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Research article

A remark on the invariant energy quadratization (IEQ) method for preserving the original energy dissipation laws

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Abstract: In this letter, we revisit the invariant energy quadratization (IEQ) method and provide a new perspective on its ability to preserve the original energy dissipation laws. The IEQ method has been widely used to design energy stable numerical schemes for phase-field or gradient flow models. Although there are many merits of the IEQ method, one major disadvantage is that the IEQ method usually respects a modified energy law, where the modified energy is expressed in the auxiliary variables. Still, the dissipation laws in terms of the original energy are not guaranteed by the IEQ method. Using the widely-used Cahn-Hilliard equation as an example, we demonstrate that the Runge-Kutta IEQ method indeed can preserve the original energy dissipation laws for certain situations up to arbitrary high-order accuracy. Interested readers are encouraged to extend this idea to more general cases and apply it to other thermodynamically consistent models.

Keywords: energy stable; cahn hilliard equation; invariant energy quadratization (IEQ) method

1. Introduction

A wide variety of interfacial phenomena [1–5] are driven by dissipative mechanism [6–8]. As a powerful approach to describe the dissipative mechanism, gradient flow models which respect the thermodynamic laws are commonly used. In general, consider a spatial-temporal domain $\Omega \times [0, T]$, and denote the state variable as ϕ. The dissipative dynamics takes the form of

$$\partial_t \phi(\mathbf{x}, t) = -\mathcal{G}\frac{\delta E}{\delta \phi} \quad \text{in } \Omega \times [0, T], \tag{1.1}$$

where E is a functional of ϕ known as the free energy, and $\mathcal{G}$ is a semi-positive definite operator, known as the mobility operator. The triplet $(\phi, \mathcal{G}, E)$ uniquely determines the thermodynamically consistent gradient flow model. With proper boundary conditions, the dynamics of the gradient flow model (1.1) satisfies the following energy dissipation law,

$$\frac{dE}{dt} = \Big(\frac{\delta E}{\delta \phi}, \frac{\partial \phi}{\partial t}\Big) = -(\frac{\delta E}{\delta \phi}, \mathcal{G}\frac{\delta E}{\delta \phi}) \leq 0, \tag{1.2}$$

where the L^2 inner product and its norm are defined by $(f, g) = \int_\Omega f g d\mathbf{x}$ and $\|f\|_2 = \sqrt{(f, f)}$, $\forall f, g \in L^2(\Omega)$, respectively. Due to its broad applications, many approaches [9–15] are proposed to develop numerical approximations such that the energy dissipation property (1.2) can be preserved in the discrete level.

Among these existing numerical approaches, the invariant energy quadratization (IEQ) method [15] has been extensively used to design numerical algorithms for a broad class of phase field models [16]. Meanwhile, by combing it with the Runge-Kutta method, arbitrarily high-order schemes could be developed [17]. However, there is still one limitation of the IEQ method that has not been adequately addressed in the numerical analysis community. The numerical schemes based on the IEQ method mainly respect a modified energy law, where the modified energy is expressed with auxiliary variables. The original energy and the modified energy are equivalent with respect to the analytical solutions. But they are not necessarily equal with respect to the numerical solutions. Whether the numerical schemes based on the IEQ method respect the original energy law is still unknown. To remedy this issue, we introduced a relaxation technique in our early work [18, 19] for solving phase-field equations with the IEQ method and the scalar auxiliary variable (SAV) approach. By adding a relaxation parameter, we penalize the numerical difference between the modified energy and the original energy so that the numerical solutions of the phase-field equations will follow more closely to the original energy dissipation law. Nevertheless, it is still an open question whether the numerical schemes based on the IEQ method respect the original energy law or not.

In this letter, we attempt to shed light on this issue. Inspired by some recent advances on designing high-order structure-preserving schemes for Hamiltonian systems [20, 21], we discover that some numerical schemes based on the IEQ method indeed can respect the original energy dissipation laws for certain types of gradient flow models. Particularly, we revisit our early work on developing arbitrarily high-order numerical schemes for dissipative systems [17, 22–24]. Eventually, we come up with a new perspective on the IEQ method. We conclude that specific Runge-Kutta type numerical schemes derived by the IEQ method indeed can preserve the original energy dissipation laws for certain situations up to arbitrary high-order accuracy.

