Explicit high-order energy-preserving methods for general Hamiltonian partial differential equations

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Abstract

A novel class of explicit high-order energy-preserving methods are proposed for general Hamiltonian partial differential equations with non-canonical structure matrix. When the energy is not quadratic, it is firstly done that the original system is reformulated into an equivalent form with a modified quadratic energy conservation law by the energy quadratization approach. Then the resulting system that satisfies the quadratic energy conservation law is discretized in time by combining explicit high-order Runge-Kutta methods with orthogonal projection techniques. The proposed schemes are shown to share the order of explicit Runge-Kutta method and thus can reach the desired high-order accuracy. Moreover, the methods are energy-preserving and explicit because the projection step can be solved explicitly. Numerical results are addressed to demonstrate the remarkable superiority of the proposed schemes in comparison with other structure-preserving methods.

AMS subject classification: 65M06, 65M70

Keywords: explicit Runge-Kutta method, orthogonal projection, energy quadratization approach, Hamiltonian system.

1 Introduction

Hamiltonian partial differential equations (PDEs) play an important role in science and engineering, some particularly important examples include: quantum mechanics, fluid mechanics and electromagnetics etc. The general form of Hamiltonian PDEs is given by

\[
\partial_t z = D(z) \frac{\delta H}{\delta z},
\]

(1.1)

where \(D(z)\) is a skew-adjoint operator for any \(z\). One of the most famous geometric characteristics of (1.1) is that the exact flow has the invariant (also called first integral) \(H=\text{const}\). A numerical scheme that preserves one or more invariants of Hamiltonian PDEs (1.1) is known as an energy-preserving scheme or integral-preserving scheme. During the past decade, it has been shown that non-energy-preserving schemes may easily show nonlinear blow-up or lead to instability (see Ref. [20]). This is because such

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schemes may introduce truncation errors that destroy the physical law numerically. In addition, the energy-preserving property has been showed to be a crucial role in the proof of stability, convergence, existence and uniqueness of the solution for numerical methods (e.g., see Ref. [31]).

As a matter of fact, over the years, there has been an increasing interest in energy-preserving numerical methods for convertive systems. In Ref. [16], Cooper proved that all RK methods conserve linear invariants and an irreducible RK method can preserve all quadratic invariants if and only if their coefficients \((A \in \mathbb{R}^{s \times s}, b \in \mathbb{R}^s)\) satisfy
\[
b_{i} a_{i,j} + b_{j} a_{j,i} - b_{i} b_{j} = 0 \quad \text{for all } i,j = 1, \cdots, s.
\]
However, no RK method can preserve arbitrary polynomial invariants of degree 3 or higher of arbitrary vector fields [11]. To overcome this difficulty, various different numerical methods which can preserve general invariants are proposed such as the discrete gradient method [35] (including the averaged vector field (AVF) method [7, 12, 21, 32, 37]), discrete variational derivative methods [17, 19, 34], the energy quadratization (EQ) approach [8, 26] and the Kahan’s method [18]. However, to our best knowledge, most of the existing energy-preserving schemes are only second order in time, which can’t provide long time accurate solutions with a given large time step. Thus, how to design high-order and energy-preserving numerical schemes for conservative systems has attracted much attention in recent years. The noticeable ones include the high-order AVF methods [30, 37, 43], Hamiltonian Boundary Value Methods (HBVMs) [1, 2, 3], continuous stage Runge-Kutta (CSRK) methods [15, 24, 36, 42] as well as projection methods [5, 23, 29]. More recently, Jiang et al [28] developed a class of arbitrarily high-order energy-preserving schemes for Camassa-Holm equation by combining the methodology of the invariant energy quadratization (IEQ) approach introduced in Refs. [22, 44, 47] with a symplectic RK method (see e.g., Refs. [38, 39]). Other high-order energy-preserving schemes can be found in Refs. [13, 33, 45]. Despite the exciting high-order schemes are energy-preserving and achieve high-order accuracy in time, all of them are fully implicit which further implies that the practical implementation of the methods is complicated and expensive unless a fast nonlinear solver is proposed [4, 36].

