \\ -R(t^{n+1})^2 \left(\frac{h(\phi^n)}{E[\phi^n]} - \frac{h(\phi(t^n))}{E[\phi(t^n)]}, e_\phi^{n+1} - e_\phi^n \right) &= R(t^{n+1})^2 \left(\frac{h(\phi^n)}{E[\phi^n]} - \frac{h(\phi(t^n))}{E[\phi(t^n)]}, \Delta t \Delta e_\mu^{n+1} - T_{\phi_{1B}}^{n+1} \right) \\ &\leq \frac{\Delta t}{12} \|\nabla e_\mu^{n+1}\|_0^2 + C \Delta t \left\| \frac{\nabla h(\phi^n)}{E[\phi^n]} - \frac{\nabla h(\phi(t^n))}{E[\phi(t^n)]} \right\|_0^2 \end{aligned}$$

$$\begin{aligned}
& + C \Delta t^2 \int_{t^n}^{t^{n+1}} \|\phi_{tt}(s)\|_{-1}^2 ds, \\
& -R(t^{n+1})^2 \left(\frac{h(\phi(t^n))}{E[\phi(t^n)]} - \frac{h(\phi(t^{n+1}))}{E[\phi(t^{n+1})]} \right) e_\phi^{n+1} - e_\phi^n = R(t^{n+1})^2 \left(\frac{h(\phi(t^n))}{E[\phi(t^n)]} - \frac{h(\phi(t^{n+1}))}{E[\phi(t^{n+1})]} \right) \Delta t \Delta e_\mu^{n+1} - T_{\phi_{1B}}^{n+1} \\
& \leq \frac{\Delta t}{12} \|\nabla e_\mu^{n+1}\|_0^2 + C \Delta t \left\| \frac{\nabla h(\phi(t^n))}{E[\phi(t^n)]} - \frac{\nabla h(\phi(t^{n+1}))}{E[\phi(t^{n+1})]} \right\|_0^2 \\
& + C \Delta t^2 \int_{t^n}^{t^{n+1}} \|\phi_{tt}(s)\|_{-1}^2 ds.
\end{aligned}$$

Next, the right-hand side terms of (A.5b) can be treated as follows.

$$\left\{ \begin{aligned}
& -\frac{\Delta t |e_R^{n+1}|^2}{E[\phi^{n+1}]} \int_{\Omega} |\nabla \mu^{n+1}|^2 dx \leq C \Delta t \|\nabla \mu^{n+1}\|_0^2 |e_R^{n+1}|^2, \\
& -\frac{\Delta t e_R^{n+1} R(t^{n+1})}{E[\phi^{n+1}]} \int_{\Omega} (|\nabla \mu^{n+1}|^2 - |\nabla \mu(t^{n+1})|^2) dx \\
& \quad \leq \frac{\Delta t e_R^{n+1}}{E[\phi^{n+1}]} \|\nabla e_\mu^{n+1}\|_0 \|\nabla \mu^{n+1} + \nabla \mu(t^{n+1})\|_0 \\
& \quad \leq C \Delta t (\|\nabla \mu^{n+1}\|_0^2 + 1) |e_R^{n+1}|^2 + \frac{\Delta t}{12} \|\nabla e_\mu^{n+1}\|_0^2, \\
& -\Delta t R(t^{n+1}) e_R^{n+1} \left(\frac{1}{E[\phi^{n+1}]} - \frac{1}{E[\phi(t^{n+1})]} \right) \int_{\Omega} |\nabla \mu(t^{n+1})|^2 dx \\
& \quad \leq C \Delta t (|e_R^{n+1}|^2 + |E[\phi^{n+1}] - E[\phi(t^{n+1})]|^2), \\
& -2e_R^{n+1} T_{R_{1B}}^{n+1} \leq \Delta t |e_R^{n+1}|^2 + \frac{\Delta t}{12} |T_{R_{1B}}^{n+1}|^2 \\
& \quad \leq \Delta t |e_R^{n+1}|^2 + C \Delta t^2 \int_{t^n}^{t^{n+1}} \left| \frac{d^2 R(s)}{dt^2} \right|^2 ds.
\end{aligned} \right.$$

Combining (2.51), (2.52), (2.53) and the above inequalities with (A.5a) and (A.5b), we have

$$\begin{aligned}
& \frac{1}{2} (\|\nabla e_\phi^{n+1}\|_0^2 - \|\nabla e_\phi^n\|_0^2) + \frac{\lambda}{2} (\|e_\phi^{n+1}\|_0^2 - \|e_\phi^n\|_0^2) + |e_R^{n+1}|^2 - |e_R^n|^2 + \frac{\Delta t}{2} \|\nabla e_\mu^{n+1}\|_0^2 \\
& + \frac{1}{2} \|\nabla e_\phi^{n+1} - \nabla e_\phi^n\|_0^2 + \frac{\lambda}{2} \|e_\phi^{n+1} - e_\phi^n\|_0^2 + |e_R^{n+1} - e_R^n|^2 \\
& \leq C \Delta t (1 + \|\nabla \mu^{n+1}\|_0^2) |e_R^{n+1}|^2 + C \Delta t (\|\nabla e_\phi^{n+1}\|_0^2 + \|e_\phi^{n+1}\|_0^2 + \|\nabla e_\phi^n\|_0^2 + \|e_\phi^n\|_0^2 + |e_R^n|^2) \\
& + C \Delta t^2 \int_{t^n}^{t^{n+1}} (\|\phi_{tt}(s)\|_{-1}^2 + \|\phi_t(s)\|_1^2) ds + C \Delta t^2 \int_{t^n}^{t^{n+1}} \left(\left| \frac{d^2 R(s)}{dt^2} \right|^2 + \left| \frac{dR(s)}{dt} \right|^2 \right) ds. \tag{A.6}
\end{aligned}$$

Summing up these equations for the indices from 0 to n and using the discrete Gronwall lemma 2.3 conclude the proof. \square

Theorem 2.19. Suppose $\phi_{in} \in H^3(\Omega)$ and the condition (2.14) holds. The following inequality holds for all n with the scheme (2.65),

$$\begin{aligned}
& \|\nabla \phi^{n+1}\|_0^2 + \|\nabla(2\phi^{n+1} - \phi^n)\|_0^2 + \frac{1}{2} \|\nabla(\phi^{n+1} - \phi^n)\|_0^2 + \frac{\lambda}{2} (\|\phi^{n+1}\|_0^2 + \|2\phi^{n+1} - \phi^n\|_0^2) \\
& + \lambda \Delta t \|\Delta \phi^{n+1}\|_0^2 + \frac{3\Delta t}{2} \|\nabla \Delta \phi^{n+1}\|_0^2 + \frac{\Delta t}{2} \|\nabla \Delta(\phi^{n+1} - \phi^n)\|_0^2 + \Delta t \sum_{k=0}^n \|\nabla \mu^{k+1}\|_0^2 \leq \widehat{C}_5,
\end{aligned}$$

where $\widehat{C}_5 = (2\|\nabla \phi^0\|_0^2 + \lambda\|\phi^0\|_0^2 + \lambda\Delta t \|\Delta \phi^0\|_0^2 + \frac{3\Delta t}{2} \|\nabla \Delta \phi^0\|_0^2) \exp(C(M)T)$.