2. A brief review of the IEQ method

2.1. A generic model reformulation using the IEQ method

Now, we briefly explain the invariant energy quadratization (IEQ) method that was introduced in [15]. Without loss of generality, we consider the generic form of the effective free energy

$$E(\phi) = \frac{1}{2}(\phi, \mathcal{L}_0\phi) + (g(\phi), 1), \tag{2.1}$$

where $\mathcal{L}_0$ is a linear operator and $g(\phi)$ is a potential function density. With the effective free energy (2.1), the gradient flow model (1.1) could be written as

$$\partial_t \phi = -\mathcal{G}(\mathcal{L}_0\phi + g'(\phi)). \tag{2.2}$$

For simplicity of presentation, we only consider periodic boundary conditions in this letter. Therefore, the gradient flow system (2.2) satisfies the following energy dissipation law

$$\frac{d}{dt}E(\phi) = (\mathcal{L}_0\phi + g'(\phi), \partial_t\phi) = -\Big(\mathcal{L}_0\phi + g'(\phi), \mathcal{G}(\mathcal{L}_0\phi + g'(\phi))\Big) \le 0. \tag{2.3}$$

An energy stable scheme for (2.2) means the numerical solutions from the scheme will also respect the energy dissipation law of (2.3) in the discrete level. The IEQ method [15] is shown to be effective in guiding the design of energy stable schemes. The idea of the IEQ method is to reformulate the original PDE in (2.2) into an equivalent form, for which the energy stable schemes can be effectively designed. Specifically, we can introduce the auxiliary function

$$q(\mathbf{x}, t) := \sqrt{2(g(\phi) + C_0)}, \tag{2.4}$$

where $C_0 > 0$ is a constant making sure the auxiliary function is well-defined [25]. The energy functional (2.1) could be rewritten as a quadratic form

$$F(\phi, q) = \frac{1}{2}(\phi, \mathcal{L}_0\phi) + \frac{1}{2}(q, q) - C_0|\Omega|. \tag{2.5}$$

Then we can rewrite the original gradient flow system (2.2) into the IEQ reformulated system

$$\begin{cases} \partial_t\phi = -\mathcal{G}\Big(\mathcal{L}_0\phi + \dfrac{qg'(\phi)}{\sqrt{2(g(\phi) + C_0)}}\Big), \\ \partial_t q = \dfrac{g'(\phi)}{\sqrt{2(g(\phi) + C_0)}}\partial_t\phi, \quad q(\mathbf{x}, 0) = \sqrt{2(g(\phi|_{t=0}) + C_0)}. \end{cases} \tag{2.6}$$

By a straightforward calculation, the new system (2.6) possesses the following energy dissipation law

$$\frac{d}{dt}F(\phi, q) = -\Big(\mathcal{L}_0\phi + \frac{qg'(\phi)}{\sqrt{2(g(\phi) + C_0)}}, \mathcal{G}(\mathcal{L}_0\phi + \frac{qg'(\phi)}{\sqrt{2(g(\phi) + C_0)}})\Big) \le 0. \tag{2.7}$$

Lemma 1. *Systems* (2.2) *and* (2.6) *are equivalent.*

This lemma can be easily shown. So the details are omitted. Notice the fact that we can get

$$q(\mathbf{x}, t) - \sqrt{2(g(\phi) + C_0)} = 0 \tag{2.8}$$

from (2.4). Hence the original energy (2.1) and the modified energy (2.5) are equivalent, and the original energy law (2.3) and the modified energy law (2.7) are equivalent as well. However, we emphasize that the consistent condition in (2.8) might not be satisfied numerically.

2.2. Arbitrarily high-order numerical schemes

Given the reformulated system (2.6) is equivalent to the original system (2.2), a numerical scheme that solves (2.6) will provide the numerical solutions for (2.2).

To solve (2.6), we revisit the IEQ-RK schemes in our previous work [17]. Consider the time domain $t \in [0, T]$. We discretize it into equally distanced meshes, $0 = t_0 < t_1 < \cdots < t_N = T$, with $t_i = i\Delta t$ and $\Delta t = \frac{T}{N}$. And we use ϕ^{n+1} to represent the numerical solution of $\phi(\mathbf{x}, t)$ at t_{n+1}. Similar notations apply to other variables as well.

Scheme 1 (s-stage IEQ-RK scheme)**.** *Let a_{ij} and b_i with $i, j = 1, 2, \cdots, s$ be real numbers (the Runge-Kutta coefficients). Use the consistent initial condition $q^0 = \sqrt{2(g(\phi^0) + C_0)}$. Given (ϕ^n, q^n), we can calculate (ϕ^{n+1}, q^{n+1}) through the following Runge-Kutta (RK) numerical scheme*

$$\phi^{n+1} = \phi^n + \Delta t \sum_{i=1}^{s} b_i k_i^n, \tag{2.9}$$

$$q^{n+1} = q^n + \Delta t \sum_{i=1}^{s} b_i l_i^n, \tag{2.10}$$

where the intermediate terms are calculated from

$$\begin{aligned}
\phi_i^n &= \phi^n + \Delta t \sum_{j=1}^{s} a_{ij} k_j^n, \\
q_i^n &= q^n + \Delta t \sum_{j=1}^{s} a_{ij} l_j^n, \\
k_i^n &= -\mathcal{G}\Big(\mathcal{L}_0 \phi_i^n + \frac{q_i^n g'(\phi_i^n)}{\sqrt{2(g(\phi_i^n) + C_0)}}\Big), \\
l_i^n &= \frac{g'(\phi_i^n)}{\sqrt{2(g(\phi_i^n) + C_0)}} k_i^n,
\end{aligned} \tag{2.11}$$

with $i = 1, 2, \cdots, s$.