Compared to the fully implicit methods, explicit ones are simple and easy to implementation. Thus, in the past few decades, there have been many existing attempts to develop explicit high-order energy-preserving methods. In Ref. [6], del Buono and Mastroserio proposed an explicit fourth-order rational RK method which preserve a quadratic invariant. Later on, Calvo et al. [9] developed a novel class of high-order explicit methods to preserve quadratic invariants in the numerical integration of the underling system by using the incremental direction projection technique associated with explicit RK methods. Further studies on such method have been carried out in Ref. [10]. However, for general invariants, their methods need to solve a nonlinear equations, at every time level, which may lead to expensive costs. Recently, Zhang et al. [46] constructed a class of explicit high-order numerical methods that can preserve a quadratic invariant for the perturbed Kepler two-body system and the one dimensional nonlinear Schrödinger equation, respectively, by using the incremental direction projection and the EQ strategy. In this paper, we will propose a framework for developing explicit high-order energy-preserving methods for general Hamiltonian PDEs (1.1), based on the idea of the IEQ approach and the orthogonal projection technique. We first utilize the idea of the IEQ approach to reformulate the system (1.1) where the energy is not quadratic, into a reformulated system, which inherits a quadratic invariant. Then, the resulting system is solved by the orthogonal projection method associated with explicit RK methods. We show that the Lagrange multiplier of the projected methods can be explicitly obtained, and the resulting methods can retain the order of the RK method. Thus, our methods are energy-preserving, explicit and can achieve desired high-order
accuracy. Moreover, different from Ref. [46], in this paper, we mainly focus on the Hamiltonian PDEs (1.1) where the invariant is boundness (i.e., defined in the senses of a norm). This is because the boundness of numerical solution can be directly obtained by these discrete invariants. Therefore it is valuable to expect that the proposed methods for this class of systems will produce richer information. For illustration purposes, we solve the two-dimensional nonlinear Schrödinger equation and the one and two-dimensional sine-Gordon equation to demonstrate the effectiveness of the selected new scheme, respectively. To show their accuracy and efficiency, we also compare our proposed scheme with the Gauss collocation method and the one provided by incremental direction projection.

The rest of this paper is organized as follows. In Section 2, we use the idea of the IEQ approach to reformulate the system (1.1) into an equivalent form. In Section 3, the explicit high-order energy-preserving schemes are introduced, and their energy-preservation is discussed. In Sections 4, several numerical examples are shown to illustrate the power of our proposed explicit high-order schemes. We draw some conclusions in Section 5.

2 Model reformulation

In this section, we apply the IEQ approach to reformulate the Hamiltonian PDEs (1.1) when the energy is not quadratic. The reformulated model satisfies a quadratic energy conservation law, which is equivalent to the original system in the continuous level. This process provides an elegant platform for developing explicit high-order energy-preserving schemes.

For the purpose of illustration, we assume the energy is given by the following

\[ H = \frac{1}{2} \langle z, Bz \rangle + (f(z), 1), \]  

(2.1)

where \( B \) is a linear, self-adjoint, positive definite operator, and \( f(z) \) is a lower bounded function that only depends on \( z \) itself, but not its spatial derivatives. Then the energy (2.1) can be rewritten as a quadratic form

\[ H = \frac{1}{2} \langle z, Bz \rangle + \frac{1}{2} \| q \|^2 - C_0, \]  

(2.2)

by introducing an auxiliary variable \( q = \sqrt{2(f(z) + C_0 |Ω|)} \), where \( C_0 \) is a constant large enough to make \( q \) well-defined for all \( z \).

Denote \( g(z) = \frac{f'(z)}{\sqrt{2(f(z) + C_0 |Ω|)}} \). We then reformulate the system (1.1) into an equivalent form

\[
\begin{align*}
\partial_t z &= D(z)(Bz + g(z)q), \\
\partial_t q &= g(z)\partial_t z,
\end{align*}
\]  

(2.3)

with the consistent initial condition

\[ q(x, 0) = \sqrt{2\left(f(z(x, 0)) + \frac{C_0}{|Ω|}\right)}. \]  

(2.4)

Denoting \( \Phi = \begin{pmatrix} z \\ q \end{pmatrix} \), the system (2.3) then can be written as the following compact form

\[ \partial_t \Phi = G(\Phi) \frac{\delta H}{\delta \Phi}, \]  

(2.5)
with a quadratic energy (2.2) and a modified structure matrix

\[ \mathcal{G}(\Phi) = \begin{pmatrix} 1 \\ g(z) \end{pmatrix} \mathcal{D}(z) \begin{pmatrix} 1 \\ g(z) \end{pmatrix}, \]

It is worth mentioning that \( \mathcal{G} \) is still skew-adjoint for any \( \Phi \), so that the quadratic energy conservation law is satisfied by the reformulated system (2.5) (or (2.3))

\[ \frac{dH}{dt} = \left( \frac{\delta H}{\delta \Phi}, \partial_t \Phi \right) = \left( \frac{\delta H}{\delta \Phi}, \mathcal{G}(\Phi) \frac{\delta H}{\delta \Phi} \right) = 0. \] (2.6)