Proof. Taking the inner product of (2.65a) and (2.65b) with $2\Delta t \mu^{n+1}$ and $3\phi^{n+1} - 4\phi^n + \phi^{n-1}$, respectively, we have

$$\begin{aligned}
& \frac{1}{2} (\|\nabla \phi^{n+1}\|_0^2 - \|\nabla \phi^n\|_0^2 + \|\nabla(2\phi^{n+1} - \phi^n)\|_0^2 - \|\nabla(2\phi^n - \phi^{n-1})\|_0^2 + \|\nabla(\phi^{n+1} - 2\phi^n + \phi^{n-1})\|_0^2) \\
& + \frac{\lambda}{2} (\|\phi^{n+1}\|_0^2 - \|\phi^n\|_0^2 + \|2\phi^{n+1} - \phi^n\|_0^2 - \|2\phi^n - \phi^{n-1}\|_0^2 + \|\phi^{n+1} - 2\phi^n + \phi^{n-1}\|_0^2) + 2\Delta t \|\nabla \mu^{n+1}\|_0^2 \\
& = -|\xi_{2A}^{n+1}|^2 (h(\bar{\phi}^n), 3\phi^{n+1} - 4\phi^n + \phi^{n-1}) \leq \Delta t \|\nabla \mu^{n+1}\|_0^2 + |\xi_{2A}^{n+1}|^4 \Delta t \|\nabla h(\bar{\phi}^n)\|_0^2. \tag{A.7}
\end{aligned}$$

Taking the inner product of (2.65a) and (2.65b) with $\Delta(2\phi^{n+1} - \phi^n)$ and $\Delta^2(2\phi^{n+1} - \phi^n)$, respectively, and by using the boundary conditions, we can re-write the two resultant equations into

$$\begin{aligned} & \frac{1}{2}(\|\nabla\phi^{n+1}\|_0^2 - \|\nabla\phi^n\|_0^2 + \|\nabla(2\phi^{n+1} - \phi^n)\|_0^2 - \|\nabla(2\phi^n - \phi^{n-1})\|_0^2 + \|\nabla(\phi^{n+1} - 2\phi^n + \phi^{n-1})\|_0^2) \\ & + 2\|\nabla(\phi^{n+1} - \phi^n)\|_0^2 + \frac{1}{2}(\|\nabla(\phi^{n+1} - \phi^n)\|_0^2 - \|\nabla(\phi^n - \phi^{n-1})\|_0^2 + \|\nabla(\phi^{n+1} - 2\phi^n + \phi^{n-1})\|_0^2) \\ & + 2\Delta t\|\nabla\Delta\phi^{n+1}\|_0^2 + \Delta t(\|\nabla\Delta\phi^{n+1}\|_0^2 - \|\nabla\Delta\phi^n\|_0^2 + \|\nabla\Delta(\phi^{n+1} - \phi^n)\|_0^2) + 2\lambda\Delta t\|\Delta\phi^{n+1}\|_0^2 \\ & + \lambda\Delta t(\|\Delta\phi^{n+1}\|_0^2 - \|\Delta\phi^n\|_0^2 + \|\Delta\phi^{n+1} - \Delta\phi^n\|_0^2) \\ & = 2|\xi_{2A}^{n+1}|^2\Delta t(\nabla h(\bar{\phi}^n), \nabla\Delta\phi^{n+1}) + 2|\xi_{2A}^{n+1}|^2\Delta t(\nabla h(\bar{\phi}^n), \nabla\Delta(\phi^{n+1} - \phi^n)) \\ & \leq \Delta t\|\nabla\Delta\phi^{n+1}\|_0^2 + \frac{\Delta t}{2}\|\nabla\Delta(\phi^{n+1} - \phi^n)\|_0^2 + 3\Delta t|\xi_{2A}^{n+1}|^4\|\nabla h(\bar{\phi}^n)\|_0^2. \end{aligned} \quad (\text{A.8})$$

Summing up (A.7) and (A.8), we have

$$\begin{aligned} & \|\nabla\phi^{n+1}\|_0^2 - \|\nabla\phi^n\|_0^2 + \|\nabla(2\phi^{n+1} - \phi^n)\|_0^2 - \|\nabla(2\phi^n - \phi^{n-1})\|_0^2 + 2\|\nabla(\phi^{n+1} - \phi^n)\|_0^2 + \Delta t\|\nabla\mu^{n+1}\|_0^2 \\ & + \frac{1}{2}(\|\nabla(\phi^{n+1} - \phi^n)\|_0^2 - \|\nabla(\phi^n - \phi^{n-1})\|_0^2) + \frac{\lambda}{2}(\|\phi^{n+1}\|_0^2 - \|\phi^n\|_0^2 + \|2\phi^{n+1} - \phi^n\|_0^2 \\ & - \|2\phi^n - \phi^{n-1}\|_0^2) + \Delta t\|\nabla\Delta\phi^{n+1}\|_0^2 + \Delta t(\|\nabla\Delta\phi^{n+1}\|_0^2 - \|\nabla\Delta\phi^n\|_0^2) + \frac{\Delta t}{2}\|\nabla\Delta(\phi^{n+1} - \phi^n)\|_0^2 \\ & + \lambda\Delta t(\|\Delta\phi^{n+1}\|_0^2 - \|\Delta\phi^n\|_0^2 + \|\Delta\phi^{n+1} - \Delta\phi^n\|_0^2) \\ & \leq 4|\xi_{2A}^{n+1}|^4\Delta t\|\nabla h(\bar{\phi}^n)\|_0^2. \end{aligned} \quad (\text{A.9})$$

