High-order mass- and energy-conserving SAV–Gauss collocation finite element methods for the nonlinear Schrödinger equation

Xiaobing Feng∗  Buyang Li†  Shu Ma†

Abstract

A family of arbitrarily high-order fully discrete space-time finite element methods are proposed for the nonlinear Schrödinger equation based on the scalar auxiliary variable formulation, which consists of a Gauss collocation temporal discretization and the finite element spatial discretization. The proposed methods are proved to be well-posed and conserving both mass and energy at the discrete level. An error bound of the form \(O(h^p + \tau^{k+1})\) in the \(L^\infty(0,T;H^1)\)-norm is established, where \(h\) and \(\tau\) denote the spatial and temporal mesh sizes, respectively, and \((p,k)\) is the degree of the space-time finite elements. Numerical experiments are provided to validate the theoretical results on the convergence rates and conservation properties. The effectiveness of the proposed methods in preserving the shape of a soliton wave is also demonstrated by numerical results.

Key words: Nonlinear Schrödinger equation, mass- and energy-conservation, high-order conserving schemes, SAV-Gauss collocation finite element method, error estimates.

1 Introduction

This paper is concerned with the development and analysis of high-order fully discrete numerical methods for the following initial-boundary value problem of the nonlinear Schrödinger (NLS) equation:

\[
\begin{align*}
    i\partial_t u - \Delta u - f(|u|^2)u &= 0 & &\text{in } \Omega \times (0,T], \quad (1.1a) \\
    u &= 0 & &\text{on } \partial\Omega \times (0,T], \quad (1.1b) \\
    u &= u_0 & &\text{in } \Omega \times \{0\}, \quad (1.1c)
\end{align*}
\]

where \(\Omega \subset \mathbb{R}^d\) is a polygonal or polyhedral domain with boundary \(\partial\Omega\), and \(u : \Omega \to \mathbb{C}\) is a complex-valued function, with \(i = \sqrt{-1}\), and \(f : \mathbb{R}_+ \to \mathbb{R}\) is the derivative of some function \(F : \mathbb{R}_+ \to \mathbb{R}\). The best known examples are

\[
f(s) = \pm s^{\frac{q+1}{2}} \quad \text{and} \quad F(s) = \pm \frac{2}{q+1} s^{\frac{q+1}{2}}, \quad \text{with} \quad q > 1,
\]

where the “−” and “+” cases are often referred to as defocusing and focusing models, respectively. In the focusing case, the solution will blow up in \(L^\infty(\Omega)\) within finite time when the

∗Department of Mathematics, The University of Tennessee, Knoxville, TN 37996, U.S.A. Email address: xfeng@math.utk.edu. The work of this author was partially supported by the NSF-grant DMS-1620168.

†Department of Applied Mathematics, The Hong Kong Polytechnic University, Hung Hom, Kowloon, Hong Kong. Email address: buyang.li@polyu.edu.hk, maisie.ma@connect.polyu.hk. The work of B. Li was partially supported by a Hong Kong RGC grant (project ID: P0031035 ZZKQ) and the work of S. Ma was partially supported by a Hong Kong RGC grant (Project No. 15300817).
initial energy is negative; see [8, 36]. The NLS equation (1.1) arises from many applications in physics and engineering, and is one of the fundamental equations in mathematical physics [8, 36, 44, 27, 30].

It is well known that the solutions of (1.1) conserve the mass and energy in the sense that for all \( t \geq 0 \)

\[
\frac{d}{dt} \int_{\Omega} |u|^2 dx = 0, \quad \text{(mass conservation)} \tag{1.3}
\]

\[
\frac{d}{dt} \int_{\Omega} \left( \frac{1}{2} |\nabla u|^2 - \frac{1}{2} F(|u|^2) \right) dx = 0. \quad \text{(energy conservation)} \tag{1.4}
\]

The development of numerical methods that can retain these conservation properties in numerical solutions is important for long-time numerical simulation, and therefore has been one of the research focuses in numerical approximation to the NLS equation.

There exists a large amount of literature on numerical solutions and numerical analysis of the NLS equation. Delfour et al. [11] proposed a second-order modified Crank–Nicolson scheme for the NLS equation to preserve both mass and energy conservations. The construction of this method was motivated by a similar scheme for the Klein–Gordon equation in [34]. Sanz-Serna [28] extended the modified Crank–Nicolson time-stepping scheme to the NLS equation with more general nonlinear term, and established an optimal order error estimate for the fully discrete finite element discretization. For the cubic NLS equation, more delicate results on the existence, uniqueness and convergence of numerical solutions of the modified Crank–Nicolson scheme were proved by Akrivis et al. in [1]. The modified Crank–Nicolson scheme has been widely used in computation and was combined with spatial finite difference methods to solve the NLS and Gross–Pitaevskii equations in [2, 4, 5, 6], and with various spatial discretization methods to approximate the NLS in [37, 21, 25, 39, 14]. Besides the modified Crank–Nicolson scheme, a second order explicit leapfrog scheme for the NLS equation was proposed by Sanz-Serna and Manoranjan in [29]. This scheme was proved to preserve mass conservation at the discrete level. Optimal rates of convergence of the fully discrete leapfrog finite element method was established in [28]. To avoid solving nonlinear systems, a linearly implicit leapfrog scheme was proposed by Fei et al. in [45] for the NLS equation, and a linearly implicit relaxation scheme was proposed by Besse in [7]. Both schemes preserve mass and energy conservations at the discrete level. More recently, Feng et al. [13] constructed a class of second-order mass- and energy-conserving schemes for the NLS equation, including the modified Crank–Nicolson method, the implicit leapfrog method and a class of modified backward differentiation formulae as special cases.

To the best of our knowledge, all the existing mass- and energy-conserving methods have only second-order accuracy in time. No higher-order time-stepping schemes, which conserve both mass and energy, have been reported in the literature. Moreover, the existing error estimates for nonlinearly implicit schemes for the NLS equation generally require certain grid-ratio conditions. The standard grid-ratio conditions in the literature are \( \tau = o(h^2) \) for the cubic NLS equation and \( \tau = o(h^4) \) for general nonlinearity, where \( h \) and \( \tau \) denote the spatial and temporal mesh sizes. Karakashian and Makridakis [22, 23] proposed some continuous and discontinuous space-time Galerkin finite element methods for the cubic NLS equation and proved optimal-order convergence under a weaker grid-ratio condition \( \tau^{k-1} \ln h \to 0 \) in two dimensions, where \( k \geq 2 \) is the degree of finite elements in time. For the defocusing cubic NLS equation (or the focusing cubic NLS equation with sufficiently small initial data), using the energy conservation of the numerical scheme, error estimates were established without grid-ratio condition in [17, 38]. For
general nonlinearity (possibly focusing), Wang [37] established an error estimate for a linearized semi-implicit scheme without grid-ratio condition; Henning and Peterseim [20] established an error estimate for the nonlinearly implicit Crank–Nicolson finite element method without grid-ratio condition. Both [37] and [20] used an error splitting technique in which they proved boundedness of the numerical solutions by establishing an $L^\infty$-norm error estimate between the fully discrete and the semidiscrete-in-time numerical solutions. The error splitting technique allows to avoid grid-ratio conditions in using the inverse inequality.

The objective of this paper is to develop a family of arbitrarily higher-order mass- and energy-conserving fully discrete space-time finite element methods based on the scalar auxiliary variable (SAV) formulation of the NLS equation, and to establish the existence, uniqueness and optimal order convergence of numerical solutions without grid-ratio condition. Two key ideas are utilized in our construction of the method. First, the SAV reformulation of the NLS equation is used. This approach was introduced in [32, 31] as an enhanced version of the invariant energy quadratization (IEQ) approach [40, 41, 42, 43], for developing energy-decay methods for dissipative (gradient flow) systems. Here we adapt the SAV approach to the dispersive NLS equation, and the SAV reformulation is essential to enable our methods to maintain the energy conservation property at the discrete level. Second, the Gauss collocation method is used for time discretization in the SAV formulation of the NLS equation. The method can be viewed as an efficient implementation of the space-time finite element methods for the SAV formulation with Gauss quadrature in time. The Gauss collocation method was combined with IEQ and SAV to preserve energy decay in solving phase field equations in [3, 18, 19]. We adopt this method here to preserve mass conservation without affecting the energy conservation structure of the SAV formulation.

The SAV formulation introduces new difficulties to error analysis for the NLS equation due to the presence of $\partial_t u$ in the equation of $r$, see equation (2.6b), which leads to a consistency error of sub-optimal order in time and introduces new difficulty in obtaining the stability estimate. As far as we know, rigorous analysis for convergence of numerical methods based on SAV formulations has not been done for any wave equation so far. These difficulties are overcome by combining three techniques. First, inspired by the error analysis of Karakashian and Makridakis [23], our proof makes use of properties of the Legendre polynomials on each interval $I_n$, rewriting the Gauss collocation method into a space-time Galerkin finite element method, which makes it easier to choose suitable test functions in the error estimation. Second, we introduce a temporal Ritz projection and use a super-approximation result of the temporal local $L^2$ projection to eliminate the sub-optimal temporal consistency error caused by $\partial_t u$ in the equation of $r$; see Remark 3.1 (hence, the proof of optimal order in Theorem 3.3 is one of our main contributions). Third, we estimate the time derivative of the error in $H^{-1}(\Omega)$ with a duality argument following an $H^1$-norm error estimate. As a result, we obtain an optimal-order $H^1$-norm error estimate in the end. We prove the existence, uniqueness and optimal-order convergence of numerical solutions based on Schaefer’s fixed point theorem in an $L^\infty$-neighborhood of the exact solution. This avoids grid-ratio conditions for the NLS equation with general nonlinearity.