**Remark 2.1.** On the one hand, the energy quadratization reformulation is not necessary for conservation systems whose invariant is quadratic. For example, the mass of the nonlinear Schrödinger equation is a quadratic invariant (see Section 4). On the other hand, the energy quadratization approach can also work for a more general \( f \) which depends on \( z \) and its spatial derivatives. If \( f \) is unbounded from below, we can use the splitting strategy to divide \( f \) into several differences which are bounded from below. Then the energy can be transformed into a quadratic form by introducing multiple auxiliary variables and the corresponding model reformulation can be derived (see [27]).

Since the EQ-reformulated form in (2.3) has a quadratic energy, we next discuss how to devise explicit high-order energy-preserving schemes for it.

3 Explicit high-order energy-preserving methods

In this section, a class of explicit high-order energy-preserving methods is proposed for the energy-quadratized system (2.5) by utilizing explicit high-order RK methods and orthogonal projection techniques. For simplicity of notations, we denote \( \mathcal{F}(\Phi) = \mathcal{G}(\Phi) \frac{\delta H}{\delta \Phi} \) and then rewrite the EQ reformulation (2.5) into the following form

\[ \partial_t \Phi = \mathcal{F}(\Phi), \] (3.1)

which conserves the quadratic energy \( \mathcal{H} = \frac{1}{2} \langle \Phi, L \Phi \rangle \) with \( L = \text{diag}(B, 1) \). We here focus on developing time-discrete methods. Denote \( t_n = n\tau, n = 0, 1, 2, \cdots \), where \( \tau \) is the time step. The approximation of the function \( \Phi(x, t) \) at time \( t^n \) is denoted by \( \Phi^n \).

3.1 Explicit schemes for modular Hamiltonian PDE systems

In this subsection, we consider the system (3.1) with the special energy \( \mathcal{H} = \frac{1}{2} \| \Phi \|^2 \), which is called a modular Hamiltonian system. Combining the explicit RK methods and the orthogonal projection technique, we obtain the following explicit energy-preserving methods for the modular conservative system:

**Scheme 3.1.** For given \( \Phi^n \), \( \Phi^{n+1} \) is calculated by the following two steps

1. **Explicit RK:** we compute \( \tilde{\Phi}^{n+1} \) using

\[
\begin{align*}
    k_1 &= \mathcal{F}(\Phi^n), \\
    k_i &= \mathcal{F} \left( \Phi^n + \tau \sum_{j=1}^{i-1} a_{ij} k_j \right), \quad i = 2, \cdots, s, \\
    \tilde{\Phi}^{n+1} &= \Phi^n + \tau \sum_{i=1}^{s} b_i k_i,
\end{align*}
\] (3.2)

where \( b_i, a_{ij} \) are RK coefficients.
2. **Projection:** we update \( \Phi_{n+1} \) via
\[
\Phi_{n+1}^{\text{proj}} = \frac{\|\Phi_n\|}{\|\Phi_{n+1}\|} \Phi_{n+1}.
\] (3.3)

**Theorem 3.1.** If the explicit RK step has order \( p \) and \( \Phi^n \neq 0 \), then there exists \( \tau^* > 0 \) such that Scheme 3.1 has at least order \( p \) for all \( \tau \in (0, \tau^*) \). Moreover, Scheme 3.1 preserves the discrete energy conservation law
\[
\mathcal{H}^{n+1} = \mathcal{H}^n, \quad \mathcal{H}^n = \frac{1}{2} \|\Phi^n\|^2, \quad \forall n \geq 0.
\] (3.4)

**Proof.** Since the explicit RK step has order \( p \), we have the local error
\[
\hat{\Phi}_{n+1} = \Phi(t_n + \tau) + C_{p+1}(\Phi^n)\tau^{p+1} + O(\tau^{p+2}),
\] (3.5)
which leads to
\[
\|\hat{\Phi}_{n+1}\|^2 = \|\Phi(t_n + \tau)\|^2 + O(\tau^{p+1}).
\] (3.6)
Noticing that the modular conservative system (3.1) satisfies the energy conservation
\[
\frac{1}{2} \|\Phi(t_n + \tau)\|^2 = \frac{1}{2} \|\Phi^n\|^2,
\] (3.7)
therefore, we can deduce from (3.7)
\[
\frac{\|\Phi^n\|}{\|\Phi_{n+1}\|} = 1 + O(\tau^{p+1}).
\] (3.8)
Using (3.5) and (3.8) leads to
\[
\Phi_{n+1} = \frac{\|\Phi^n\|}{\|\Phi_{n+1}\|} \hat{\Phi}_{n+1} = \Phi(t_n + \tau) + O(\tau^{p+1}).
\] (3.9)