Using Lemma 2.1, one finds

$$4|\xi_{2A}^{n+1}|^4\|\nabla h(\bar{\phi}^n)\|_0^2 \leq 4|\xi_{2A}^{n+1}|^4\|h'(\bar{\phi}^n)\|_{0,\infty}^2\|\nabla\bar{\phi}^n\|_0^2 \leq 4C|\xi_{2A}^{n+1}|^4\|\nabla\bar{\phi}^n\|_0^2(1 + \|\bar{\phi}^n\|_{0,\infty}^4). \quad (\text{A.10})$$

By using the same technique as in the proof of Theorem 2.8, the Cauchy Schwarz inequality and the triangle inequality, we have

$$4|\xi_{2A}^{n+1}|^4\|\nabla h(\bar{\phi}^n)\|_0^2 \leq \begin{cases} C(M)\|\nabla\bar{\phi}^n\|_0^2 & \text{for } d = 1, \\ C(M)\|\nabla\bar{\phi}^n\|_0^2 + C(\varepsilon_1, M)\|\nabla\bar{\phi}^n\|_0^2 + \varepsilon_1\|\nabla\Delta\bar{\phi}^n\|_0^2 & \text{for } d = 2, \\ C(M)\|\nabla\bar{\phi}^n\|_0^2 + C(\varepsilon_2, M)\|\nabla\bar{\phi}^n\|_0^2 + \varepsilon_2\|\nabla\Delta\bar{\phi}^n\|_0^2 & \text{for } d = 3. \end{cases}$$

Noting that

$$\|\nabla\Delta\bar{\phi}^n\|_0^2 \leq 2\|\nabla\Delta\phi^n\|_0^2 + 2\|\nabla\Delta(\phi^n - \phi^{n-1})\|_0^2,$$

and by setting $\varepsilon_1 = \varepsilon_2 = \frac{1}{4}$ and combining the above inequalities with (A.9), we obtain

$$\begin{aligned} & \|\nabla\phi^{n+1}\|_0^2 - \|\nabla\phi^n\|_0^2 + \|\nabla(2\phi^{n+1} - \phi^n)\|_0^2 - \|\nabla(2\phi^n - \phi^{n-1})\|_0^2 + \Delta t\|\nabla\mu^{n+1}\|_0^2 \\ & + \frac{1}{2}(\|\nabla(\phi^{n+1} - \phi^n)\|_0^2 - \|\nabla(\phi^n - \phi^{n-1})\|_0^2) + \frac{\lambda}{2}(\|\phi^{n+1}\|_0^2 - \|\phi^n\|_0^2 + \|2\phi^{n+1} - \phi^n\|_0^2 \\ & - \|2\phi^n - \phi^{n-1}\|_0^2) + \lambda\Delta t(\|\Delta\phi^{n+1}\|_0^2 - \|\Delta\phi^n\|_0^2) + \frac{3\Delta t}{2}(\|\nabla\Delta\phi^{n+1}\|_0^2 - \|\nabla\Delta\phi^n\|_0^2) \\ & + \frac{\Delta t}{2}(\|\nabla\Delta(\phi^{n+1} - \phi^n)\|_0^2 - \|\nabla\Delta(\phi^n - \phi^{n-1})\|_0^2) \\ & \leq C(M)\Delta t\|\nabla\bar{\phi}^n\|_0^2 \leq C(M)\Delta t(\|\nabla\phi^n\|_0^2 + \|\nabla\phi^{n-1}\|_0^2). \end{aligned} \quad (\text{A.11})$$

We conclude the proof by taking the sum of (A.11) for the indices from 0 to n and using the discrete Gronwall lemma 2.4. \square

Theorem 2.20. Suppose $\phi_{in} \in H^4(\Omega)$, and the conditions for Lemmas 2.1 and 2.2 hold. The following inequality holds for all n with the scheme (2.65),

$$\begin{aligned} & \frac{1}{2}\|\Delta\phi^{n+1}\|_0^2 + \frac{1}{2}\|\Delta(2\phi^{n+1} - \phi^n)\|_0^2 + \frac{1}{2}\|\Delta(\phi^{n+1} - \phi^n)\|_0^2 + \lambda\Delta t\|\nabla\Delta\phi^{n+1}\|_0^2 \\ & + \frac{3\Delta t}{2}\|\Delta^2\phi^{n+1}\|_0^2 + \frac{\Delta t}{2}\|\Delta^2(\phi^{n+1} - \phi^n)\|_0^2 + \lambda\Delta t\sum_{k=0}^n\|\nabla\Delta\phi^{k+1}\|_0^2 \leq \hat{C}_6, \end{aligned}$$

where $\hat{C}_6 = \|\Delta\phi^0\|_0^2 + \frac{3\Delta t}{2}\|\Delta^2\phi^0\|_0^2 + \lambda\Delta t\|\nabla\Delta\phi^0\|_0^2 + C(M)T$.

Proof. Multiplying (2.65a) by $2\Delta t \Delta^2(2\phi^{n+1} - \phi^n)$ and combining (2.65a) with (2.65b), we obtain

$$\begin{aligned} & \frac{1}{2} (\|\Delta\phi^{n+1}\|_0^2 - \|\Delta\phi^n\|_0^2 + \|\Delta(2\phi^{n+1} - \phi^n)\|_0^2 - \|\Delta(2\phi^n - \phi^{n-1})\|_0^2 + \|\Delta(\phi^{n+1} - 2\phi^n + \phi^{n-1})\|_0^2) \\ & + 2\|\Delta(\phi^{n+1} - \phi^n)\|_0^2 + \frac{1}{2} (\|\Delta(\phi^{n+1} - \phi^n)\|_0^2 - \|\Delta(\phi^n - \phi^{n-1})\|_0^2 + \|\Delta(\phi^{n+1} - 2\phi^n + \phi^{n-1})\|_0^2) \\ & + 2\Delta t \|\Delta^2\phi^{n+1}\|_0^2 + \Delta t (\|\Delta^2\phi^{n+1}\|_0^2 - \|\Delta^2\phi^n\|_0^2 + \|\Delta^2(\phi^{n+1} - \phi^n)\|_0^2) \\ & + 2\lambda\Delta t \|\nabla\Delta\phi^{n+1}\|_0^2 + \lambda\Delta t (\|\nabla\Delta\phi^{n+1}\|_0^2 - \|\nabla\Delta\phi^n\|_0^2 + \|\nabla\Delta(\phi^{n+1} - \phi^n)\|_0^2) \\ & = 2|\xi_{2A}^{n+1}|^2 \Delta t (\Delta h(\bar{\phi}^n), \Delta^2\phi^{n+1}) + 2|\xi_{2A}^{n+1}|^2 \Delta t (\Delta h(\bar{\phi}^n), \Delta^2(\phi^{n+1} - \phi^n)) \\ & \leq \frac{\Delta t}{2} \|\Delta^2\phi^{n+1}\|_0^2 + \frac{\Delta t}{2} \|\Delta^2(\phi^{n+1} - \phi^n)\|_0^2 + 4|\xi_{2A}^{n+1}|^4 \Delta t \|\Delta h(\bar{\phi}^n)\|_0^2. \end{aligned} \quad (\text{A.12})$$