For simplicity of notations, we organize the s-stage RK coefficients in the Butcher table as below.

$$\begin{array}{c|c} \mathbf{c} & \mathbf{A} \\ \hline & \mathbf{b}^T \end{array} = \begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & & \vdots \\ c_s & a_{s1} & \cdots & a_{ss} \\ \hline & b_1 & \cdots & b_s \end{array},$$

where $\mathbf{A} \in \mathbb{R}^{s,s}$, $\mathbf{b} \in \mathbb{R}^s$, and $\mathbf{c} = \mathbf{A}\mathbf{l}$ with $\mathbf{l} = (1, 1, \cdots, 1)^T \in \mathbb{R}^s$. The RK coefficients based on the 2nd, 4th, and 6th order Gaussian collocation methods [26] are summarized in Table 1.

Table 1. Butcher tableaus of Gauss methods of 2, 4 and 6.

$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2} - \frac{\sqrt{3}}{6}$	$\frac{1}{4}$	$\frac{1}{4} - \frac{\sqrt{3}}{6}$	$\frac{1}{2} - \frac{\sqrt{15}}{10}$	$\frac{5}{36}$	$\frac{2}{9} - \frac{\sqrt{15}}{15}$	$\frac{5}{36} - \frac{\sqrt{15}}{30}$
					$\frac{1}{2}$	$\frac{5}{36} + \frac{\sqrt{15}}{24}$	$\frac{2}{9}$	$\frac{5}{36} - \frac{\sqrt{15}}{24}$
	1	$\frac{1}{2} + \frac{\sqrt{3}}{6}$	$\frac{1}{4} + \frac{\sqrt{3}}{6}$	$\frac{1}{4}$	$\frac{1}{2} + \frac{\sqrt{15}}{10}$	$\frac{5}{36} + \frac{\sqrt{15}}{30}$	$\frac{2}{9} + \frac{\sqrt{15}}{15}$	$\frac{5}{36}$
			$\frac{1}{2}$	$\frac{1}{2}$		$\frac{5}{18}$	$\frac{4}{9}$	$\frac{5}{18}$

Definition 1 (Symplectic Condition). Define a symmetric matrix $\mathbf{S} \in \mathbb{R}^{s,s}$ as

$$S_{ij} = b_i a_{ij} + b_j a_{ji} - b_i b_j, \quad i, j = 1, 2, \cdots s.$$

The symplectic condition is defined as

$$S_{ij} = 0, \quad b_i \geq 0, \quad i, j = 1, 2, \cdots s. \tag{2.12}$$

It is easy to verify that the RK coefficients in Table 1 satisfy the symplectic condition in (2.12). In other words, the set of RK coefficients that satisfy the symplectic condition in (2.12) is not empty.

3. Numerical schemes respecting the original energy dissipation laws

Now, we are ready to present the main contribution of this letter. In this letter, we point out that the s-stage IEQ-RK scheme that satisfies the symplectic condition in (2.12) indeed respects the original energy dissipation laws given that the auxiliary function in (2.4) is a quadratic function of ϕ.

3.1. The IEQ method for the Cahn-Hilliard equation

To better explain this new perspective, we restrict our presentation on the widely-used Cahn-Hilliard equation in this letter. Recall the widely-used Cahn-Hilliard equation with periodic boundary conditions

$$\begin{cases} \partial_t \phi = M\Delta\mu, \\ \mu = -\varepsilon\Delta\phi + \dfrac{1}{\varepsilon}(\phi^3 - \phi). \end{cases} \tag{3.1}$$

which can be written in an energy variation form of (1.1) with $\mathcal{G} = -M\Delta$ and the free energy $E(\phi)$ defined as

$$E(\phi) = \int_\Omega \Big[\frac{\varepsilon}{2}|\nabla\phi|^2 + \frac{1}{4\varepsilon}(\phi^2 - 1)^2\Big] d\mathbf{x}. \tag{3.2}$$

This model has an energy dissipation law

$$\frac{d}{dt}E(\phi) = (M\Delta\mu, \mu) = -\int_\Omega M|\nabla\mu|^2 d\mathbf{x} \leq 0. \tag{3.3}$$