The discrete energy conservation (3.4) is clearly held by following the projection step (3.3). This completes the proof. \( \square \)

**Remark 3.1.** If the initial condition is taken as \( \Phi^0 = 0 \), then the modular conservation system here satisfies the zero exact solution. So we’re only thinking about the case where \( \Phi^0 \) is non-zero. It’s not hard to see that Scheme 3.1 can work when \( \hat{\Phi}_{n+1} \neq 0 \). Eq. (3.7) implies \( \hat{\Phi}_{n+1} \neq 0 \) for sufficiently small \( \tau \). Therefore, if \( \hat{\Phi}_{n+1} \) is calculated to be zero in numerical calculations, the time step \( \tau \) needs to be reduced to recalculate \( \hat{\Phi}_{n+1} \) that is not zero.

**Remark 3.2.** Quadratic invariants of the form \( \mathcal{H} = \frac{1}{2} \|\Phi\|^2 \) appear in many physical problems, such as the nonlinear Schrödinger equation and the Korteweg-de Vries equation. The proposed methods here will be considered for the nonlinear Schrödinger equation in this paper.

**Remark 3.3.** As a matter of fact, the projection step (3.3) is explicit and can be derived by the standard projection method
\[
\frac{1}{2} \|\Phi_{n+1} - \hat{\Phi}_{n+1}\|^2 \rightarrow \text{min} \quad \text{subject to} \quad \frac{1}{2} \|\Phi_{n+1}\|^2 = \frac{1}{2} \|\Phi^n\|^2.
\] (3.10)
However, for general quadratic energy \( \mathcal{H} = \frac{1}{2}(\Phi, L\Phi) \) where \( L \neq I \), the standard projection method always derives an implicit format, which needs to be solved by a nonlinear iteration.

5
3.2 Explicit schemes for general Hamiltonian PDE systems

In this subsection, we are committed to developing explicit energy-preserving methods for the EQ system (3.1) with general quadratic energy \( H = \frac{1}{2}(\Phi, L\Phi) \). Changing the standard projection method in Scheme 3.1 to the modified projection technique (see P. 111 of Ref. [25]), we derive the following explicit schemes for general Hamiltonian PDEs:

**Scheme 3.2.** For given \( \Phi^n, \Phi^{n+1} \) is calculated by the following two steps

1. Explicit RK: we calculate \( \Phi^n_{n+1} \) through an explicit RK method (3.2).
2. Modified projection: we update \( \Phi^{n+1} \) via
   
   \[
   \Phi^{n+1} = (I + \lambda_n L)\tilde{\Phi}^{n+1},
   \]
   
   where \( \lambda_n \) is a constant given by
   
   \[
   \lambda_n = \frac{-\delta_n}{\beta_n + \sqrt{\beta_n^2 - \alpha_n \delta_n}},
   \]
   
   and \( \alpha_n = (\Phi^{n+1}, L^3\Phi^{n+1}), \beta_n = (\Phi^{n+1}, L^2\Phi^{n+1}), \delta_n = (\Phi^{n+1}, L\Phi^{n+1}) - (\Phi^n, L\Phi^n) \).

**Theorem 3.2.** If the explicit RK step has order \( p \) and \( L\Phi^n \neq 0 \), then there exists \( \tau^* > 0 \) such that Scheme 3.2 has at least order \( p \) for all \( \tau \in (0, \tau^*) \). Scheme 3.2 preserves the discrete energy conservation law

\[
H^{n+1} = H^n = \frac{1}{2}(\Phi^n, L\Phi^n), \quad \forall n \geq 0.
\]

**Proof.** Since the explicit RK step has order \( p \), we have the local error

\[
\Phi^{n+1} = \Phi(t_n + \tau) + O(\tau^{p+1}) = \Phi^n + O(\tau),
\]

which leads to

\[
\alpha_n = (\Phi^n, L^3\Phi^n) + O(\tau), \quad \beta_n = (\Phi^n, L^2\Phi^n) + O(\tau), \quad \delta_n = (\Phi(t_n + \tau), L\Phi(t_n + \tau)) - (\Phi^n, L\Phi^n) + O(\tau^{p+1}).
\]