According to (2.18), for any $\varepsilon > 0$, there exists a constant $C(\varepsilon, M)$ depending on ε such that

$$4|\xi_{2A}^{n+1}|^4 \Delta t \|\Delta h(\bar{\phi}^n)\|_0^2 \leq C(M) \Delta t (1 + \|\Delta^2\bar{\phi}^n\|_0^{2\sigma}) \leq \varepsilon \Delta t \|\Delta^2\bar{\phi}^n\|_0^2 + C(\varepsilon, M) \Delta t.$$

By the triangle inequality, we have

$$\|\Delta^2\bar{\phi}^n\|_0^2 \leq 2\|\Delta^2\phi^n\|_0^2 + 2\|\Delta^2(\phi^n - \phi^{n-1})\|_0^2.$$

Combining the above inequalities with (A.12) and choosing $\varepsilon = \frac{1}{4}$, we have

$$\begin{aligned} & \frac{1}{2} (\|\Delta\phi^{n+1}\|_0^2 - \|\Delta\phi^n\|_0^2 + \|\Delta(2\phi^{n+1} - \phi^n)\|_0^2 - \|\Delta(2\phi^n - \phi^{n-1})\|_0^2 + \|\Delta(\phi^{n+1} - 2\phi^n + \phi^{n-1})\|_0^2) \\ & + 2\|\Delta(\phi^{n+1} - \phi^n)\|_0^2 + \frac{1}{2} (\|\Delta(\phi^{n+1} - \phi^n)\|_0^2 - \|\Delta(\phi^n - \phi^{n-1})\|_0^2 + \|\Delta(\phi^{n+1} - 2\phi^n + \phi^{n-1})\|_0^2) \\ & + \Delta t \|\Delta^2\phi^{n+1}\|_0^2 + \frac{3\Delta t}{2} (\|\Delta^2\phi^{n+1}\|_0^2 - \|\Delta^2\phi^n\|_0^2) + \frac{\Delta t}{2} (\|\Delta^2(\phi^{n+1} - \phi^n)\|_0^2 - \|\Delta^2(\phi^n - \phi^{n-1})\|_0^2) \\ & + 2\lambda\Delta t \|\nabla\Delta\phi^{n+1}\|_0^2 + \lambda\Delta t (\|\nabla\Delta\phi^{n+1}\|_0^2 - \|\nabla\Delta\phi^n\|_0^2 + \|\nabla\Delta(\phi^{n+1} - \phi^n)\|_0^2) \\ & \leq C(M) \Delta t. \end{aligned} \quad (\text{A.13})$$

We conclude the proof by taking the sum of this inequality for the indices from 0 to n . \square

Theorem 2.23. Suppose $\phi_{in} \in H^3(\Omega)$ and the condition (2.14) holds. The following inequality holds for all n with the scheme (2.70),

$$\begin{aligned} & \|\nabla\phi^{n+1}\|_0^2 + \|\nabla(2\phi^{n+1} - \phi^n)\|_0^2 + \frac{1}{2} \|\nabla(\phi^{n+1} - \phi^n)\|_0^2 + \frac{\lambda}{2} (\|\phi^{n+1}\|_0^2 + \|2\phi^{n+1} - \phi^n\|_0^2) \\ & + \lambda\Delta t \|\Delta\phi^{n+1}\|_0^2 + \frac{3\Delta t}{2} \|\nabla\Delta\phi^{n+1}\|_0^2 + \frac{\Delta t}{2} \|\nabla\Delta(\phi^{n+1} - \phi^n)\|_0^2 + \Delta t \sum_{k=0}^n \|\nabla\mu^{k+1}\|_0^2 \leq \widehat{C}_5, \end{aligned}$$

where \widehat{C}_5 is given in Theorem 2.19.

Proof. By Lemma 2.22, $\widehat{\xi}_{2B}^n$ satisfies the conditions $|\widehat{\xi}_{2B}^n| \leq \frac{3M}{\sqrt{C_0}}$ and $|\widehat{\xi}_{2B}^n| \leq \frac{C(M)}{\|\phi\|_1}$. In parallel to the proof of Theorem 2.19, we take the same steps therein but replace ξ_{2A}^{n+1} by $\widehat{\xi}_{2B}^n$. \square

Theorem 2.24. Suppose $\phi^0 \in H^4(\Omega)$, and the conditions for Lemmas 2.1 and 2.2 hold. Then the following inequality holds with the scheme (2.70),

$$\begin{aligned} & \frac{1}{2} \|\Delta\phi^{n+1}\|_0^2 + \frac{1}{2} \|\Delta(2\phi^{n+1} - \phi^n)\|_0^2 + \frac{1}{2} \|\Delta(\phi^{n+1} - \phi^n)\|_0^2 + \lambda\Delta t \|\nabla\Delta\phi^{n+1}\|_0^2 \\ & + \frac{3\Delta t}{2} \|\Delta^2\phi^{n+1}\|_0^2 + \frac{\Delta t}{2} \|\Delta^2(\phi^{n+1} - \phi^n)\|_0^2 + \lambda\Delta t \sum_{k=0}^n \|\nabla\Delta\phi^{k+1}\|_0^2 \leq \widehat{C}_6, \end{aligned}$$

where \widehat{C}_6 is given in Theorem 2.20.