The rest of this paper is organized as follows. In Section 2, we present the SAV reformulation of the NLS equation and introduce our SAV space-time Gauss collocation finite element method. In Section 3, we first present an integral reformulation of the proposed numerical method and then establish its mass and energy conservation properties. We also derive a consistency error estimate for the proposed method, which is vitally used to prove an error estimate in the subsequent section. In Section 4, we first establish the well-posedness of the numerical method
and then prove an error bound of the form \(O(h^p + \tau^{k+1})\) in the energy norm, where \(\tau\) and \(h\) denote the temporal and spatial mesh sizes, respectively, with \((p,k)\) denoting the degree of polynomials in the space-time finite element method. Finally, in Section 5, we present a few numerical experiments to validate the theoretical results, and to demonstrate the effectiveness of the proposed method in preserving the shape of a soliton wave.

Throughout this paper, unless stated otherwise, \(C\) will be used to denote a generic positive constant which is independent of \(\tau\), \(h\), \(n\) and \(N\), but may depend on \(T\) and the regularity of solution.

2 Formulation of the SAV–Gauss collocation finite element method

In this section, we construct a Gauss collocation finite element method based on the SAV reformulation of the NLS equation, and prove some desired properties of the numerical method, including the mass and energy conservation.

2.1 Function spaces

Let \(H^k(\Omega)\), \(k \geq 0\), be the conventional complex-valued Sobolev space of functions on \(\Omega\), and denote

\[
L^2(\Omega) = H^0(\Omega) \quad \text{and} \quad H^1_0(\Omega) = \{v \in H^1(\Omega) : u = 0 \text{ on } \partial \Omega\}.
\]

We denote by \((\cdot, \cdot)\) and \(\|\cdot\|\) the inner product and norm of the complex-valued Hilbert space \(L^2(\Omega)\), respectively, defined by

\[
(u, v) := \int_\Omega u \overline{v} \text{d}x \quad \text{and} \quad \|u\| := \sqrt{(u, u)}.
\]

For \(m, s \geq 0\) and \(1 \leq p \leq \infty\), the notation \(W^{m,p}(0, T; H^s(\Omega))\) stands for the space-time Sobolev space of functions which are \(W^{m,p}\) in time and \(H^s\) in space; see [12, Chapter 5.9]. We abbreviate the norms of \(H^s(\Omega)\) and \(W^{m,p}(0, T; H^s(\Omega))\) as \(\|\cdot\|_{H^s}\) and \(\|\cdot\|_{W^{m,p}(0, T; H^s)}\), respectively, omitting the dependence on \(\Omega\) in the subscripts.

2.2 The SAV reformulation of (1.1)

The SAV formulation of the NLS equation (cf. [31]) introduces a scalar auxiliary variable

\[
r = \sqrt{\int_\Omega \frac{1}{2} F(|u|^2) \text{d}x + c_0} \quad \text{with} \quad g(u) = \frac{f(|u|^2)}{\sqrt{\int_\Omega \frac{1}{2} F(|u|^2) \text{d}x + c_0}},
\]

with a positive \(c_0\) (which guarantees that the function \(r\) has a positive lower bound), and reformulate (1.1) as

\[
\begin{align*}
i \partial_t u - \Delta u - rg(u)u &= 0 \quad \text{in } \Omega \times (0, T], \quad (2.6a) \\
\frac{\text{d}r}{\text{d}t} &= \text{Re}(\frac{1}{2}g(u)u, \partial_t u) \quad \text{in } \Omega \times (0, T], \quad (2.6b) \\
u &= 0 \quad \text{on } \partial \Omega \times (0, T], \quad (2.6c) \\
u &= u_0, \quad r = r_0 \quad \text{in } \Omega \times \{0\}, \quad (2.6d)
\end{align*}
\]
where \( r_0 = \sqrt{\int_\Omega \frac{1}{2} F(|u_0|^2)dx + c_0} \). The mass and energy conservation in the SAV formulation are

\[
\frac{d}{dt} \int_\Omega |u|^2 dx = 0, \quad \text{and} \quad \frac{d}{dt} \left( \frac{1}{2} \int_\Omega |\nabla u|^2 dx - r^2 \right) = 0. \tag{2.7}
\]

### 2.3 Space-time finite element spaces

Let \( \mathcal{T}_h \) be a shape-regular and quasi-uniform triangulation of \( \Omega \) with mesh size \( h \in (0,1) \) and \( \{t_n\}_{n=0}^N \) be a uniform partition of \([0,T]\) with the time step size \( \tau \in (0,1) \), where \( N \) is a positive integer and hence \( \tau = \frac{T}{N} \). For an integer \( p \geq 1 \) we denote by \( \mathbb{Q}^p \) the space of complex-valued polynomials of degree \( \leq p \) in space, and we denote by \( S_h \) the complex-valued Lagrange finite element space subject to the triangulation of \( \Omega \), defined by

\[
S_h = \{ v \in C(\overline{\Omega}) : v|_K \in \mathbb{Q}^p \text{ for all } K \in \mathcal{T}_h, \ v = 0 \text{ on } \partial \Omega \},
\]

where \( C(\overline{\Omega}) \) denotes the space of complex-valued uniformly continuous functions on \( \Omega \). Then \( S_h \) is a complex Hilbert spaces with the inner product \( (\cdot, \cdot) \) and norm \( \| \cdot \| \).

For an integer \( k \geq 1 \), let \( \mathbb{P}^k \) denote the space of real-valued polynomials of degree \( \leq k \) in \( t \). For a Banach space \( X \), such as \( X = L^2(\Omega) \) or \( X = S_h \), we define the following tensor-product space:

\[
\mathbb{P}^k \otimes X := \text{span} \left\{ p(t)\phi(x) : p \in \mathbb{P}^k, \phi \in X \right\} = \left\{ \sum_{j=0}^k t^j \phi_j : \phi_j \in X \right\}. \tag{2.8}
\]

Moreover, let \( P_h : L^2(\Omega) \to S_h \) denote the \( L^2 \) projection operator defined by

\[
(w - P_h w, v_h) = 0 \quad \forall v_h \in S_h, \ \forall w \in L^2(\Omega).
\]

The following stability properties are well-known (cf. [9]):

\[
\|P_h w\| \leq \|w\| \quad \forall w \in L^2(\Omega), \tag{2.9a}
\]

\[
\|P_h w\|_{H^1} \leq C\|w\|_{H^1} \quad \forall w \in H^1(\Omega), \tag{2.9b}
\]

where \( C \) depends only on the shape-regularity and quasi-uniformity of the mesh.

We also introduce the global space-time finite element spaces

\[
X_{\tau,h} = \{ v_h \in C([0,T];S_h) : v_h|_{I_n} \in \mathbb{P}^k \otimes S_h \text{ for } n = 1, \ldots, N \}, \tag{2.10}
\]

\[
Y_{\tau,h} = \{ q_h \in C([0,T]) : q_h|_{I_n} \in \mathbb{P}^k \text{ for } n = 1, \ldots, N \}. \tag{2.11}
\]

### 2.4 SAV–Gauss collocation finite element method

Let \( c_j \) and \( w_j, j = 1, \ldots, k \), be the nodes and weights of the \( k \)-point Gauss quadrature rule in the interval \([-1,1]\) (see [33, Table 3.1]), and let \( t_{nj} = t_{n-1} + (1 + c_j)\tau/2, j = 1, \ldots, k \) denote the Gauss points in the interval \( I_n = [t_{n-1}, t_n] \). We define the following Gauss collocation finite element method for (2.6).

**Main Algorithm**

**Step 1:** Set \( u^0_h := I_h u_0 \) and \( r^0_h := r_0 \), where \( I_h \) is the Lagrange interpolation operator onto the finite element space. Determine \((u_h, r_h) \in X_{\tau,h} \times Y_{\tau,h}\) by the following two steps.
Step 2: For \( n = 1, 2, \cdots, N \), define \( \{ (u_h(t_{nj}), r_h(t_{nj})) \}_{j=1}^{k} \subset S_h \times \mathbb{R} \) by solving recursively (in \( n \)) the following nonlinear (algebraic) system:

\[
\begin{align*}
&(i) (\partial_t u_h(t_{nj}), v_h) + (\nabla u_h(t_{nj}), \nabla v_h) \\
&\quad - (r_h(t_{nj}) g(u_h(t_{nj}))(u_h(t_{nj}), v_h) = 0, \quad \forall v_h \in S_h, \tag{2.12a} \\
&\partial_t r_h(t_{nj}) = \frac{1}{2} \text{Re}(g(u_h(t_{nj}))(\partial_t u_h(t_{nj})), \tag{2.12b} \\
&u_h(t_{n-1}) = u_h^{n-1} \quad \text{and} \quad r_h(t_{n-1}) = r_h^{n-1}. \tag{2.12c}
\end{align*}
\]

Step 3: Set \( u_h^n := u_h(t_n) \) and \( r_h^n := r_h(t_n) \).