To utilize the IEQ method, we can introduce an auxiliary function

$$q(\mathbf{x}, t) := \phi^2 - 1 - C, \tag{3.4}$$

where C is a constant to be specified by the users [25]. With the auxiliary function $q(\mathbf{x}, t)$, we reformulate the CH equation (3.1) as

$$\begin{cases} \partial_t \phi = M\Delta\mu, \\ \mu = -\varepsilon\Delta\phi + \dfrac{1}{\varepsilon}\phi(q + C), \\ \partial_t q = 2\phi\partial_t\phi, \quad q(\mathbf{x}, 0) = \phi^2(\mathbf{x}, 0) - 1 - C. \end{cases} \tag{3.5}$$

Here $q(\mathbf{x},0)=\phi^2(\mathbf{x},0)-1-C$ is the consistent initial condition. The reformulated model (3.5) satisfies a modified energy law

$$\frac{d}{dt}F(\phi,q)=-\int_\Omega M\Big|\nabla\Big(-\varepsilon\Delta\phi+\frac{1}{\varepsilon}\phi(q+C)\Big)\Big|^2d\mathbf{x}\le 0, \tag{3.6}$$

with the modified energy $F(\phi,q)$ given as

$$F(\phi,q)=\int_\Omega\Big[\frac{\varepsilon}{2}|\nabla\phi|^2+\frac{C}{2\varepsilon}\phi^2+\frac{1}{4\varepsilon}\Big(q^2-C^2-2C\Big)\Big]d\mathbf{x}. \tag{3.7}$$

Scheme 2 (s-stage IEQ-RK scheme for the CH equation)**.** *Let a_{ij} and b_i with $i,j=1,2,\cdots,s$ be real numbers (the Runge-Kutta coefficients). Use the consistent initial condition $q^0=(\phi^0)^2-1-C$. Given (ϕ^n,q^n), we can calculate (ϕ^{n+1},q^{n+1}) through the following numerical scheme*

$$\phi^{n+1}=\phi^n+\Delta t\sum_{i=1}^s b_ik_i^n, \tag{3.8}$$

$$q^{n+1}=q^n+\Delta t\sum_{i=1}^s b_il_i^n, \tag{3.9}$$

where the intermediate terms are calculated from

$$\begin{aligned}
\phi_i^n&=\phi^n+\Delta t\sum_{j=1}^s a_{ij}k_j^n,\\
q_i^n&=q^n+\Delta t\sum_{j=1}^s a_{ij}l_j^n,\\
k_i^n&=M\Delta\Big(-\varepsilon\Delta\phi_i^n+\frac{1}{\varepsilon}\phi_i^n(q_i^n+C)\Big),\\
l_i^n&=2\phi_i^nk_i^n,
\end{aligned} \tag{3.10}$$

with $i=1,2,\cdots,s$.

Lemma 2. *Assume that the RK coefficients a_{ij},b_i satisfy the symplectic condition in* (2.12)*. From Scheme 2, we have*

$$q^{n+1}=(\phi^{n+1})^2-1-C,\quad \forall n\ge 0. \tag{3.11}$$

Proof. First of all, we will show that

$$q^{n+1}-q^n=(\phi^{n+1})^2-(\phi^n)^2.$$

From (3.9), we have

$$\begin{aligned} q^{n+1} - q^n &= \Delta t \sum_{i=1}^{s} b_i l_i^n = 2\Delta t \sum_{i=1}^{s} b_i \phi_i^n k_i^n \\ &= 2\Delta t \sum_{i=1}^{s} b_i k_i^n (\phi^n + \Delta t \sum_{j=1}^{s} a_{ij} k_j^n) \\ &= 2\Delta t \sum_{i=1}^{s} b_i k_i^n \phi^n + 2(\Delta t)^2 \sum_{i=1}^{s}\sum_{j=1}^{s} b_i a_{ij} k_i^n k_j^n \\ &= 2\Delta t \sum_{i=1}^{s} b_i k_i^n \phi^n + (\Delta t)^2 \sum_{i=1}^{s}\sum_{j=1}^{s} (b_i a_{ij} + b_j a_{ji}) k_i^n k_j^n \\ &= 2\Delta t \sum_{i=1}^{s} b_i k_i^n \phi^n + (\Delta t)^2 \sum_{i=1}^{s}\sum_{j=1}^{s} b_i b_j k_i^n k_j^n. \end{aligned} \tag{3.12}$$