Noticing the energy conservation \( \frac{1}{2}(\Phi(t_n + \tau), L\Phi(t_n + \tau)) = \frac{1}{2}(\Phi^0, L\Phi^0) = \frac{1}{2}(\Phi^n, L\Phi^n) \), we obtain

\[
\delta_n = O(\tau^{p+1}).
\]

Using (3.15), (3.16) and (3.18), we can derive

\[
\beta_n^2 - \alpha_n \delta_n = (\Phi^n, L^2\Phi^n)^2 + O(\tau).
\]

According to (3.16), (3.19) and \( L\Phi^n \neq 0 \), there exists \( \tau^* > 0 \) such that \( \beta_n > 0, \beta_n^2 - \alpha_n \delta_n > 0 \) for all \( \tau \in (0, \tau^*) \), which makes \( \lambda_n \) well-defined. In addition, we can derive from Eqs. (3.16), (3.18) and (3.19)

\[
\lambda_n = O(\tau^{p+1}).
\]

Therefore, Scheme 3.2 has at least order \( p \).

By a direct calculation, the discrete energy conservation (3.13) is readily proved by following the projection step (3.11). This completes the proof.
Remark 3.4. For general conservation system, the energy $H = \frac{1}{2}(\Phi, L\Phi)$ is generally nonzero, which implies $L\Phi \neq 0$. If $\beta_n$ is calculated to be zero or $\beta_n^2 - \alpha_n\delta_n \leq 0$, the time step $\tau$ needs to be reduced to recalculate $\tilde{\Phi}^{n+1}$ so that $\beta_n > 0, \beta_n^2 - \alpha_n\delta_n > 0$.

Remark 3.5. In this paper, we focus on the case that the operator $L$ is self-adjoint and positive definite so that the energy $H$ is bounded. In this case, the developed energy-preserving methods may produce some unexpected nonlinear stability. In addition, we give numerical examples in a classical RK method of order 4, where their coefficients are given by the following Butcher table

\[
\begin{array}{c|ccc}
0 & 1/2 & 1/2 \\
1/2 & 0 & 1/2 \\
1 & 0 & 0 & 1 \\
\hline
1/6 & 2/6 & 2/6 & 1/6
\end{array}
\]

The standard Fourier pseudo-spectral method is employed for spatial discretization, which is omitted here due to space limitation. Interested readers are referred to Refs. [14, 40] for details.

4 Numerical results

In the previous sections, we present some explicit high-order energy-preserving schemes for general Hamiltonian PDEs. In this section, we apply the proposed Schemes 3.1 and 3.2 to solve two benchmark Hamiltonian PDE systems, the nonlinear Schrödinger (NLS) equation and the sine-Gordon (SG) equation, respectively.

4.1 Nonlinear Schrödinger equation

We consider the two dimensional nonlinear Schrödinger equation given as follows

\[ i\partial_t u + \Delta u + \beta |u|^2 u = 0, \quad (4.1) \]

where $i = \sqrt{-1}$ is the complex unit, $u$ is the complex-valued wave function, $\Delta$ is the usual Laplace operator, and $\beta$ is a given real constant.

If we suppose $u = p + iq$, the nonlinear Schrödinger equation (4.1) is rewritten into

\[
\begin{align*}
\partial_t p &= -\Delta q - \beta(p^2 + q^2)q, \\
\partial_t q &= \Delta p + \beta(p^2 + q^2)p.
\end{align*}
\]

(4.2)

Denoting $\Phi = \begin{pmatrix} p \\ q \end{pmatrix}$, then the system (4.2) is equivalently transformed into the system (2.5) with a quadratic invariant

\[ H = \frac{1}{2}\|\Phi\|^2 = \frac{1}{2}(\|p\|^2 + \|q\|^2), \quad (4.3) \]

and a structure matrix operator

\[ G(\Phi) = \begin{pmatrix} \Delta + \beta(p^2 + q^2) & -\Delta - \beta(p^2 + q^2) \\
\Delta + \beta(p^2 + q^2) & \Delta - \beta(p^2 + q^2) \end{pmatrix}. \]

Applying Scheme 3.1 to system (4.2), we obtain

**Scheme 4.1.** For given $(p^n, q^n)$, $(p^{n+1}, q^{n+1})$ is calculated by the following two steps

0. \quad \begin{align*}
\partial_t p &= -\Delta q - \beta(p^2 + q^2)q, \\
\partial_t q &= \Delta p + \beta(p^2 + q^2)p.
\end{align*}