Remark 2.1 (a) We note that in (2.12a) and (2.12b), \( \partial_t u_h(t_{nj}) = \partial_t u_h(t)|_{t=t_{nj}} \) and \( \partial_t r_h(t_{nj}) = \partial_t r_h(t)|_{t=t_{nj}} \). Main Algorithm really computes \( \{ (u_h(t_{nj}), r_h(t_{nj})) \}_{j=1}^{k} \) for each \( n \geq 1 \), however, since any \( k \)th order polynomial on \( I_n \) is uniquely determined by its initial value at \( t_{n-1} \) and its values at the \( k \) Gauss points \( t_{nj}, j = 1, \ldots, k \), then the Gauss-point values generated by Main Algorithm uniquely determine the pair \( (u_h, r_h) \in X_{\tau,h} \times Y_{\tau,h} \).

(b) Each of (2.12a) and (2.12b) consists of nonlinear algebraic equations, note that the test functions \( v_h \) and \( q_h \) can be different for different \( j \), and one “side/initial condition” is prescribed for each of \( u_h \) and \( r_h \) for each \( n \). The number of equations imposed is the same as the degree of freedoms which equals the dimension of the space \( \mathbb{P}^k \otimes S_h \) for each \( n \).

(c) Main Algorithm can be obtained by applying the Gauss quadrature rule (in time) to a (continuous) space-time finite element method for (2.6). See Section 3.1.

3 Conservation, stability and consistency analysis

3.1 A reformulation of scheme (2.12a)–(2.12b)

In this subsection, we present several integral identities, including a reformulation of Main Algorithm, and inequalities related to the proposed numerical method. These identities and inequalities will be used in the subsequent analysis of existence, uniqueness and convergence of numerical solutions.

Consider the interval \( I_n = [t_{n-1}, t_n] \), then we define \( P^n_\tau : L^2(I_n; L^2(\Omega)) \to \mathbb{P}^{k-1} \otimes L^2(\Omega) \) to be the \( L^2 \) projection defined by

\[
\int_{I_n} (u - P_\tau^n u)v \, dt = 0 \quad \forall v \in \mathbb{P}^{k-1} \otimes L^2(\Omega). \tag{3.13}
\]

Thus \( u - P_\tau^n u \) is orthogonal to all temporal polynomials of degree \( \leq k - 1 \), which means that if \( u \in \mathbb{P}^k \otimes L^2(\Omega) \) then

\[
u - P_\tau^n u = \phi_{n-1} L_k, \tag{3.14}
\]

where \( \phi_{n-1} \in L^2(\Omega) \) and

\[
L_k(t) := \frac{2t - t_{n-1} - t_n}{\tau} \tag{3.15}
\]
is the shifted Legendre polynomial (orthogonal to polynomials of lower degree on $I_n$). The temporal $L^2$ projection operator $P^n_T$ has the following approximation property (cf. [10]):

$$
\max_{t \in I_n} \| v - P^n_T v \|_X \leq C \tau^m \max_{t \in I_n} \| \partial_t^m v \|_X, \quad 0 \leq m \leq k,
$$

(3.16)

for all $v \in C^k([0, T]; X)$, where $X = \mathbb{R}$ or $X = H^s(\Omega)$ for some $s \in \mathbb{R}$.

Since the $k$-point Gauss quadrature holds exactly for polynomials of degree $2k - 1$ (cf. [16, p. 222]), and the Gauss points $t_{nj}, j = 1, \ldots, k$, are the roots of the Legendre polynomial $L_k(t)$ (cf. [24, p. 33]), it follows that the following two identities hold:

$$
\int_{I_n} v(t) dt = \frac{\tau}{2} \sum_{j=1}^k v(t_{nj}) w_j \quad \forall v \in \mathbb{P}^{2k-1} \otimes S_h,
$$

(3.17)

$$
v(t_{nj}) = P^n_T v(t_{nj}) \quad \forall v \in \mathbb{P}^k \otimes S_h.
$$

(3.18)

By choosing $v_h = \frac{\tau}{2} v(t_{nj}) w_j$ in (2.12a) and summing up the results for $j = 1, \ldots, k$, and using (3.17)–(3.18) in the first two terms, we obtain the following integral identity:

$$
\int_{I_n} i (\partial_t u_h, v_h) dt + \int_{I_n} (\nabla P^n_T u_h, \nabla v_h) dt
\quad
- \frac{\tau}{2} \sum_{j=1}^k w_j (r_h(t_{nj}) g(u_h(t_{nj})) u_h(t_{nj}), v_h(t_{nj})) = 0 \quad \forall v_h \in \mathbb{P}^k \otimes S_h.
$$

(3.19)

Similarly, multiplying (2.12b) by $\frac{\tau}{2} q_h(t_{nj}) w_j$ and summing up the results for $j = 1, \ldots, k$, and using (3.17) in the first term, we have

$$
\int_{I_n} \partial_t q_h v_h dt = \frac{\tau}{2} \sum_{j=1}^k w_j \frac{\tau}{2} \left( \Re (g(u_h(t_{nj})) u_h(t_{nj}), \partial_t u_h(t_{nj}) q_h(t_{nj})) \right) \quad \forall q_h \in \mathbb{P}^k.
$$

(3.20)

(3.19)–(3.20) provides a reformulation of Main Algorithm. It will be crucially used to show mass and energy conservations, as well as existence, uniqueness and convergence of numerical solutions.

From (3.14) we get

$$
\| \phi_{n-1} \| = \frac{1}{|L_k(t_{n-1})|} \| u_h(t_{n-1}) - P^n_T u_h(t_{n-1}) \|
\leq C \| u_h(t_{n-1}) \| + C \left( \frac{1}{\tau} \int_{I_n} \| P^n_T u_h(t) \|^2 dt \right)^{\frac{1}{2}},
$$

where we have used the inverse inequality in time. Thus, by using (3.14) again, we obtain the following inequality:

$$
\int_{I_n} \| u_h \|^2 dt \leq C \int_{I_n} \| P^n_T u_h \|^2 dt + C \tau \| u_h(t_{n-1}) \|^2 \quad \forall u_h \in \mathbb{P}^k \otimes S_h.
$$

(3.21)

By using the two identities (3.17)–(3.18), one can also prove the following inequality:

$$
\frac{\tau}{2} \sum_{j=1}^k w_j \| v_h(t_{nj}) \|^2 = \int_{I_n} \| P^n_T v_h(t) \|^2 dt \leq \int_{I_n} \| v_h(t) \|^2 dt \quad \forall v_h \in \mathbb{P}^k \otimes S_h.
$$

(3.22)

The inequalities (3.21)–(3.22) will be frequently used in the subsequent error analysis.
3.2 Mass and energy conservation properties

In this subsection, we prove the following conservation properties of the numerical solution, which comprise of the first main theorem of this paper.

**Theorem 3.1** Let \((u_h, r_h) \in X_{\tau, h} \times Y_{\tau, h}\) be a solution of Main Algorithm, then the following mass and energy conservations hold:

\[
\begin{align*}
\frac{1}{2} \| u_h(t_n) \|^2 &= \frac{1}{2} \| u_h(t_0) \|^2 \quad \text{for } n \geq 1, \\
\frac{1}{2} \| \nabla u_h(t_n) \|^2 - |r_h(t_n)|^2 &= \frac{1}{2} \| \nabla u_h(t_0) \|^2 - |r_h(t_0)|^2 \quad \text{for } n \geq 1.
\end{align*}
\]

**Proof.** Setting \(v_h = u_h \in P^k \otimes S_h\) in (3.19) and taking the imaginary part yield

\[
\text{Im} \int_{I_n} i(\partial_t u_h, u_h) dt = -\text{Im} \int_{I_n} (\nabla P^n_{\tau} u_h, \nabla u_h) dt + \text{Im} \left[ \frac{\tau}{2} \sum_{j=1}^k w_j (r_h(t_{n_j}) g(u_h(t_{n_j})), |u_h(t_{n_j})|^2) \right] = 0,
\]

where we have used the definition of the projection operator \(P^n_{\tau}\), which implies

\[
\text{Im} \int_{I_n} (\nabla P^n_{\tau} u_h, \nabla u_h) dt = \text{Im} \int_{I_n} (\nabla P^n_{\tau} u_h, \nabla P^n_{\tau} u_h) dt = 0.
\]

Then the mass conservation follows from (3.23) and the identity

\[
\text{Im} \int_{I_n} i(\partial_t u_h, u_h) dt = \frac{1}{2} \| u_h(t_n) \|^2 - \frac{1}{2} \| u_h(t_{n-1}) \|^2.
\]

Alternatively, setting \(v_h = \partial_t u_h\) and \(q_h = 2r_h\) in (3.19) and (3.20), respectively, and taking the real parts yield

\[
\text{Re} \int_{I_n} (\nabla P^n_{\tau} u_h, \nabla \partial_t u_h) dt = \frac{\tau}{2} \text{Re} \sum_{j=1}^k w_j (r_h(t_{n_j}) g(u_h(t_{n_j})) u_h(t_{n_j}), \partial_t u_h(t_{n_j}))
\]

\[
|r_h(t_{n_j})|^2 - |r_h(t_{n_{j-1}})|^2 = \frac{\tau}{2} \text{Re} \sum_{j=1}^k w_j (r_h(t_{n_j}) g(u_h(t_{n_j})) u_h(t_{n_j}), \partial_t u_h(t_{n_j})).
\]