From (3.8), we have

$$\begin{aligned} (\phi^{n+1})^2 - (\phi^n)^2 &= (2\phi^n + \Delta t \sum_{i=1}^{s} b_i k_i^n)(\Delta t \sum_{i=1}^{s} b_i k_i^n) \\ &= 2\Delta t \sum_{i=1}^{s} b_i k_i^n \phi^n + (\Delta t)^2 \sum_{i=1}^{s}\sum_{j=1}^{s} b_i b_j k_i^n k_j^n. \end{aligned} \tag{3.13}$$

Comparing the Eqs (3.12) and (3.13), we immediately find

$$q^{n+1} - q^n = (\phi^{n+1})^2 - (\phi^n)^2. \tag{3.14}$$

Also, notice the fact $q^0 = (\phi^0)^2 - 1 - C$. Therefore, by induction, we get

$$q^{n+1} = (\phi^{n+1})^2 - 1 - C, \quad \forall n \geq 0. \tag{3.15}$$

Now, we are ready to present the major result of this letter.

Theorem 1. Assume that the RK coefficients a_{ij}, b_i satisfy the symplectic condition in (2.12). Scheme 2 obeys the following energy dissipation law

$$E(\phi^{n+1}) - E(\phi^n) = -\Delta t \sum_{i=1}^{s} b_i \Big\| \sqrt{M}\nabla\Big(-\varepsilon\Delta\phi_i^n + \frac{1}{\varepsilon}\phi_i^n(q_i^n + C)\Big)\Big\|^2 \leq 0, \tag{3.16}$$

with $E(\phi)$ defined in (3.2). In other words, the numerical solutions respect the original energy dissipation laws.

Proof. Denote $\mathcal{L} = -\varepsilon\Delta + \frac{1}{\varepsilon}C$. First, we will show that

$$E(\phi^{n+1}) - E(\phi^n) = F(\phi^{n+1}, q^{n+1}) - F(\phi^n, q^n)$$

The original energy functional (3.3) can be rewritten as the following quadratic form

$$E(\phi) = \frac{1}{2}(\phi, \mathcal{L}\phi) - \frac{C}{2\varepsilon}(\phi, \phi) + \frac{1}{4\varepsilon}(\phi^2 - 1, \phi^2 - 1). \tag{3.17}$$

Similarly, the modified energy functional (3.7) can be rewritten as follows

$$F(\phi, q) = \frac{1}{2}(\phi, \mathcal{L}\phi) + \frac{1}{4\varepsilon}(q, q) - \frac{C^2 + 2C}{4\varepsilon}|\Omega|. \tag{3.18}$$

From (3.17), (3.18) and Lemma 2, we have

$$\begin{aligned} F(\phi^{n+1}, q^{n+1}) &= \frac{1}{2}(\phi^{n+1}, \mathcal{L}\phi^{n+1}) + \frac{1}{4\varepsilon}(q^{n+1}, q^{n+1}) - \frac{C^2 + 2C}{4\varepsilon}|\Omega| \\ &= \frac{1}{2}(\phi^{n+1}, \mathcal{L}\phi^{n+1}) + \frac{1}{4\varepsilon}\Big(((\phi^{n+1})^2 - 1 - C, (\phi^{n+1})^2 - 1 - C)\Big) - \frac{C^2 + 2C}{4\varepsilon}|\Omega| \\ &= \frac{1}{2}(\phi^{n+1}, \mathcal{L}\phi^{n+1}) + \frac{1}{4\varepsilon}((\phi^{n+1})^2 - 1, (\phi^{n+1})^2 - 1) - \frac{C}{2\varepsilon}(\phi^{n+1}, \phi^{n+1}) \\ &= E(\phi^{n+1}). \end{aligned} \tag{3.19}$$

Therefore, we can get

$$\begin{aligned} E(\phi^{n+1}) - E(\phi^n) &= F(\phi^{n+1}, q^{n+1}) - F(\phi^n, q^n) \\ &= \frac{1}{2}(\phi^{n+1}, \mathcal{L}\phi^{n+1}) + \frac{1}{4\varepsilon}(q^{n+1}, q^{n+1}) - \Big[\frac{1}{2}(\phi^n, \mathcal{L}\phi^n) + \frac{1}{4\varepsilon}(q^n, q^n)\Big]. \end{aligned} \tag{3.20}$$