1. \quad \begin{align*}
p^{n+1} &= p^n + \tau G(p^n)q^n, \\
q^{n+1} &= q^n + \tau G(q^n)p^n.
\end{align*}
1. Explicit RK: we compute \((\tilde{p}^{n+1}, \tilde{q}^{n+1})\) using

\[
\begin{align*}
P_1 &= p^n, \quad P_i = p^n + \tau \sum_{j=1}^{i-1} a_{ij} k_j, \\
Q_1 &= q^n, \quad Q_i = q^n + \tau \sum_{j=1}^{i-1} a_{ij} l_j, \\
k_i &= -\Delta Q_i - \beta (P_i^2 + Q_i^2) Q_i, \\
l_i &= \Delta P_i + \beta (P_i^2 + Q_i^2) P_i, \\
\tilde{p}^{n+1} &= p^n + \tau \sum_{i=1}^{s} b_i k_i, \\
\tilde{q}^{n+1} &= q^n + \tau \sum_{i=1}^{s} b_i l_i,
\end{align*}
\]

(4.4)

where \(b_i, a_{ij}\) are RK coefficients.

2. Projection: we update \((p^{n+1}, q^{n+1})\) via

\[
\begin{align*}
p^{n+1} &= \sqrt{\|p^n\|^2 + \|q^n\|^2} \tilde{p}^{n+1}, \\
q^{n+1} &= \sqrt{\|p^n\|^2 + \|q^n\|^2} \tilde{q}^{n+1}.
\end{align*}
\]

(4.5)

First of all, we present the time mesh refinement tests to show the order of accuracy of the proposed schemes. Also, the following high-order schemes for preserving the discrete quadratic energy are chosen for comparisons:

- 4th-order GM: the 2-stage Gauss method described in Refs. [38, 39];
- 4th-order PM: the projection method for quadratic invariants proposed in Refs. [9, 46].

As a summary, the properties of these schemes have been given in Tab. 1.

**Table. 1: Comparison of properties of different numerical schemes**

| Property                        | Scheme                  | 4th-order GM | 4th-order PM | The proposed method |
|---------------------------------|-------------------------|--------------|--------------|---------------------|
| Conserving quadratic energy     | Yes                     | Yes          | Yes          | Yes                 |
| Temporal accuracy               | 4th                     | 4th          | 4th          |                     |
| Explicit                        | No                      | Yes          | Yes          |                     |

The two dimensional nonlinear Schrödinger equation (4.1) possesses the following analytical solution

\[
u(x, y, t) = A \exp(i(k_1 x + k_2 y - \omega t)), \quad \omega = k_1^2 + k_2^2 - \beta |A|^2.
\]

(4.6)

Here we use computational domain \(\Omega = [0, 2\pi]^2\) and choose parameters \(A = 1, k_1 = k_2 = 1\) and \(\beta = -2\). To test the temporal discretization errors of the three numerical schemes, we fix the Fourier node \(32 \times 32\) such that the spatial discretization errors are negligible.

The \(L^2\) errors and \(L^\infty\) errors in numerical solution of \(u\) at \(t = 1\) are calculated using three different numerical schemes with various time steps, and the results are displayed.
in Fig. 1. In Fig. 2, we show the global $L^2$ errors and $L^\infty$ errors of $u$ versus the CPU time using the three different schemes at $t = 1$. From Figs. 1 and 2 we can draw the following observations: (i) all methods have fourth order accuracy in time; (ii) the error provided by the 4th-order GM is smallest, and the one provided by the proposed scheme has the same order of magnitude as the one of the 4th-order PM; (iii) for a given global error, the cost of 4th-order GM is most expensive while the one of our scheme is cheapest.

To further investigate the energy-preservation of the proposed scheme, we provide the energy errors using the three numerical schemes for the two dimensional Schrödinger equation over the time interval $t \in [0, 100]$ in Fig. 3, which shows that all three methods can exactly preserve the quadratic invariant (4.3), the 4th-order GM admits smallest energy error, and the error provided by the proposed scheme is much smaller than the one of the 4th-order PM.

![Fig. 1: Time step refinement tests using the three numerical schemes for the Schrödinger equation.](image)

![Fig. 2: The numerical error versus the CPU time using the three numerical schemes for the Schrödinger equation.](image)
Fig. 3: The energy deviation using the three numerical schemes with time step $\tau = 0.01$ and spatial step $h = \frac{\pi}{8}$ for the two dimensional Schrödinger equation.