Since

\[
\text{Re} \int_{I_n} (\nabla P^n_{\tau} u_h, \nabla \partial_t u_h) dt = \text{Re} \int_{I_n} (P^n_{\tau} \nabla u_h, \nabla \partial_t u_h) dt = \text{Re} \int_{I_n} (\nabla u_h, \nabla \partial_t u_h) dt
\]

\[
= \frac{1}{2} \| \nabla u_h(t_n) \|^2 - \frac{1}{2} \| \nabla u_h(t_{n-1}) \|^2,
\]

it follows that

\[
\frac{1}{2} \| \nabla u_h(t_n) \|^2 - \frac{1}{2} \| \nabla u_h(t_{n-1}) \|^2 = \frac{\tau}{2} \text{Re} \sum_{j=1}^k w_j (r_h(t_{n_j}) g(u_h(t_{n_j})) u_h(t_{n_j}), \partial_t u_h(t_{n_j})).
\]
Subtracting (3.25) from (3.26) yields
\[ \frac{1}{2} \| \nabla u_h(t_n) \|^2 - |r_h(t_n)|^2 = \frac{1}{2} \| \nabla u_h(t_{n-1}) \|^2 - |r_h(t_{n-1})|^2 \quad \text{for } n \geq 1. \]  
(3.27)

Thus, the energy conservation holds. The proof is complete. \[ \square \]

### 3.3 An upper bound of mass at internal stages

In this subsection, we prove that the average mass of numerical solutions at internal stages has an upper bound unconditionally (independent of the regularity of solutions). This property furthermore strengthens the stability of numerical solutions when the exact solution is not smooth (for example, close to blow up).

**Theorem 3.2** Let \((u_h, r_h) \in X_{\tau, h} \times Y_{\tau, h}\) be a solution of Main Algorithm, then the following inequalities hold:

\[
\begin{align*}
\max_{1 \leq n \leq N} & \frac{1}{\tau} \int_{I_n} \| P^n_\tau u_h(t) \|^2 \, dt \leq \| u_h(0) \|^2, \quad (3.28a) \\
\max_{1 \leq n \leq N} & \max_{1 \leq j \leq k} \| u_h(t_{nj}) \| \leq C \| u_h(0) \|, \quad (3.28b)
\end{align*}
\]

where \(C\) is a constant independent of \(\tau, h\) and the regularity of the solution.

**Proof.** By the definition of the temporal \(L^2\) projection \(P^n_\tau\), we get

\[
\begin{align*}
\int_{I_n} \| P^n_\tau u_h(t) \|^2 \, dt &= \text{Re} \int_{I_n} (u_h(t), P^n_\tau u_h(t)) \, dt \\
&= \text{Re} \int_{I_n} (u_h(t_{n-1}), P^n_\tau u_h(t_{n-1})) \, dt \\
&\quad + \text{Re} \int_{I_n} \int_{t_{n-1}}^t \left[ (\partial_s u_h(s), P^n_\tau u_h(s)) + (u_h(s), \partial_s P^n_\tau u_h(s)) \right] ds \, dt \\
&= \text{Re} \int_{I_n} (u_h(t_{n-1}), P^n_\tau u_h(t_{n-1})) \, \tau + \text{Re} \int_{I_n} \int_{t_{n-1}}^{t_{n-1}} (\partial_t u_h(t), (t_n - t) P^n_\tau u_h(t)) \, dt \\
&\quad + \text{Re} \int_{I_n} (u_h(t), (t_n - t) \partial_t P^n_\tau u_h(t)) \, dt \\
&=: J_1 + J_2 + J_3,
\end{align*}
\]

where we have interchanged the order of integration in deriving the second to last equality. Using Hölder’s and Young’s inequalities, we have

\[
J_1 = \text{Re} (u_h(t_{n-1}), P^n_\tau u_h(t_{n-1})) \tau \leq \| u_h(t_{n-1}) \| \| P^n_\tau u_h(t_{n-1}) \| \tau \\
\leq \frac{\tau}{2} \| u_h(t_{n-1}) \|^2 + \frac{\tau}{2} \| P^n_\tau u_h(t_{n-1}) \|^2.
\]

Setting \(v_h = (t_n - t) P^n_\tau u_h\) in (3.19) and taking the imaginary part yield

\[
J_2 = \text{Re} \int_{I_n} \int_{t_{n-1}}^{t_{n-1}} (\partial_t u_h(t), (t_n - t) P^n_\tau u_h(t)) \, dt = \text{Im} \int_{I_n} (\partial_t u_h(t), (t_n - t) P^n_\tau u_h(t)) \, dt \\
= \text{Im} \tau \sum_{j=1}^k w_j (r_h(t_{nj}) g(u_h(t_{nj})), \| u_h(t_{nj}) \|^2) (t_n - t_{nj})
\]

9
-

\[ - \text{Im} \int_{I_n} \| \nabla P^n_\tau u_h \|^2 (t_n - t) \, dt = 0, \]

where we have used (3.18) in deriving the first term on the right-hand side. Since \((t_n - t) \partial_t P^n_\tau u_h(t)\) is a polynomial of degree \(k - 1\) in \(t\), it follows that

\[
\int_{I_n} (u_h(t), (t_n - t) \partial_t P^n_\tau u_h(t)) \, dt = \int_{I_n} (P^n_\tau u_h(t), (t_n - t) \partial_t P^n_\tau u_h(t)) \, dt.
\]

Hence,

\[
J_3 = \text{Re} \int_{I_n} (P^n_\tau u_h(t), (t_n - t) \partial_t P^n_\tau u_h(t)) \, dt = \int_{I_n} \frac{1}{2} \frac{d}{dt} \| P^n_\tau u_h(t) \|^2 (t_n - t) \, dt
\]

\[
= -\frac{\tau}{2} \| P^n_\tau u_h(t_{n-1}) \|^2 + \int_{I_n} \frac{1}{2} \| P^n_\tau u_h(t) \|^2 \, dt.
\]

Substituting the estimates of \(J_1, J_2\) and \(J_3\) into (3.29), we obtain

\[
\int_{I_n} \| P^n_\tau u_h \|^2 \, dt \leq \tau \| u_h(t_{n-1}) \|^2 = \tau \| u_h(0) \|^2,
\]

where the last equality follows from mass conservation proved in Theorem 3.1. This proves (3.28a) holds.

Substituting (3.30) into (3.21) and using the mass conservation again, we obtain \(\int_{I_n} \| u_h \|^2 \, dt \leq C \tau \| u_h(0) \|^2\). Then, by using the inverse inequality, we obtain

\[
\max_{t \in I_n} \| u_h(t) \| \leq C \| u_h(0) \|,
\]

which proves (3.28b). The proof is complete. \(\square\)

### 3.4 Temporal and spatial Ritz projections

Let \(P^n_\tau u\) and \(P^n_\tau r\) be the temporal Lagrange interpolation polynomials of \(u\) and \(r\), respectively, interpolated at the \(k + 1\) points \(t_{n-1}\) and \(t_{nj}, j = 1, \ldots, k\). Both \(P^n_\tau u\) and \(P^n_\tau r\) are temporal polynomials of degree \(\leq k\). The one-dimensional temporal Lagrange interpolation operator \(P^n_\tau\) has the following approximation property (cf. [10]):

\[
\max_{t \in I_n} (\| v - P^n_\tau v \|_X + \tau \| \partial_t (v - P^n_\tau v) \|_X) \leq C \tau^{m+1} \max_{t \in I_n} \| \partial_t^{m+1} v \|_X
\]

(3.31)

for all \(v \in C^{m+1}([0, T]; X), 0 \leq m \leq k\), and \(X = \mathbb{R}\) or \(X = H^s(\Omega)\) for some \(s \in \mathbb{R}\).

To analyze the error of numerical solutions due to temporal discretization, we define a temporal Ritz projection operator \(R^n_\tau : W^{1,\infty}(I_n; L^2(\Omega)) \rightarrow \mathbb{P}^k \otimes L^2(\Omega)\) by the following two conditions:

\[
\int_{I_n} (\partial_t (u - R^n_\tau u), v) \, dt = 0 \quad \forall \, v \in \mathbb{P}^{k-1} \otimes L^2(\Omega),
\]

(3.32)

\[
u(t_{n-1}) - R^n_\tau u(t_{n-1}) = 0.
\]

(3.33)

Clearly, \(\partial_t R^n_\tau u\) is the temporal \(L^2\) projection of \(\partial_t u\) onto \(\mathbb{P}^{k-1} \otimes L^2(\Omega)\). By using this property and the shifted Legendre polynomials defined in (3.15), we can express the temporal Ritz projection as

\[
R^n_\tau u(t) = u(t_{n-1}) + \sum_{j=0}^{k-1} \int_{I_n} L_j(s) \partial_s u(s) \, ds \int_{t_{n-1}}^t L_j(s) \, ds.
\]

(3.34)
This expression implies that if \( X \supset L^2(\Omega) \) is a Banach space and \( u \in W^{1,\infty}(I_n; X) \), then \( R^n u \) is automatically in \( \mathbb{P}^k \otimes X \). Meanwhile, this temporal Ritz projection has the following approximation property.