Proof. The proof is essentially the same as for Theorem 2.20. One can refer to the proof of Theorem 2.20. \square

Theorem 2.25. Suppose the condition (2.76), and the conditions for Theorems 2.23 and 2.24 hold. The following inequality holds for sufficiently small Δt ,

$$\frac{1}{2} (\|\nabla e_\phi^{n+1}\|_0^2 + \|\nabla(2e_\phi^{n+1} - e_\phi^n)\|_0^2) + \frac{\lambda}{2} (\|e_\phi^{n+1}\|_0^2 + \|2e_\phi^{n+1} - e_\phi^n\|_0^2) + \frac{\Delta t}{2} \|\nabla e_\mu^{n+1}\|_0^2 + |e_R^{n+1}|^2 \leq \widehat{C}_7 \Delta t^4,$$

where $\widehat{C}_7 = C \exp(\Delta t \sum_{k=0}^{n+1} \frac{r^{k+1/2}}{1-r^{k+1/2} \Delta t}) \int_0^{t^{n+1}} (\|\phi_t(s)\|_1^4 + \|\phi_t(s)\|_1^2 + \|\phi_{tt}(s)\|_1^2 + \|\phi_{ttt}(s)\|_{-1}^2) ds$, $r^{k+1/2} = 1 + \|\nabla \mu^{k+1/2}\|_0^2$, and the constant C depends on T , ϕ_{in} , Ω , $\|\phi\|_{L^\infty(0,T;W^{3,\infty}(\Omega))}$, $\|\phi_t\|_{L^\infty(0,T;L^2(\Omega))}$ and $\|\mu\|_{L^\infty(0,T;H^1(\Omega))}$.

Proof. By subtracting (2.79) from (2.70), we have

$$\frac{3e_\phi^{n+1} - 4e_\phi^n + e_\phi^{n-1}}{\Delta t} = \Delta e_\mu^{n+1} - \frac{1}{\Delta t} T_{\phi_{2B}}^{n+1}, \quad (\text{A.14a})$$

$$e_\phi^{n+1} = -\Delta e_\phi^{n+1} + \lambda e_\phi^{n+1} + A_5^{n+1}, \quad (\text{A.14b})$$

$$\frac{e_R^{n+1} - e_R^n}{\Delta t} = -\frac{1}{2} A_6^{n+1} - \frac{1}{\Delta t} T_{R_{2B}}^{n+1}, \quad (\text{A.14c})$$

where

$$\begin{aligned} A_5^{n+1} &= |\widehat{\xi}_{2B}^n|^2 h(\bar{\phi}^n) - \frac{R(t^{n+1})^2}{E[\phi(t^{n+1})]} h(\phi(t^{n+1})) \\ &= \frac{(\bar{R}^n)^2 - \bar{R}(t^n)^2}{E[\bar{\phi}^n]} h(\bar{\phi}^n) + \frac{R(t^n)^2 - R(t^{n+1})^2}{E[\bar{\phi}^n]} h(\bar{\phi}^n) + R(t^{n+1})^2 \left(\frac{h(\bar{\phi}^n)}{E[\bar{\phi}^n]} - \frac{h(\bar{\phi}(t^n))}{E[\bar{\phi}(t^n)]} \right) \\ &\quad + R(t^{n+1})^2 \left(\frac{h(\bar{\phi}(t^n))}{E[\bar{\phi}(t^n)]} - \frac{h(\phi(t^{n+1}))}{E[\phi(t^{n+1})]} \right), \\ A_6^{n+1} &= \frac{\xi_{2B}^{n+1}}{\sqrt{E[\bar{\phi}^{n+1/2}]}} \int_\Omega |\nabla \mu^{n+1/2}|^2 dx - \frac{R(t^{n+1})}{\sqrt{E[\phi(t^{n+1})]}} \frac{1}{\sqrt{E[\phi(t^{n+1/2})]}} \int_\Omega |\nabla \mu(t^{n+1/2})|^2 dx \\ &= \frac{e_R^{n+1}}{\sqrt{E[\bar{\phi}^{n+1/2}]E[\phi^{n+1}]}} \int_\Omega |\nabla \mu^{n+1/2}|^2 dx + \frac{R(t^{n+1})}{\sqrt{E[\bar{\phi}^{n+1/2}]E[\phi^{n+1}]}} \int_\Omega (|\nabla \mu^{n+1/2}|^2 - |\nabla \mu(t^{n+1/2})|^2) dx \\ &\quad + \frac{R(t^{n+1})}{\sqrt{E[\phi^{n+1}]}} \left(\frac{1}{\sqrt{E[\bar{\phi}^{n+1/2}]}} - \frac{1}{\sqrt{E[\phi(t^{n+1/2})]}} \right) \int_\Omega |\nabla \mu(t^{n+1/2})|^2 dx \\ &\quad + \frac{R(t^{n+1})}{\sqrt{E[\phi(t^{n+1/2})]}} \left(\frac{1}{\sqrt{E[\bar{\phi}^{n+1}]}} - \frac{1}{\sqrt{E[\phi(t^{n+1})]}} \right) \int_\Omega |\nabla \mu(t^{n+1/2})|^2 dx. \end{aligned}$$

Taking the inner product of (A.14a) with $2\Delta t e_\mu^{n+1}$ and (A.14b) with $3e_\phi^{n+1} - 4e_\phi^n + e_\phi^{n-1}$, and multiplying (A.14c) with $2\Delta t e_R^{n+1}$, we get the following:

$$\frac{1}{2} (\|\nabla e_\phi^{n+1}\|_0^2 - \|\nabla e_\phi^n\|_0^2 + \|\nabla(2e_\phi^{n+1} - e_\phi^n)\|_0^2 - \|\nabla(2e_\phi^n - e_\phi^{n-1})\|_0^2) + 2\Delta t \|\nabla e_\mu^{n+1}\|_0^2 + \frac{\lambda}{2} (\|e_\phi^{n+1}\|_0^2 - \|e_\phi^n\|_0^2 + \|2e_\phi^{n+1} - e_\phi^n\|_0^2 - \|2e_\phi^n - e_\phi^{n-1}\|_0^2) \leq -(A_5^{n+1}, 3e_\phi^{n+1} - 4e_\phi^n + e_\phi^{n-1}) - 2(T_{\phi_{2B}}^{n+1}, e_\mu^{n+1}), \quad (\text{A.15a})$$

$$|e_R^{n+1}|^2 - |e_R^n|^2 + |e_R^{n+1} - e_R^n|^2 = -\Delta t A_6^{n+1} e_R^{n+1} - 2e_R^{n+1} T_{R_{2B}}^{n+1}. \quad (\text{A.15b})$$