### 4.2 Sine-Gordon equation

In this subsection, we focus on the sine-Gordon equation given as follows

$$\partial_{tt} u - \Delta u + \sin(u) = 0,$$  \hspace{1cm} (4.7)

where the Hamiltonian energy functional is given by

$$\mathcal{H} = \frac{1}{2} ( ||v||^2 + (u, -\Delta u) + 2(1 - \cos(u), 1)).$$  \hspace{1cm} (4.8)

We let $q = \sqrt{2 \left( (1 - \cos(u)) + \frac{C_0}{||\Omega||} \right)}$, and rewrite the Hamiltonian energy functional as

$$\mathcal{H} = \frac{1}{2} ( ||v||^2 + (u, -\Delta u) + ||r||^2) - C_0.$$  \hspace{1cm} (4.9)

According to the IEQ reformulation, we obtain the following equivalent system

$$\begin{cases}
\partial_t u = v, \\
\partial_t v = \Delta u - \frac{\sin(u)q}{\sqrt{2 \left( (1 - \cos(u)) + \frac{C_0}{||\Omega||} \right)}}, \\
\partial_t q = \frac{\sin(u)\partial_t u}{\sqrt{2 \left( (1 - \cos(u)) + \frac{C_0}{||\Omega||} \right)}}.
\end{cases}$$  \hspace{1cm} (4.10)

with the consistent initial condition

$$\begin{cases}
u(t = 0) = u_0, \\
q(t = 0) = \sqrt{2 \left( (1 - \cos(u_0)) + \frac{C_0}{||\Omega||} \right)}.
\end{cases}$$  \hspace{1cm} (4.11)

Supposing $\Phi = \begin{pmatrix} u \\ v \\ q \end{pmatrix}$, then the system (4.10) is equivalently reformulated into the system (3.1) with a quadratic energy

$$\mathcal{H} = \frac{1}{2} (\Phi, \mathcal{L}\Phi), \quad \mathcal{L} = \begin{pmatrix} -\Delta & 1 \\ 1 & 1 \end{pmatrix}.$$  \hspace{1cm} (4.12)
and a modified structure matrix

\[
\mathcal{G}(\Phi) = \begin{pmatrix}
0 & 1 & 0 & 0 \\
-1 & 0 & \frac{-\sin(u)}{\sqrt{2}} & \sqrt{2}\left(1 - \cos(u) + \frac{c_0}{|\Omega|}\right) \\
0 & \frac{\sin(u)}{\sqrt{2}} & (1 - \cos(u)) + \frac{c_0}{|\Omega|} & 0
\end{pmatrix}.
\]

Applying Scheme 3.2 to system (4.11), we have

**Scheme 4.2.** For given \((u^n, v^n, q^n)\), \((u^{n+1}, v^{n+1}, q^{n+1})\) is calculated by the following two steps:

1. **Explicit RK:** we compute \((\tilde{u}^{n+1}, \tilde{v}^{n+1}, \tilde{q}^{n+1})\) using

\[
\begin{align*}
U_1 &= u^n, \quad U_i = u^n + \tau \sum_{j=1}^{i-1} a_{ij} k_j, \\
V_1 &= v^n, \quad V_i = v^n + \tau \sum_{j=1}^{i-1} a_{ij} l_j, \\
Q_1 &= q^n, \quad Q_i = q^n + \tau \sum_{j=1}^{i-1} a_{ij} m_j, \\
k_i &= V_i, \\
l_i &= \Delta U_i - \frac{\sin(U_i) Q_i}{\sqrt{2}\left(1 - \cos(U_i) + \frac{c_0}{|\Omega|}\right)},
\end{align*}
\]

\[
\begin{align*}
\tilde{u}^{n+1} &= u^n + \tau \sum_{i=1}^{s} b_i k_i, \\
\tilde{v}^{n+1} &= v^n + \tau \sum_{i=1}^{s} b_i l_i, \\
\tilde{q}^{n+1} &= q^n + \tau \sum_{i=1}^{s} b_i m_i,
\end{align*}
\]

where \(b_i, a_{ij}\) are RK coefficients.

2. **Projection:** we update \((u^{n+1}, v^{n+1}, q^{n+1})\) via

\[
\begin{align*}
u^{n+1} &= \tilde{u}^{n+1} + \lambda_n (-\Delta \tilde{u}^{n+1}), \\
v^{n+1} &= \tilde{v}^{n+1} + \lambda_n \tilde{v}^{n+1}, \\
q^{n+1} &= \tilde{q}^{n+1} + \lambda_n \tilde{q}^{n+1},
\end{align*}
\]

where \(\lambda_n\) is given by (3.12).