**Lemma 3.1** Let \( X = \mathbb{R} \) or \( H^s(\Omega) \) for some \( s \geq 0 \). For \( u \in W^{m+1,\infty}(I_n; X) \), with \( 0 \leq m \leq k \), the following approximation property holds:

\[
\|u - R^n u\|_{L^\infty(I_n; X)} + \tau \|\partial_t (u - R^n u)\|_{L^\infty(I_n; X)} \leq C \tau^{m+1} \|u\|_{W^{m+1,\infty}(I_n; X)}.
\]

**Proof.** We prove the result for the case \( X = H^s(\Omega) \) with \( s \geq 0 \). To this end, we denote by \( H^s(\Omega)' \) the dual space of \( H^s(\Omega) \). Then, by the Riesz representation theorem, there exists a continuous linear bijection \( J : H^s(\Omega)' \to H^s(\Omega) \) such that

\[
(u, Jv)_{H^s} = \langle u, v \rangle \quad \forall u \in H^s(\Omega) \text{ and } v \in H^s(\Omega)', \tag{3.35}
\]

where \( \langle \cdot, \cdot \rangle_{H^s} \) is the inner product of \( H^s(\Omega) \), and \( \langle \cdot, \cdot \rangle \) denotes the pairing between \( H^s(\Omega) \) and its dual space \( H^s(\Omega)' \), satisfying

\[
\langle w, v \rangle = \langle w, v \rangle \quad \forall w \in H^s(\Omega), \ v \in L^2(\Omega) \leftrightarrow H^s(\Omega)'.
\]

Then (3.32) implies that

\[
\int_{I_n} (\partial_t (u - R^n u), Jv)_{H^s} dt = 0 \quad \forall v \in \mathbb{P}^{k-1} \otimes L^2(\Omega). \tag{3.36}
\]

Since \( L^2(\Omega) \) is dense in \( H^s(\Omega)' \), it follows that (3.36) actually holds for all \( v \in \mathbb{P}^{k-1} \otimes H^s(\Omega)' \). Since for any \( w \in \mathbb{P}^{k-1} \otimes H^s(\Omega) \) there exists \( v \in \mathbb{P}^{k-1} \otimes H^s(\Omega)' \) satisfying \( Jv = w \), it follows that (3.36) can be equivalently written as

\[
\int_{I_n} (\partial_t (u - R^n u), w)_{H^s} dt = 0 \quad \forall w \in \mathbb{P}^{k-1} \otimes H^s(\Omega). \tag{3.37}
\]

By using the inverse inequality in time and the property (3.37), we have

\[
\|\partial_t (u - R^n u)\|_{L^\infty(I_n; H^s)} \leq C \tau^{-1} \int_{I_n} (\partial_t (u - R^n u), \partial_t (u - R^n u))_{H^s} dt \tag{3.38}
\]

\[
= C \tau^{-1} \int_{I_n} (\partial_t (u - R^n u), \partial_t (u - g))_{H^s} dt \leq C \|\partial_t (u - R^n u)\|_{L^\infty(I_n; H^s)} \|\partial_t (u - g)\|_{L^\infty(I_n; H^s)},
\]

where \( g \) can be an arbitrary function in \( \mathbb{P}^k \otimes H^s(\Omega) \), which implies \( \partial_t (g - R^n u) \in \mathbb{P}^{k-1} \otimes H^s(\Omega) \). The inequality above implies

\[
\|\partial_t (u - R^n u)\|_{L^\infty(I_n; H^s)} \leq C \inf_{g \in \mathbb{P}^k \otimes H^s(\Omega)} \|\partial_t (u - g)\|_{L^\infty(I_n; H^s)} \tag{3.39}
\]

\[
\leq C \|\partial_t (u - R^n u)\|_{L^\infty(I_n; H^s)}.
\]

This and the approximation property (3.31) together imply the following inequality:

\[
\|\partial_t (u - R^n u)\|_{L^\infty(I_n; H^s)} \leq C \tau^m \|u\|_{W^{m+1,\infty}(I_n; H^s)}. \tag{3.40}
\]
To estimate \( \|u - R^m_\tau u\|_{L^\infty(I_n;H^s)} \), we use a duality argument in time. Let \( w \in W^{1,\infty}(I_n;H^s(\Omega)) \) be the solution of the following IVP:

\[
\partial_t w(t) = u(t) - (R^m_\tau u)(t), \quad w(t_n) = 0.
\] (3.41)

Then, testing (3.41) by \( J^{-1}(u - R^m_\tau u) \), with the operator \( J \) defined in (3.35), we obtain

\[
\int_{I_n} \|u - R^m_\tau u\|_{H^s}^2 dt = \int_{I_n} (\partial_t w, u - R^m_\tau u)_{H^s} dt
= - \int_{I_n} (w, \partial_t (u - R^m_\tau u))_{H^s} dt
= - \int_{I_n} (w - I^m_\tau w, \partial_t (u - R^m_\tau u))_{H^s} dt \quad (\text{here (3.37) is used})
\leq C\tau \|w - I^m_\tau w\|_{L^\infty(I_n;H^s)} \|\partial_t (u - R^m_\tau u)\|_{L^\infty(I_n;H^s)}
\leq C\tau^{m+1} \|\partial_t w\|_{L^\infty(I_n;H^s)} \|u\|_{W^{m+1,\infty}(I_n;H^s)},
\]

where we have used (3.40) in the last inequality. By applying the temporal inverse inequality and (3.41), we have

\[
\|u - R^m_\tau u\|_{L^\infty(I_n;H^s)} \leq C\tau^{-m} \|u\|_{W^{m+1,\infty}(I_n;H^s)}.
\] (3.42)

This completes the proof of Lemma 3.1.

In addition to the above optimal-order approximation result, we also have the following super-convergence result.

**Lemma 3.2** (A super-approximation property) Let \( X = \mathbb{R} \) or \( H^s(\Omega) \) for some \( s \geq 0 \). If \( w \in W^{k,\infty}(I_n;W^{s,\infty}(\Omega)) \) and \( v \in \mathbb{P}^{k-1} \otimes X \), then

\[
\|wv - P^m_\tau(wv)\|_{L^2(I_n;X)} \leq C\tau \|v\|_{L^2(I_n;X)}.
\]

**Proof.** We only give a proof for the case \( X = H^s(\Omega) \) because the other cases are similar. By applying (3.16) with \( m = k \), we have

\[
\|wv - P^m_\tau(wv)\|_{L^2(I_n;H^s)} \leq C\tau^{k+\frac{1}{2}} \|wv - P^m_\tau(wv)\|_{L^\infty(I_n;H^s)}
\leq C\tau^{k+1} \|\partial^k_t (wv)\|_{L^\infty(I_n;H^s)}
\leq C \sum_{m=0}^{k-1} \tau^{k+m} \|\partial^{k-m}_t w \partial^m v\|_{L^\infty(I_n;H^s)} \quad (\text{since } \partial^k_t v = 0)
\leq C \sum_{m=0}^{k-1} \tau^{k+m} \|\partial^{k-m}_t w\|_{L^\infty(I_n;W^{s,\infty})} \|\partial^m v\|_{L^\infty(I_n;H^s)}
\]

12
and the discrete Laplacian operator $\Delta_h$ and (3.32), we can express these consistency errors by

$$d = C \sum_{m=0}^{k-1} \tau^{k+\frac{1}{2}-m} \|v\|_{L^\infty(I_n;H^s)}$$

$$\leq C \tau^2 \|v\|_{L^\infty(I_n;H^s)}$$

$$\leq C \tau \|v\|_{L^2(I_n;H^s)}.$$  

Here we have used the inverse inequality in time twice above. The proof is complete. \( \square \)

Finally, we also recall the (spatial) Ritz projection operator $R_h : H^1(\Omega) \to S_h$ defined by

$$(\nabla(w - R_h w), \nabla v_h) = 0 \quad \forall v_h \in S_h, \quad \forall w \in H^1_0(\Omega),$$

and the discrete Laplacian operator $\Delta_h : S_h \to S_h$ defined by

$$(\Delta_h \phi_h, \chi_h) := -(\nabla \phi_h, \nabla \chi_h) \quad \forall \phi_h, \chi_h \in S_h. \quad (3.44)$$

It is known [9] that there hold the following identities:

$$P_h \Delta v = \Delta_h R_h v \quad \forall v \in H^1_0(\Omega), \quad (3.45a)$$

$$R^n_h R_h v = R_h R^n_h v \quad \forall v \in W^{1,\infty}(I_n; H^1_0(\Omega)), \quad (3.45b)$$

$$R^n_h \Delta_h v_h = \Delta_h R^n_h v_h \quad \forall v \in W^{1,\infty}(I_n; S_h). \quad (3.45c)$$

Moreover, there holds the following approximation property (cf. [9]):

$$\|v - R_h v\|_{H^1} \leq C h^p \|v\|_{H^{p+1}} \quad \forall v \in H^1_0(\Omega) \cap H^{p+1}(\Omega). \quad (3.46)$$