Next, from (3.8), we have

$$\begin{aligned} &\frac{1}{2}(\phi^{n+1}, \mathcal{L}\phi^{n+1}) - \frac{1}{2}(\phi^n, \mathcal{L}\phi^n) \\ =&\frac{1}{2}(\phi^n + \Delta t \sum_{i=1}^{s} b_i k_i^n, \mathcal{L}\phi^n + \Delta t \sum_{i=1}^{s} b_i \mathcal{L}k_i^n) - \frac{1}{2}(\phi^n, \mathcal{L}\phi^n) \\ =&\Delta t \sum_{i=1}^{s} b_i (k_i^n, \mathcal{L}\phi^n) + \frac{1}{2}(\Delta t)^2 \sum_{i=1}^{s}\sum_{j=1}^{s} b_i b_j (k_i^n, \mathcal{L}k_j^n) \\ =&\Delta t \sum_{i=1}^{s} b_i (k_i^n, \mathcal{L}\phi_i^n - \Delta t \sum_{j=1}^{s} a_{ij}\mathcal{L}k_j^n) + \frac{1}{2}(\Delta t)^2 \sum_{i=1}^{s}\sum_{j=1}^{s} b_i b_j (k_i^n, \mathcal{L}k_j^n) \\ =&\Delta t \sum_{i=1}^{s} b_i (k_i^n, \mathcal{L}\phi_i^n) - (\Delta t)^2 \sum_{i=1}^{s}\sum_{j=1}^{s} b_i a_{ij} (k_i^n, \mathcal{L}k_j^n) + \frac{1}{2}(\Delta t)^2 \sum_{i=1}^{s}\sum_{j=1}^{s} b_i b_j (k_i^n, \mathcal{L}k_j^n) \\ =&\Delta t \sum_{i=1}^{s} b_i (k_i^n, \mathcal{L}\phi_i^n) - \frac{1}{2}(\Delta t)^2 \sum_{i=1}^{s}\sum_{j=1}^{s} \Big[b_i a_{ij} + b_j a_{ji} - b_i b_j\Big](k_i^n, \mathcal{L}k_j^n) \\ =&\Delta t \sum_{i=1}^{s} b_i (k_i^n, \mathcal{L}\phi_i^n). \end{aligned} \tag{3.21}$$

Meanwhile, from (3.9), we have

$$\begin{aligned}
&\frac{1}{2}(q^{n+1}, q^{n+1}) - \frac{1}{2}(q^n, q^n) \\
=&\frac{1}{2}(q^n + \Delta t \sum_{i=1}^{s} b_i l_i^n, q^n + \Delta t \sum_{i=1}^{s} b_i l_i^n) - \frac{1}{2}(q^n, q^n) \\
=&\Delta t \sum_{i=1}^{s} b_i (l_i^n, q^n) + \frac{1}{2}(\Delta t)^2 \sum_{i=1}^{s}\sum_{j=1}^{s} b_i b_j (l_i^n, l_j^n) \\
=&\Delta t \sum_{i=1}^{s} b_i (l_i^n, q_i^n - \Delta t \sum_{j=1}^{s} a_{ij} l_j^n) + \frac{1}{2}(\Delta t)^2 \sum_{i=1}^{s}\sum_{j=1}^{s} b_i b_j (l_i^n, l_j^n) \\
=&\Delta t \sum_{i=1}^{s} b_i (l_i^n, q_i^n) - \frac{1}{2}(\Delta t)^2 \sum_{i=1}^{s}\sum_{j=1}^{s} \Big[b_i a_{ij} + b_j a_{ji} - b_i b_j\Big](l_i^n, l_j^n) \\
=&\Delta t \sum_{i=1}^{s} b_i (l_i^n, q_i^n) = \Delta t \sum_{i=1}^{s} b_i (k_i^n, 2\phi_i^n q_i^n).
\end{aligned} \tag{3.22}$$

So, from (3.21) and (3.22), we conclude

$$\begin{aligned}
&\frac{1}{2}(\phi^{n+1}, \mathcal{L}\phi^{n+1}) + \frac{1}{4\varepsilon}(q^{n+1}, q^{n+1}) - \Big[\frac{1}{2}(\phi^n, \mathcal{L}\phi^n) + \frac{1}{4\varepsilon}(q^n, q^n)\Big] \\
=&\Delta t \sum_{i=1}^{s} b_i (k_i^n, \mathcal{L}\phi_i^n) + \frac{\Delta t}{2\varepsilon} \sum_{i=1}^{s} b_i (k_i^n, 2\phi_i^n q_i^n) \\
=&\Delta t \sum_{i=1}^{s} b_i (k_i^n, \mathcal{L}\phi_i^n + \frac{1}{\varepsilon}\phi_i^n q_i^n) \\
=&\Delta t \sum_{i=1}^{s} b_i (M\Delta(\mathcal{L}\phi_i^n + \frac{1}{\varepsilon}\phi_i^n q_i^n), \mathcal{L}\phi_i^n + \frac{1}{\varepsilon}\phi_i^n q_i^n).
\end{aligned} \tag{3.23}$$