We repeat the time step refinement test first and choose the parameter \(C_0 = 1\). The one dimensional sine-Gordon equation (4.7) admits the analytical solution

\[
u(x, t) = 4 \arctan(t \text{sech}(x)).
\]
We set computational domain $\Omega = [-50, 50]$ with a periodic boundary. The $L^2$ errors and $L^\infty$ errors of $u$ using the three schemes (see Table 1), spatial step $h = \frac{25}{128}$ and various time steps are showed in Fig. 4. Moreover, we plot the global $L^2$ errors and $L^\infty$ errors of $u$ versus the the CPU time using the different schemes and the spatial step $h = \frac{25}{1024}$ in Fig. 5. Here we observe similar results, i.e., all methods have fourth order accuracy in time errors, the error provided by the 4th-order GM is smallest, and our scheme admits much smaller error than the 4th-order PM. Analogously, for a given global error, our scheme is computationally cheapest and the 4th-order GM is most expensive. In Fig. 6, we display the errors of the quadratic energy (4.12) for the one dimensional sine-Gordon equation over the time interval $t \in [0, 1000]$, which behaves similarly as that of Fig. 3.
Next, we apply the proposed scheme to simulate the collision of four ring solitons for the two dimensional sine-Gordon equation with initial conditions given as follows \[41\]

\[
\begin{align*}
 u(x, y, 0) &= 4 \tan^{-1}\left[ \exp\left( \frac{4 - \sqrt{(x + 3)^2 + (y + 7)^2}}{0.436} \right) \right], \\
 u_t(x, y, 0) &= \frac{4.13}{\cosh\left( \frac{4 - \sqrt{(x+3)^2+(y+7)^2}}{0.436} \right)}, \quad (x, y) \in \Omega.
\end{align*}
\]

We choose the computational domain as \( \Omega = [-30, 10]^2 \) and a periodic boundary condition. The collision precisely among four expanding circular ring solitons are summarized in Fig. 7 showing a strong agreement with the existing results presented in Ref. \[41\]. Here, one should notice that the numerical solutions includes the extension across \( x = -10 \) and \( y = -10 \) by symmetry properties of the problem. The corresponding errors of the quadratic energy \(4.12\) over the time interval \( t \in [0, 100] \) are calculated with different schemes and the results are summarized in Fig. 8 which behaves similarly as those given in Figs. 3 and 6.
Fig. 7: The profile of $\sin(u/2)$ at $t = 0, 2.5, 5, 7.5$ and 10 using time step $\tau = 0.1$ and spatial step $h = 0.2$ with the proposed scheme.

Fig. 8: The energy deviation with the three numerical schemes for the two dimensional sine-Gordon equation.

5 Concluding remarks

In this paper, we have presented a new systematic and unified way to develop explicit high-order energy-preserving methods for general Hamiltonian PDEs by combining the orthogonal projection method with the explicit RK methods. Numerical examples are addressed to illustrate the accuracy, CPU time and invariants-preservation of the proposed methods. Compared with the two existing energy-preserving schemes of same order, the proposed high-order schemes show remarkable efficiency.

We conclude this paper with some remarks. First, compared with the incremental direction method proposed in Ref. [9], the proposed method required to evaluate the gradient of the energy, and can not preserve linear invariants and affine invariants, however, for the quadratic invariant, the analytical expression of the gradient for the invariant is easily obtained and numerical results show the computation cost of our method is much cheaper than the incremental direction method. In addition, the expression of
the Lagrange multiplier $\lambda_n$ (see (3.12)) is more concise. Second, the proposed method might not work well for highly unstable systems, thus, implicit projections (e.g., see Ref. [5]) become necessary. However, such trade-offs among methods should be further investigated. Finally, for several invariants, the Lagrange multiplier of the proposed projection can not be explicitly obtained. Thus, a possible future work is to develop explicit high-order multiple invariants-preserving methods.

Acknowledgments

Chaolong Jiang’s work is partially supported by the National Natural Science Foundation of China (Grant No. 11901513), the Yunnan Provincial Department of Education Science Research Fund Project (Grant No. 2019J0956) and the Science and Technology Innovation Team on Applied Mathematics in Universities of Yunnan. Yushun Wang’s work is partially supported by the National Natural Science Foundation of China (Grant No. 11771213). Yuezheng Gong’s work is partially supported by the Natural Science Foundation of Jiangsu Province (Grant No. BK20180413) and the National Natural Science Foundation of China (Grant No. 11801269).

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