### 3.5 Consistency of scheme (2.12a)–(2.12b)

We define a pair of intermediate solutions (for comparison with the numerical solutions)

$$u_h^* = R^n_h R_h u \quad \text{and} \quad r_h^* = R^n_h r.$$

Then, testing (2.6a) and (2.6b) by $P^n_r v_h$ and $P^n_q q_h$, respectively, we obtain the following equations for $u_h^*$ and $r_h^*$:

$$\int_{I_n} i (\partial_t u_h^*, P^n_r v_h) dt + \int_{I_n} (\nabla u_h^*, \nabla P^n_r v_h) dt$$

$$+ \frac{\tau}{2} \sum_{j=1}^k w_j (r_h^*(t_{nj}) g(u_h^*(t_{nj})) u_h^*(t_{nj}), P^n_r v_h(t_{nj})) = \int_{I_n} (d^n_u, P^n_r v_h) dt,$$

$$\int_{I_n} \partial_t r_h^* P^n_r q_h dt = \frac{\tau}{4} \sum_{j=1}^k w_j \text{Re} (P^n_r q_h(t_{nj}) g(u_h^*(t_{nj})) u_h^*(t_{nj}), \partial_t u_h^*(t_{nj}))$$

$$+ \int_{I_n} d^n_q P^n_r q_h dt,$$

where $d^n_u$ and $d^n_q$ are consistency errors of the numerical method. By using the identities (3.17) and (3.32), we can express these consistency errors by

$$d^n_u = i \partial_t R^n_r (R_h u - u) + \Delta_h R_h (u - R^n_r u) + r g(u) u - I^n_r [r_h^* g(u_h^*) u_h^*], \quad (3.49)$$

13
\[
d_r^n = \frac{1}{2} \text{Re} \left[ (g(u_t u) - I^n_t (g(u^*_h)u^*_h, \partial_t u^*_h) \right]. \tag{3.50}
\]

After using (3.13) and (3.18), equations (3.47)–(3.48) can be rewritten as
\[
\int_{I_n} i(\partial_t u^*_h, v_h) dt + \int_{I_n} (\nabla P^n u^*_h, \nabla v_h) dt \tag{3.51}
\]
\[
- \frac{\tau}{2} \sum_{j=1}^{k} w_j (r^*_h(t_{nj})g(u^*_h(t_{nj})u^*_h(t_{nj}), v_h(t_{nj})) = \int_{I_n} (P^n d^n_r, v_h) dt, \tag{3.52}
\]
\[
\int_{I_n} \partial_t r^*_h q_h dt = \frac{\tau}{4} \sum_{j=1}^{k} w_j \text{Re} \left( q_h(t_{nj})g(u^*_h(t_{nj})u^*_h(t_{nj}), \partial_t u^*_h(t_{nj})) \right)
\]
\[
+ \int_{I_n} P^n d^n_r q_h dt.
\]

**Theorem 3.3** Suppose that the solution of (1.1) is sufficiently smooth, then \(d^n_u \in C(I_n; H^1_0(\Omega))\) and there hold
\[
\sup_{t \in I_n} \|d^n_u\|_{H^1} \leq C(h^p + \tau^{k+1}) \quad \text{and} \quad \sup_{t \in I_n} |P^n d^n_r| \leq C(h^p + \tau^{k+1}). \tag{3.53}
\]

**Remark 3.1** The key observation for the consistency errors is that, although (3.50) contains an \(O(h^p + \tau^k)\) error from \(\partial_t u - \partial_t u^*_h\), the temporal \(L^2\) projection operator \(P^n_r\) acting on \(d^n_r\) furthermore reduces this error to \(O(h^p + \tau^{k+1})\). This is proved by using the super-approximation result in Lemma 3.2.

**Proof.** Since the spatial Ritz projection \(R_h\) maps \(H^1_0(\Omega)\) into \(S_h \subset H^1_0(\Omega)\), and the temporal Ritz projection \(R^n_t\) maps \(W^{1,\infty}(I_n; H^1_0(\Omega))\) into \(\mathbb{P}^k \otimes H^1_0(\Omega)\), it follows that every term in (3.49) is in \(C(I_n; H^1_0(\Omega))\). This implies \(d^n_u \in C(I_n; H^1_0(\Omega))\).

By using the triangle inequality, from (3.49) we get
\[
\max_{t \in I_n} \|d^n_u\|_{H^1} \leq \max_{t \in I_n} \left( \|\partial_t R^n_t (R_h u - u)\|_{H^1} + \|\Delta_h R_h (u - R^n_u)\|_{H^1} \right. \tag{3.54}
\]
\[
\left. + \max_{t \in I_n} \left( \|r g(u) - I^n_t [rg(u)u]\|_{H^1} + \|r g(u)u - r^*_h g(u^*_h)u^*_h\|_{H^1} \right) \right)
\]
\[
= : D^u_1 + D^u_2 + D^u_3 + D^u_4.
\]

Choosing \(m = 0\) in Lemma 3.1, we obtain the following stability result:
\[
\|R^n_t u\|_{W^{1,\infty}(I_n; H^s)} \leq C\|u\|_{W^{1,\infty}(I_n; H^s)}. \tag{3.55}
\]

Using (3.55) and (3.46), we can estimate \(D^u_1\) as follows:
\[
D^u_1 = \max_{t \in I_n} \|\partial_t R^n_t (R_h u - u)\|_{H^1} \leq \|R_h u - u\|_{W^{1,\infty}(I_n; H^1)} \leq C h^p \|R_h u - u\|_{W^{1,\infty}(I_n; H^{p+1})}.
\]

Similarly, using identity (3.45) and Lemma 3.1, we have
\[
D^u_2 = \max_{t \in I_n} \|\Delta_h R_h (u - R^n_u)\|_{H^1} = \max_{t \in I_n} \|P_h \Delta (u - R^n_u)\|_{H^1}.
\]
\[ \leq \max_{t \in I_n} \| u - R^n \tau u \|_{H^3} \]
\[ \leq C \tau^{k+1} \| u \|_{W^{k+1, \infty}(I_n; H^3)}, \]

and
\[ D^u_n = \max_{t \in I_n} \| rg(u)u - I^n \tau [rg(u)u] \|_{H^1} \leq C \tau^{k+1}. \]

By using the triangle inequality, we decompose \( D^u_n \) into two parts,

\[ D^u_n \leq \max_{t \in I_n} \left( \| rg(u)u - rg(R_h u)R_h u \|_{H^1} + \| rg(R_h u)R_h u - R^n \tau RG(R^n \tau R_h u)R^n \tau R_h u \|_{H^1} \right) \]
\[ \leq C h^p + C \tau^{k+1}. \]

Then, substituting the estimates of \( D_j^u, \ j = 1, 2, 3, 4, \) into (3.54), we obtain the desired estimate for \( \| d^u_n \|_{H^1} \).

To estimate \( |P^n \tau d^n \tau| \), we rewrite (3.50) as
\[ d^n \tau = \frac{1}{2} \text{Re} \left[ (g(u)u, \partial_t (u - u^*_h)) + (g(u)u - g(u^*_h)u^*_h, \partial_t u^*_h) \right] \]
\[ + \frac{1}{2} \text{Re} \left[ (g(u^*_h)u^*_h, \partial_t u^*_h) - I^n \tau (g(u^*_h)u^*_h, \partial_t u^*_h) \right] \]
and test this expression by \( P^n \tau d^n \tau v \) in the time interval \( I_n \), with \( v \in \mathbb{P}^k \). This yields
\[
\int_{I_n} P^n \tau d^n \tau v \, dt = \int_{I_n} d^n \tau P^n \tau v \, dt \tag{3.56}
\]
\[ \leq \frac{1}{2} \text{Re} \int_{I_n} (g(u)u, \partial_t (u - u^*_h)) P^n \tau v \, dt \]
\[ + C \tau^{\frac{1}{2}} \|(g(u)u - g(u^*_h)u^*_h, \partial_t u^*_h)\|_{L^\infty(I_n)} \| v \|_{L^2(I_n)} \]
\[ + C \tau^{k+\frac{3}{2}} \| \partial_t^{k+1} (g(u^*_h)u^*_h, \partial_t u^*_h) \|_{L^\infty(I_n)} \| v \|_{L^2(I_n)} \]
\[ \leq \frac{1}{2} \text{Re} \int_{I_n} (g(u)u, \partial_t (u - u^*_h)) P^n \tau v \, dt + C \tau^{\frac{1}{2}} (h^p + \tau^{k+1}) \| v \|_{L^2(I_n)}. \]