Noticing the semi-definite property of $\mathcal{G} = -M\Delta$ and $b_i \geq 0$, $\forall i$, (3.20) and (3.23) together lead to

$$\begin{aligned}
E(\phi^{n+1}) - E(\phi^n) &= \Delta t \sum_{i=1}^{s} b_i (M\Delta(\mathcal{L}\phi_i^n + \frac{1}{\varepsilon}\phi_i^n q_i^n), \mathcal{L}\phi_i^n + \frac{1}{\varepsilon}\phi_i^n q_i^n) \\
&= -\Delta t \sum_{i=1}^{s} b_i \Big\| \sqrt{M}\nabla\Big(- \varepsilon\Delta\phi_i^n + \frac{1}{\varepsilon}\phi_i^n (q_i^n + C)\Big)\Big\|^2 \\
&\leq 0,
\end{aligned} \tag{3.24}$$

where $E(\phi)$ is defined in (3.2).

We emphasize that this idea not only applies to the Cahn-Hilliard equation, but it also works for other phase-field equations or gradient flow models with similar free energies. Additionally, we can conclude similar results for the generic gradient flow models when the potential function density, $g(\phi)$, is a polynomial of ϕ. Under this condition, we can always introduce single or multiple auxiliary functions that are linear or quadratic. Then by the same techniques used in the proof of Theorem 1, we

can show that our EQ-RK schemes with specified Runge-Kutta coefficients can preserve the original energy dissipation laws. Meanwhile, how to resolve the inconsistency issues of the IEQ method for the gradient flow models with other kinds of nonlinear potential function density still remains a challenge. We plan to address these issues in our future research.

3.2. Connections with the classical implicit schemes

The previous sub-section clarifies that the IEQ method can be used to derive arbitrarily high-order accurate numerical schemes for the Cahn-Hilliard equation that preserve the original energy dissipation laws. Now, we attempt to clarify their connections with the classical implicit schemes.

From Lemma 2, we have $q^{n+1} = (\phi^{n+1})^2 - 1 - C$, $\forall n \geq 0$. Plugging them into the Scheme 2, we get

$$\phi^{n+1} = \phi^n + \Delta t \sum_{i=1}^{s} b_i k_i^n, \tag{3.25}$$

where the intermediate terms are calculated from

$$\begin{aligned} \phi_i^n &= \phi^n + \Delta t \sum_{j=1}^{s} a_{ij} k_j^n, \\ k_i^n &= M\Delta\Big(- \varepsilon\Delta\phi_i^n + \frac{1}{\varepsilon}\phi_i^n\Big[(\phi^n)^2 - 1 + \Delta t \sum_{j=1}^{s} a_{ij} 2\phi_j^n k_j^n\Big]\Big), \end{aligned} \tag{3.26}$$

with $i = 1, 2, \cdots, s$. This is an implicit multi-stage scheme.

In particular, when $s = 1$, we have the RK coefficients in Table 1. Scheme 2 is reduced as

$$\begin{aligned} \phi^{n+1} &= \phi^n + \Delta t k_1^n, \\ q^{n+1} &= q^n + \Delta t l_1^n, \\ \phi_1^n &= \phi^n + \frac{1}{2}\Delta t k_1^n, \\ q_1^n &= q^n + \frac{1}{2}\Delta t l_1^n, \\ k_1^n &= M\Delta(-\varepsilon\Delta\phi_1^n + \frac{1}{\varepsilon}\phi_1^n(q_1^n + C)), \\ l_1^n &= 2\phi_1^n k_1^n, \end{aligned} \tag{3.27}$$

with the consistent initial condition $q^0 = (\phi^0)^2 - 1 - C$.

Theorem 2. The numerical scheme in (3.27) is equivalent to the implicit scheme

$$\begin{aligned} &\frac{\phi^{n+1} - \phi^n}{\Delta t} = M\Delta\mu^{n+\frac{1}{2}}, \\ &\mu^{n+\frac{1}{2}} = -\varepsilon\Delta\frac{\phi^{n+1} + \phi^n}{2} + \frac{1}{2\varepsilon}(\phi^{n+1} + \phi^n)\Big[\frac{1}{2}((\phi^{n+1})^2 + (\phi^n)^2) - 1\Big]. \end{aligned} \tag{3.28}$$

Proof. From (3.27), we have

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} = k_1^n, \tag{3.29}$$

so that

$$\phi_1^n = \phi^n + \frac{1}{2}\Delta t\frac{\phi^{n+1} - \phi^n}{\Delta t} = \frac{1}{2}(\phi^{n+1} + \phi^n).$$

Similarly, we have $q_1^n = \frac{1}{2}(q^n + q^{n+1})$.