The terms on the right hand side of (A.15a) can be treated as follows.

$$\begin{aligned} \bar{e}_R^n (\bar{R}^n + \bar{R}(t^n)) \left(\frac{h(\bar{\phi}^n)}{E[\bar{\phi}^n]}, 3e_\phi^{n+1} - 4e_\phi^n + e_\phi^{n-1} \right) &= \bar{e}_R^n (\bar{R}^n + \bar{R}(t^n)) \left(\frac{h(\bar{\phi}^n)}{E[\bar{\phi}^n]}, 2\Delta t \Delta e_\mu^{n+1} - 2T_{\phi_{2B}}^{n+1} \right) \\ &\leq C \bar{e}_R^n \left(\Delta t \|\nabla e_\mu^{n+1}\|_0 + \|(-\Delta)^{-1/2} T_{\phi_{2B}}^{n+1}\|_0 \right) \left\| \frac{\nabla h(\bar{\phi}^n)}{E[\bar{\phi}^n]} \right\|_0 \\ &\leq \frac{\Delta t}{5} \|\nabla e_\mu^{n+1}\|_0^2 + C \Delta t |\bar{e}_R^n|^2 + C \Delta t^4 \int_{t^{n-1}}^{t^{n+1}} \|\phi_{ttt}(s)\|_{-1}^2 ds, \\ (\bar{R}(t^n)^2 - R(t^{n+1})^2) \left(\frac{h(\bar{\phi}^n)}{E[\bar{\phi}^n]}, 3e_\phi^{n+1} - 4e_\phi^n + e_\phi^{n-1} \right) &\leq \frac{\Delta t}{5} \|\nabla e_\mu^{n+1}\|_0^2 + C \Delta t |\bar{R}(t^n) - R(t^{n+1})|^2 \\ &\quad + C \Delta t^4 \int_{t^{n-1}}^{t^{n+1}} \|\phi_{ttt}(s)\|_{-1}^2 ds, \\ R(t^{n+1})^2 \left(\frac{h(\bar{\phi}^n)}{E[\bar{\phi}^n]} - \frac{h(\bar{\phi}(t^n))}{E[\bar{\phi}(t^n)]}, 3e_\phi^{n+1} - 4e_\phi^n + e_\phi^{n-1} \right) &\leq \frac{\Delta t}{5} \|\nabla e_\mu^{n+1}\|_0^2 + C \Delta t \left\| \frac{\nabla h(\bar{\phi}^n)}{E[\bar{\phi}^n]} - \frac{\nabla h(\bar{\phi}(t^n))}{E[\bar{\phi}(t^n)]} \right\|_0^2 \end{aligned}$$

$$\begin{aligned}
& + C \Delta t^4 \int_{t^{n-1}}^{t^{n+1}} \|\phi_{ttt}(s)\|_{-1}^2 ds, \\
R(t^{n+1})^2 & \left(\frac{h(\bar{\phi}(t^n))}{E[\bar{\phi}(t^n)]} - \frac{h(\phi(t^{n+1}))}{E[\phi(t^{n+1})]} \right) \leq \frac{\Delta t}{5} \|\nabla e_\mu^{n+1}\|_0^2 + C \Delta t^2 \int_{t^{n-1}}^{t^{n+1}} \|\phi_{ttt}(s)\|_{-1}^2 ds \\
& + C \Delta t \left\| \frac{\nabla h(\bar{\phi}(t^n))}{E[\bar{\phi}(t^n)]} - \frac{\nabla h(\phi(t^{n+1}))}{E[\phi(t^{n+1})]} \right\|_0^2, \\
-2(T_{\phi_{2B}}^{n+1}, e_\mu^{n+1}) & \leq \frac{\Delta t}{5} \|\nabla e_\mu^{n+1}\|_0^2 + \frac{C}{\Delta t} \|(-\Delta)^{-1/2} T_{\phi_{2B}}^{n+1}\|_0^2 \leq \frac{\Delta t}{5} \|\nabla e_\mu^{n+1}\|_0^2 + C \Delta t^4 \int_{t^{n-1}}^{t^{n+1}} \|\phi_{ttt}(s)\|_{-1}^2 ds.
\end{aligned}$$

Next, the right-hand side terms of (A.15b) can be treated as follows.

$$\begin{aligned}
-2e_R^{n+1} T_{R_{2B}}^{n+1} & \leq \Delta t |e_R^{n+1}|^2 + \frac{C}{\Delta t} |T_{R_{2B}}^{n+1}|^2 \leq \Delta t |e_R^{n+1}|^2 + C \Delta t^4 \int_{t^n}^{t^{n+1}} \left| \frac{d^3 R(s)}{dt^3} \right|^2 ds, \\
- \frac{\Delta t |e_R^{n+1}|^2}{\sqrt{E[\bar{\phi}^{n+1/2}]} E[\phi^{n+1}]} \int_{\Omega} |\nabla \mu^{n+1/2}|^2 dx & \leq C \Delta t \|\nabla \mu^{n+1/2}\|_0^2 |e_R^{n+1}|^2, \\
- \frac{\Delta t e_R^{n+1} R(t^{n+1})}{\sqrt{E[\bar{\phi}^{n+1/2}]} E[\phi^{n+1}]} \int_{\Omega} (|\nabla \mu^{n+1/2}|^2 - |\nabla \mu(t^{n+1/2})|^2) dx & \leq C \Delta t e_R^{n+1} \|\nabla e_\mu^{n+1/2}\|_0 \|\nabla \mu^{n+1/2} + \nabla \mu(t^{n+1/2})\|_0 \\
& \leq C \Delta t (\|\nabla \mu^{n+1/2}\|_0^2 + 1) |e_R^{n+1}|^2 + \frac{\Delta t}{2} (\|\nabla e_\mu^{n+1}\|_0^2 + \|\nabla e_\mu^n\|_0^2), \\
- \frac{\Delta t R(t^{n+1}) e_R^{n+1}}{\sqrt{E[\phi^{n+1}]}} \left(\frac{1}{\sqrt{E[\bar{\phi}^{n+1/2}]}} - \frac{1}{\sqrt{E[\phi(t^{n+1/2})]}} \right) \int_{\Omega} |\nabla \mu(t^{n+1/2})|^2 dx & \\
& \leq C \Delta t e_R^{n+1} \left| \frac{1}{\sqrt{E[\bar{\phi}^{n+1/2}]}} - \frac{1}{\sqrt{E[\phi(t^{n+1/2})]}} \right| \leq C \Delta t |e_R^{n+1}|^2 + C \Delta t \left| \frac{1}{\sqrt{E[\bar{\phi}^{n+1/2}]}} - \frac{1}{\sqrt{E[\phi(t^{n+1/2})]}} \right|^2, \\
- \frac{\Delta t R(t^{n+1}) e_R^{n+1}}{\sqrt{E[\phi(t^{n+1/2})]}} \left(\frac{1}{\sqrt{E[\phi^{n+1}]}} - \frac{1}{\sqrt{E[\phi(t^{n+1})]}} \right) \int_{\Omega} |\nabla \mu(t^{n+1/2})|^2 dx & \\
& \leq C \Delta t e_R^{n+1} \left| \frac{1}{\sqrt{E[\phi^{n+1}]}} - \frac{1}{\sqrt{E[\phi(t^{n+1})]}} \right| \leq C \Delta t |e_R^{n+1}|^2 + C \Delta t \left| \frac{1}{\sqrt{E[\phi^{n+1}]}} - \frac{1}{\sqrt{E[\phi(t^{n+1})]}} \right|^2.
\end{aligned}$$