The first term on the right-hand side of (3.56) can be estimated as follows.
\[
\frac{1}{2} \text{Re} \int_{I_n} (g(u)u, \partial_t (u - u^*_h)) P^n \tau v \, dt = \int_{I_n} (g(u)u, \partial_t (u - R^n \tau u)) P^n \tau v \, dt \tag{3.57}
\]
\[ + \int_{I_n} (g(u)u, \partial_t R^n \tau (u - R_h u)) P^n \tau v \, dt \]
\[ =: D^1_i + D^2_i, \]

where
\[ D^1_i = \int_{I_n} (g(u)u P^n \tau v, \partial_t (u - R^n \tau u)) \, dt \]
\[ = \int_{I_n} (g(u)u P^n \tau v - P^n \tau (g(u)u P^n \tau v), \partial_t (u - R^n \tau u)) \, dt \]
\[ \leq C \tau^{\frac{1}{2}} \|(g(u)u P^n \tau v - P^n \tau (g(u)u P^n \tau v))\|_{L^2(I_n; L^2)} \| \partial_t (u - R^n \tau u) \|_{L^\infty(I_n; L^2)} \].
\[ \leq C \tau^{\frac{3}{2}} \| P_\tau^n v \|_{L^2(I_n;L^2)} \| \partial_t (u - R^n u) \|_{L^\infty(I_n;L^2)} \quad (\text{we have used Lemma 3.2}) \]

\[ \leq C \tau^{k+\frac{3}{2}} \| v \|_{L^2(I_n)} \| \tau^{k+1} u \|_{L^\infty(I_n;L^2)} \quad (\text{we have used Lemma 3.1}), \]

\[ D_2^n \leq C \tau^{\frac{1}{2}} \| g(u) u \|_{L^\infty(I_n;L^2)} \| u - R_h u \|_{W^{1,\infty}(I_n;L^2)} \| v \|_{L^2(I_n)} \]

\[ \leq C \tau^{\frac{1}{2}} h^p \| v \|_{L^2(I_n)} \| u \|_{W^{1,\infty}(I_n;H^{p+1})}. \]

Substituting these estimates into (3.56), we obtain

\[ \left| \int_{I_n} P_\tau^n d^n_r v \ dt \right| \leq C \tau^{\frac{1}{2}} (h^p + \tau^{k+1}) \| v \|_{L^2(I_n)}. \]

Since this inequality holds for arbitrary \( v \in L^2(I_n) \), it follows that

\[ \| P_\tau^n d^n_r \|_{L^2(I_n)} \leq C \tau^{\frac{1}{2}} (h^p + \tau^{k+1}). \]

Then, using the inverse inequality in time, we obtain the desired estimate for \( |P^n d^n_r| \). \square

4 Well-posedness and convergence analysis

We define the error functions \( e^n_h = u_h - u^n_h \) and \( e^r_h = r_h - r_h^e \), with the following abbreviations:

\[ e^n_{nj} = e^n_h(t_{nj}) \quad \text{and} \quad e^r_{nj} = e^r_h(t_{nj}), \]
\[ u_{nj} = u_h(t_{nj}) \quad \text{and} \quad r_{nj} = r_h(t_{nj}), \]
\[ u^*_{nj} = u^*_h(t_{nj}) \quad \text{and} \quad r^*_{nj} = r^*_h(t_{nj}), \]
\[ v_{nj} = v_h(t_{nj}) \quad \text{and} \quad q_{nj} = q_h(t_{nj}). \]

Subtracting (3.51)–(3.52) from (3.19)–(3.20), we obtain the following error equations:

\[ i \int_{I_n} (\partial_t e^n_h, v_h) \ dt = - \int_{I_n} \left( \nabla P_\tau^n e^n_h, \nabla v_h \right) \ dt + \frac{\tau}{2} \sum_{j=1}^k w_j \left( e^n_{nj} g(u_{nj}) u_{nj}, v_{nj} \right) \]
\[ + \frac{\tau}{2} \sum_{j=1}^k w_j \left( r^*_{nj} [g(u_{nj}) u_{nj} - g(u^*_{nj}) u^*_{nj}], v_{nj} \right) - \int_{I_n} (P^n d^n_r, u_h) dt, \quad (4.58a) \]

\[ \int_{I_n} \partial_t e^n_h q_h dt = \frac{\tau}{4} \sum_{j=1}^k w_j \text{Re} \left( q_{nj} (g(u_{nj}) u_{nj} - g(u^*_{nj}) u^*_{nj}), \partial_t e^n_h(t_{nj}) \right) \]
\[ + \frac{\tau}{4} \sum_{j=1}^k w_j \text{Re} \left( q_{nj} g(u_{nj}) u_{nj}, \partial_t e^n_h(t_{nj}) \right) - \int_{I_n} P^n d^n_r q_h dt, \quad (4.58b) \]

which hold for all test functions \( v_h \in \mathbb{P}^k \otimes S_h \) and \( q_h \in \mathbb{P}^k \).

Remark 4.1 If (4.58) has a solution \( (e^n_h, e^r_h) \in X_{\tau,h} \times Y_{\tau,h} \) with \( u_h = u^n_h + e^n_h \) and \( r_h = r^*_h + e^r_h \), then \( (u_h, r_h) \) is a solution of the numerical scheme (2.12). In the following, we prove existence of a solution \( (e^n_h, e^r_h) \) to (4.58) with \( u_h = u^n_h + e^n_h \) and \( r_h = r^*_h + e^r_h \).

In this section, we prove existence and uniqueness of solutions to (4.58a)–(4.58b) by using Schaefer’s Fixed Point Theorem, which is quoted below.
Theorem 4.1 (Schaefer’s Fixed Point Theorem [12, Chapter 9.2, Theorem 4]) Let $B$ be a Banach space and let $M : B \rightarrow B$ be a continuous and compact mapping (possibly nonlinear). If the set
\[ \{ \phi \in B : \exists \theta \in [0, 1] \text{ such that } \phi = \theta M(\phi) \} \] (4.59)
is bounded in $B$, then the mapping $M$ has at least one fixed point.

We define
\[ X_{\tau,h}^* = \left\{ v_h \in X_{\tau,h} : \max_{1 \leq n \leq N} \max_{1 \leq j \leq k} \| v_h(t_{n,j}) - u_h^*(t_{n,j}) \|_{L^\infty \cap H^1} \leq \frac{1}{2} \right\}, \] (4.60)
\[ Y_{\tau,h}^* = \left\{ q_h \in Y_{\tau,h} : \max_{1 \leq n \leq N} \max_{1 \leq j \leq k} | q_h(t_{n,j}) - r_h^*(t_{n,j}) | \leq \frac{1}{2} \right\}, \] (4.61)
where the norm $\| \cdot \|_{L^\infty \cap H^1}$ is defined as
\[ \| \phi_h \|_{L^\infty \cap H^1} := \max(\| \phi_h \|_{L^\infty}, \| \phi_h \|_{H^1}). \]

For any element $(\phi_h, \varphi_h) \in X_{\tau,h} \times Y_{\tau,h}$, we define two associated numbers
\[ \rho[\phi_h] := \min \left( \frac{1}{\max_{1 \leq n \leq N} \max_{1 \leq j \leq k} \| \phi_h(t_{n,j}) \|_{L^\infty \cap H^1}}, 1 \right), \] (4.62a)
\[ \rho[\varphi_h] := \min \left( \frac{1}{\max_{1 \leq n \leq N} \max_{1 \leq j \leq k} | \varphi_h(t_{n,j}) |}, 1 \right), \] (4.62b)
which are continuous with respect to $(\phi_h, \varphi_h)$ (because all norms are equivalent in the finite-dimensional space $X_{\tau,h} \times Y_{\tau,h}$). Furthermore, the two numbers defined above satisfy the following estimates:
\[ \max_{1 \leq n \leq N} \max_{1 \leq j \leq k} \| \rho[\phi_h] \phi_h(t_{n,j}) \|_{L^\infty \cap H^1} \leq 1, \] (4.63)
\[ \max_{1 \leq n \leq N} \max_{1 \leq j \leq k} | \rho[\varphi_h] \varphi_h(t_{n,j}) | \leq 1. \] (4.64)

Then we define
\[ u^\phi := u_h^* + \rho[\phi_h] \phi_h \quad \text{and} \quad r^\varphi := r_h^* + \rho[\varphi_h] \varphi_h, \] (4.65)
with the following abbreviations:
\[ u_{n,j}^\phi = u_h^*(t_{n,j}) \quad \text{and} \quad \varphi_{n,j} = \varphi_h(t_{n,j}), \]
and define $(e_{h}^u, e_{h}^r) \in X_{\tau,h} \times Y_{\tau,h}$ to be the solution of the following linear equations:
\[ i \int_{I_n} (\partial_t e_h^u, v_h) \, dt + \int_{I_n} (\nabla P^n_r e_h^u, \nabla v_h) \, dt = \frac{\tau}{2} \sum_{j=1}^{k} w_j \left( \varphi_{n,j} g(u_{n,j}^\phi) u_{n,j}^\phi, v_{n,j} \right) \] (4.66)
\[ + \frac{\tau}{2} \sum_{j=1}^{k} w_j \left( r_{n,j}^* \left[ g(u_{n,j}^\phi) u_{n,j}^\phi - g(u_{n,j}^*) u_{n,j}^* \right], v_{n,j} \right) - \int_{I_n} (P^n_r d^n u, v_h) \, dt \]
and
\[
\int_{I_n} \partial_t e_h^r q_h \, dt = \frac{\tau}{4} \sum_{j=1}^{k} w_j \text{Re} (q_{nj} (g(u_{nj}^\phi - g(u_{nj}^*) u_{nj}^*), \partial_t u_{nj}^*(t_{nj}))) + \frac{\tau}{4} \sum_{j=1}^{k} w_j \text{Re} (q_{nj} g(u_{nj}^\phi, \partial_t \phi_h(t_{nj})) - \int_{I_n} P_n^\tau d^r \phi_h \, dt
\]
for all \( v_h \in \mathbb{P}^k \otimes S_h \) and \( q_h \in \mathbb{P}^k, n = 1, \ldots, N \). We denote by \( M: X_{\tau,h} \times Y_{\tau,h} \to X_{\tau,h} \times Y_{\tau,h} \) the mapping from \((\phi_h, \varphi_h)\) to \((e_h^u, e_h^r)\), and define the set
\[
\mathcal{B} = \{ (\phi_h, \varphi_h) \in X_{\tau,h} \times Y_{\tau,h} : \exists \theta \in [0, 1] \text{ such that } (\phi_h, \varphi_h) = \theta M(\phi_h, \varphi_h) \},
\]
and the norm following norm on \( X_{\tau,h} \times Y_{\tau,h} \): for any \((\phi_h, \varphi_h) \in X_{\tau,h} \times Y_{\tau,h}
\]
\[
\| (\phi_h, \varphi_h) \|_{X_{\tau,h} \times Y_{\tau,h}} := \| \phi_h \|_{L^\infty(0,T; H^1)} + \| \varphi_h \|_{L^\infty(0,T)}.
\]

**Lemma 4.1** The mapping \( M: X_{\tau,h} \times Y_{\tau,h} \to X_{\tau,h} \times Y_{\tau,h} \) is well defined, continuous and compact.