Based on Theorem 1, we have $q^{n+1} = (\phi^{n+1})^2 - 1 - C$. This leads to

$$q_1^n = \frac{1}{2}((\phi^{n+1})^2 + (\phi^n)^2) - 1 - C. \tag{3.30}$$

Substituting (3.30) back into the expression for k_1^n, we have

$$k_1^n = M\Delta\Big[-\varepsilon\Delta\frac{\phi^{n+1} + \phi^n}{2} + \frac{1}{2\varepsilon}(\phi^{n+1} + \phi^n)(\frac{1}{2}((\phi^{n+1})^2 + (\phi^n)^2) - 1)\Big]. \tag{3.31}$$

Combing (3.29) and (3.31), we arrive at the implicit scheme (3.28).

3.3. Numerical results

Next, we briefly present several numerical experiments to test our IEQ-RK method on the Cahn-Hilliard equation. We consider problems with periodic boundary conditions for simplicity. To make the order of accuracy in space compatible with the arbitrarily high-order in time, we will employ the Fourier pseudo-spectral method in space for Scheme 2.

Consider the domain $\Omega = [0, 1]^2$ and the parameters $\varepsilon = 10^{-2}$, $M = 1$. We set the initial condition as $\phi = 0.05(\cos(6\pi x)\cos(8\pi y) + (\cos(8\pi x)\cos(6\pi y))^2 + \cos(2\pi x - 10\pi y)\cos(4\pi x - 2\pi y))$. The dynamics driven by the CH equation is summarized in Figure 1.

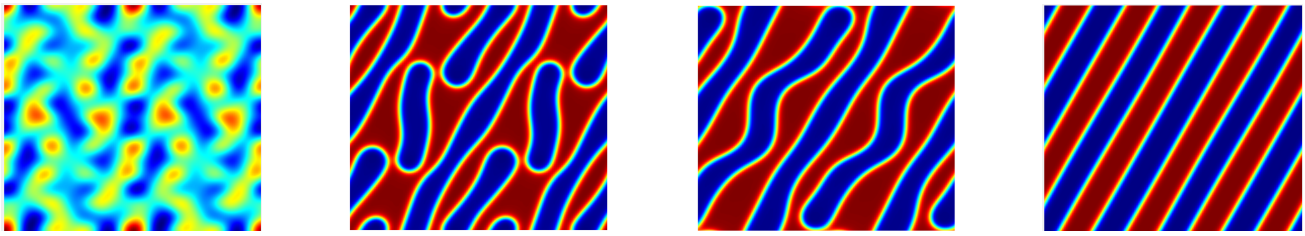

Figure 1. Dynamics driven by the Cahn-Hilliard equation with ϕ at $t = 0, 0.03, 0.07, 1$.

Meanwhile, the focus of this letter is whether the IEQ-RK schemes with specified Runge-Kutta coefficients preserve the original energy dissipation laws. We solve the problem in Figure 1 using Scheme 2 with 128^2 meshes and $\delta t = 10^{-3}$, $C = 1$ for calculation. The numerical energy using the 4th order Gaussian collocation method is summarized in Figure 2 for the CH equation, which illustrates that the scheme indeed respects the original energy dissipation law.

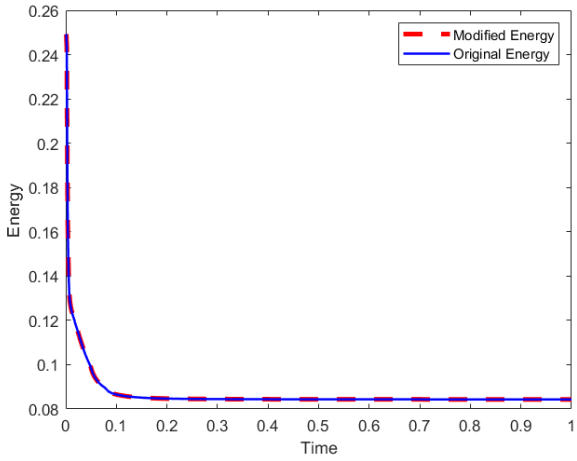

Figure 2. Numerical energies using 4th order Gaussian collocation method for the Cahn-Hilliard equation. This figure indicated that the EQ-RK schemes with specified Runge-Kutta coefficients preserve the original energy dissipation laws.

4. Concluding remarks

This letter revisited the IEQ method and EQ-RK numerical schemes for solving gradient flow models. We point out that the EQ-RK schemes with specified Runge-Kutta coefficients that satisfy the symplectic condition can preserve the energy dissipation laws with respect to the original energy expression when the auxiliary functions are quadratic functions of the original variables. This partially addresses the opening question of whether the numerical schemes based on the IEQ method respect the original energy laws. It also sheds light on further exploring the IEQ method for solving thermodynamically consistent models.

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Conflict of interest

The authors declare there is no conflicts of interest.

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