For the term $\frac{\nabla h(\bar{\phi}^n)}{E[\bar{\phi}^n]} - \frac{\nabla h(\bar{\phi}(t^n))}{E[\bar{\phi}(t^n)]}$, we rewrite it into

$$\frac{\nabla h(\bar{\phi}^n)}{E[\bar{\phi}^n]} - \frac{\nabla h(\bar{\phi}(t^n))}{E[\bar{\phi}(t^n)]} = \frac{\nabla h(\bar{\phi}^n) - \nabla h(\bar{\phi}(t^n))}{E[\bar{\phi}^n]} + \frac{\nabla h(\bar{\phi}(t^n))(E[\bar{\phi}(t^n)] - E[\bar{\phi}^n])}{E[\bar{\phi}^n] E[\bar{\phi}(t^n)]}$$

In light of the Hölder's inequality and Sobolev embedding theorem, we have

$$\begin{aligned}
\|\nabla h(\bar{\phi}^n) - \nabla h(\bar{\phi}(t^n))\|_0 & \leq \|(h'(\bar{\phi}^n) - h'(\bar{\phi}(t^n))) \nabla \bar{\phi}(t^n)\|_0 + \|h'(\bar{\phi}^n) \nabla \bar{e}_\phi^n\|_0 \\
& \leq C \|\nabla \bar{\phi}(t^n) \bar{e}_\phi^n\|_0 + C \|\nabla \bar{e}_\phi^n\|_0 \leq C (\|\nabla \bar{\phi}(t^n)\|_{0,3} \|\bar{e}_\phi^n\|_{0,6} + \|\nabla \bar{e}_\phi^n\|_0) \\
& \leq C \|\bar{\phi}(t^n)\|_2 \|\bar{e}_\phi^n\|_1 + C \|\nabla \bar{e}_\phi^n\|_0 \leq C (\|\nabla \bar{e}_\phi^n\|_0 + \|\bar{e}_\phi^n\|_0).
\end{aligned}$$

According to the definition of $E[\phi]$, we have

$$\begin{aligned}
E[\bar{\phi}^n] - E[\bar{\phi}(t^n)] & = \frac{1}{2} \int_{\Omega} (\nabla \bar{\phi}^n + \nabla \bar{\phi}(t^n)) \nabla \bar{e}_\phi^n dx + \frac{\lambda}{2} \int_{\Omega} (\bar{\phi}^n + \bar{\phi}(t^n)) \bar{e}_\phi^n dx + \int_{\Omega} (H(\bar{\phi}^n) - H(\bar{\phi}(t^n))) dx \\
& \leq C \|\nabla \bar{e}_\phi^n\|_0 + C \|\bar{e}_\phi^n\|_0 + \int_{\Omega} H'(\theta \bar{\phi}^n + (1-\theta) \bar{\phi}(t^n)) (\bar{\phi}^n - \bar{\phi}(t^n)) dx \\
& \leq C (\|\nabla \bar{e}_\phi^n\|_0 + \|\bar{e}_\phi^n\|_0).
\end{aligned} \tag{A.16}$$

Then, we have

$$\begin{aligned}
\left\| \frac{\nabla h(\bar{\phi}^n)}{E[\bar{\phi}^n]} - \frac{\nabla h(\bar{\phi}(t^n))}{E[\bar{\phi}(t^n)]} \right\|_0^2 & = \left\| \frac{\nabla h(\bar{\phi}^n) - \nabla h(\bar{\phi}(t^n))}{E[\bar{\phi}^n]} + \frac{\nabla h(\bar{\phi}(t^n))(E[\bar{\phi}(t^n)] - E[\bar{\phi}^n])}{E[\bar{\phi}^n] E[\bar{\phi}(t^n)]} \right\|_0^2 \\
& \leq C \|\nabla h(\bar{\phi}^n) - \nabla h(\bar{\phi}(t^n))\|_0^2 + C \|\nabla h(\bar{\phi}(t^n))\|_0^2 |E[\bar{\phi}(t^n)] - E[\bar{\phi}^n]|^2 \\
& \leq C (\|\nabla \bar{e}_\phi^n\|_0^2 + \|\bar{e}_\phi^n\|_0^2).
\end{aligned} \tag{A.17}$$

Similarly,

$$\left\| \frac{\nabla h(\bar{\phi}(t^n))}{E[\bar{\phi}(t^n)]} - \frac{\nabla h(\phi(t^{n+1}))}{E[\phi(t^{n+1})]} \right\|_0^2 \leq C \|\nabla h(\bar{\phi}(t^n)) - \nabla h(\phi(t^{n+1}))\|_0^2 + C \|\nabla h(\phi(t^{n+1}))\|_0^2 |E[\phi(t^{n+1})] - E[\bar{\phi}(t^n)]|^2$$

$$\begin{aligned}
& \leq C(\|\nabla\phi(t^{n+1}) - \nabla\bar{\phi}(t^n)\|_0^2 + \|\phi(t^{n+1}) - \bar{\phi}(t^n)\|_0^2) \\
& \leq C\Delta t^3 \int_{t^{n-1}}^{t^{n+1}} \|\phi_{tt}(s)\|_1^2 ds, \\
& \left| \frac{1}{\sqrt{E[\tilde{\phi}^{n+1/2}]}} - \frac{1}{\sqrt{E[\phi(t^{n+1/2})]}} \right|^2 = \frac{|E[\phi(t^{n+1/2})] - E[\tilde{\phi}^{n+1/2}]|^2}{E[\tilde{\phi}^{n+1/2}]E[\phi(t^{n+1/2})](\sqrt{E[\tilde{\phi}^{n+1/2}]} + \sqrt{E[\phi(t^{n+1/2})]})^2} \\
& \leq C|E[\phi(t^{n+1/2})] - E[\tilde{\phi}^{n+1/2}]|^2 + C|E[\tilde{\phi}^{n+1/2}] - E[\tilde{\phi}^{n+1/2}]|^2 \\
& \leq C(\|\nabla\tilde{e}_\phi^{n+1/2}\|_0^2 + \|\tilde{e}_\phi^{n+1/2}\|_0^2) + C\Delta t^3 \int_{t^{n-1}}^{t^{n+1}} \|\phi_{tt}(s)\|_1^2 ds, \\
& \left| \frac{1}{\sqrt{E[\phi^{n+1}]}} - \frac{1}{\sqrt{E[\phi(t^{n+1})]}} \right|^2 = \frac{|E[\phi(t^{n+1})] - E[\phi^{n+1}]|^2}{E[\phi^{n+1}]E[\phi(t^{n+1})](\sqrt{E[\phi^{n+1}]} + \sqrt{E[\phi(t^{n+1})]})^2} \\
& \leq C(\|\nabla e_\phi^{n+1}\|_0^2 + \|e_\phi^{n+1}\|_0^2), \\
& |\bar{R}(t^n) - R(t^{n+1})|^2 = |2R(t^n) - R(t^{n-1}) - R(t^{n+1})|^2 \leq C\Delta t^3 \int_{t^{n-1}}^{t^{n+1}} \left| \frac{d^2 R(s)}{dt^2} \right|^2 ds. \tag{A.18}
\end{aligned}$$

By combining the above inequalities with (A.15a) and (A.15b), we have

$$\begin{aligned}
& \frac{1}{2}(\|\nabla e_\phi^{n+1}\|_0^2 - \|\nabla e_\phi^n\|_0^2 + \|\nabla(2e_\phi^{n+1} - e_\phi^n)\|_0^2 - \|\nabla(2e_\phi^n - e_\phi^{n-1})\|_0^2) + \frac{\Delta t}{2}(\|\nabla e_\mu^{n+1}\|_0^2 - \|\nabla e_\mu^n\|_0^2) \\
& \quad + \frac{\lambda}{2}(\|e_\phi^{n+1}\|_0^2 - \|e_\phi^n\|_0^2 + \|2e_\phi^{n+1} - e_\phi^n\|_0^2 - \|2e_\phi^n - e_\phi^{n-1}\|_0^2) + |e_R^{n+1}|^2 - |e_R^n|^2 + |e_R^{n+1} - e_R^n|^2 \\
& \leq C\Delta t(1 + \|\nabla\mu^{n+1/2}\|_0^2)|e_R^{n+1}|^2 + C\Delta t(\|\nabla e_\phi^{n+1}\|_0^2 + \|e_\phi^{n+1}\|_0^2 + \|\nabla e_\phi^n\|_0^2 + \|e_\phi^n\|_0^2 + \|\nabla e_\phi^{n-1}\|_0^2 \\
& \quad + \|e_\phi^{n-1}\|_0^2 + |e_R^n|^2) + C\Delta t^4 \int_{t^{n-1}}^{t^{n+1}} \left(\|\phi_{ttt}(s)\|_1^2 + \|\phi_{tt}(s)\|_1^2 + \left| \frac{d^3 R(s)}{dt^3} \right|^2 + \left| \frac{d^2 R(s)}{dt^2} \right|^2 \right) ds. \tag{A.19}
\end{aligned}$$

Summing up (A.19) for the indices from 0 to n , we get

$$\begin{aligned}
& \frac{1}{2}(\|\nabla e_\phi^{n+1}\|_0^2 + \|\nabla(2e_\phi^{n+1} - e_\phi^n)\|_0^2) + \frac{\lambda}{2}(\|e_\phi^{n+1}\|_0^2 + \|2e_\phi^{n+1} - e_\phi^n\|_0^2) + \frac{\Delta t}{2}\|\nabla e_\mu^{n+1}\|_0^2 + |e_R^{n+1}|^2 \\
& \leq C\Delta t \sum_{k=0}^n (1 + \|\nabla\mu^{k+1/2}\|_0^2)|e_R^{k+1}|^2 + C\Delta t \sum_{k=0}^n (\|\nabla e_\phi^{k+1}\|_0^2 + \|e_\phi^{k+1}\|_0^2 + \|\nabla e_\phi^k\|_0^2 + \|e_\phi^k\|_0^2 + \|\nabla e_\phi^{k-1}\|_0^2) \\
& \quad + C\Delta t \sum_{k=0}^n (\|e_\phi^{k-1}\|_0^2 + |e_R^k|^2 + |e_R^{k-1}|^2) + C\Delta t^4 \\
& \leq C\Delta t \sum_{k=0}^n (1 + \|\nabla\mu^{k+1/2}\|_0^2) \left(|e_R^{k+1}|^2 + \|\nabla e_\phi^{k+1}\|_0^2 + \|e_\phi^{k+1}\|_0^2 \right) + C\Delta t^4. \tag{A.20}
\end{aligned}$$

Based on Theorem 2.23 and the triangle inequality $\|\nabla\mu^{k+1/2}\|_0^2 \leq \frac{1}{2}(\|\nabla\mu^k\|_0^2 + \|\nabla\mu^{k+1}\|_0^2)$, we have

$$\Delta t \sum_{k=0}^{n+1} \|\nabla\mu^{k+1/2}\|_0^2 \leq \widehat{C}_5.$$

We then use the discrete Gronwall lemma 2.3 to finish the proof. \square

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