**Proof.** Since the right-hand sides of (4.66)–(4.67) are given, the linear equations (4.66)–(4.67) have a unique solution \((e_h^u, e_h^r) \in X_{\tau,h} \times Y_{\tau,h}\) for any given \((\phi_h, \varphi_h) \in X_{\tau,h} \times Y_{\tau,h}\). Thus the mapping is well defined. Let \( \ell^u(\phi_h, \varphi_h; v_h) \) and \( \ell^r(\phi_h, \varphi_h; q_h) \) denote the right-hand sides of (4.66) and (4.67), respectively. Since all norms are equivalent in the finite-dimensional space \( X_{\tau,h} \times Y_{\tau,h} \), it follows that
\[
|\ell^u(\phi_h, \varphi_h; v_h) - \ell^u(\hat{\phi}_h, \hat{\varphi}_h; v_h)| \leq o(1) \| v_h \|_{L^2(0,T; L^2)}, \quad \forall v_h \in L^2(0,T; L^2),
\]
\[
|\ell^r(\phi_h, \varphi_h; q_h) - \ell^r(\hat{\phi}_h, \hat{\varphi}_h; q_h)| \leq o(1) \| q_h \|_{L^2(0,T)}, \quad \forall q_h \in L^2(0,T; L^2),
\]
as \((\phi_h, \varphi_h) \to (\hat{\phi}_h, \hat{\varphi}_h)\) in \( X_{\tau,h} \times Y_{\tau,h} \). Where \( o(1) \) represents some quantity tending to zero. Using this property, it is easy to verify that \((e_h^u, e_h^r)\) is continuous with respect to \((\phi_h, \varphi_h)\).

Since \( X_{\tau,h} \times Y_{\tau,h} \) is a finite-dimensional space, a continuous mapping is automatically compact. The proof is complete. \( \square \)

We are now ready to state and prove the following key lemma.

**Lemma 4.2** Let \( 1 \leq d \leq 3 \) and assume that the solution of the NLS equation (1.1) is sufficiently smooth. Then there exist positive constants \( \tau_0 \) and \( h_0 \) such that when \( \tau \leq \tau_0 \) and \( h \leq h_0 \), the following statement holds: If \((\phi_h, \varphi_h) \in \mathcal{B} \) and \((e_h^u, e_h^r) = M(\phi_h, \varphi_h)\), then
\[
\| e_h^u \|_{L^\infty(0,T; H^1)} + \| e_h^r \|_{L^\infty(0,T)}
\]
\[
\leq \left[ \| e_h^u(0) \|_{H^1} + | e_h^r(0) | \right] + \max_{1 \leq n \leq N} \max_{t \in I_n} \left( \| d_n^u \|_{H^1} + | P_n \| d_n^r \| \right)
\]
\[
\max_{1 \leq n \leq N} \max_{1 \leq j \leq k} \| e_h^u(t_{nj}) \|_{L^\infty \cap H^1} \leq \frac{1}{2} \quad \text{and} \quad \max_{1 \leq n \leq N} \max_{1 \leq j \leq k} | e_h^r(t_{nj}) | \leq \frac{1}{2},
\]
\[
\rho[\phi_h] = 1, \quad \rho[\varphi_h] = 1.
\]

**Proof.** If \((\phi_h, \varphi_h) \in \mathcal{B} \) and \((e_h^u, e_h^r) = M(\phi_h, \varphi_h)\), then
\[
(\phi_h, \varphi_h) = \theta M(\phi_h, \varphi_h) = (\theta e_h^u, \theta e_h^r).
\]
which implies $\phi_h = \theta e_h^n$ and $\varphi_h = \theta e_h^n$. In this case, (4.66)–(4.67) can be rewritten as

$$i \int_{I_n} (\partial_t e_h^n, v_n) dt = - \int_{I_n} (\nabla P^n_\tau e_h^n, \nabla v_n) dt + \frac{\theta \tau}{2} \sum_{j=1}^k w_j \left( e_{nj}^\phi (u_{nj}^\phi) u_{nj}^\phi, v_{nj} \right)$$

$$+ \frac{\tau}{2} \sum_{j=1}^k w_j \left( r_{nj}^* \left[ g(u_{nj}^\phi) u_{nj}^\phi - g(u_{nj}^*) u_{nj}^* \right], v_{nj} \right)$$

$$- \int_{I_n} (P^n_\tau d^n_\tau v_n) dt,$$

$$\int_{I_n} \partial_t e_h^n q_h dt = \frac{\tau}{4} \sum_{j=1}^k w_j \Re \left( q_{nj} (g(u_{nj}^\phi) u_{nj}^\phi - g(u_{nj}^*) u_{nj}^*), \partial_t u_h^n (t_{nj}) \right)$$

$$+ \frac{\theta \tau}{4} \sum_{j=1}^k w_j \Re \left( q_{nj} (g(u_{nj}^\phi) u_{nj}^\phi, \partial_t e_h^n (t_{nj}) \right)$$

$$- \int_{I_n} P^n_\tau d^n_\tau q_h dt,$$

which hold for all $v_n \in \mathbb{P}^k \otimes S_h$ and $q_h \in \mathbb{P}^k$, $n = 1, \ldots, N$. In the following, we derive estimates for $e_h^n$ and $e_h^n$ based on equations (4.73)–(4.74).

From (4.63)–(4.64) and definition (4.65) we get

$$\max_{1 \leq n \leq N} \max_{1 \leq j \leq k} \| u_h^n(t_{nj}) \|_{L^\infty \cap H^1} + \max_{1 \leq n \leq N} \max_{1 \leq j \leq k} \| r_h^n(t_{nj}) \|_{L^\infty \cap H^1}$$

$$\leq \max_{1 \leq n \leq N} \max_{1 \leq j \leq k} \| u_h^n(t_{nj}) \|_{L^\infty \cap H^1} + \max_{1 \leq n \leq N} \max_{1 \leq j \leq k} \| r_h^n(t_{nj}) \|_{L^\infty \cap H^1}$$

$$+ \max_{1 \leq n \leq N} \max_{1 \leq j \leq k} \| \rho(\varphi_h) \varphi_h(t_{nj}) \|_{L^\infty \cap H^1} + \max_{1 \leq n \leq N} \max_{1 \leq j \leq k} \| \rho(\varphi_h) \varphi_h(t_{nj}) \|_{L^\infty \cap H^1}$$

$$\leq \| u_h^n \|_{L^\infty(0,T;L^\infty \cap H^1)} + \| r_h^n \|_{L^\infty(0,T;L^\infty \cap H^1)} + 2.$$
Then substituting this into (4.76) yields

\[ =: \tau(\nabla e_h^u(t_{n-1}), \nabla P^n \tau e_h^u(t_{n-1})) + J_{u1} + J_{u2}. \]

In the second to last equality, we have used the identity

\[ \int_{I_n} \left( \nabla e_h^u(t), (t_n - t) \partial_t \nabla P^n \tau e_h^u(t) \right) dt = \int_{I_n} \left( \nabla P^n \tau e_h^u(t), (t_n - t) \partial_t \nabla P^n \tau e_h^u(t) \right) dt, \]

which holds because \((t_n - t) \partial_t \nabla P^n \tau e_h^u(t)\) is a polynomial of degree \(k - 1\) in time.

Using integration by parts, we have

\[ J_{u2} = \int_{I_n} \frac{1}{2} \frac{d}{dt} \|\nabla P^n \tau e_h^u(t)\|^2 (t_n - t) dt \]
\[ = -\frac{1}{2} \|\nabla P^n \tau e_h^u(t_{n-1})\|^2 + \int_{I_n} \frac{1}{2} \|\nabla P^n \tau e_h^u(t)\|^2 dt. \]

Then substituting this into (4.76) yields

\[ \int_{I_n} \|\nabla P^n \tau e_h^u(t)\|^2 dt \leq 2\tau(\nabla e_h^u(t_{n-1}), \nabla P^n \tau e_h^u(t_{n-1})) + 2J_{u1}. \]

Setting \(v_h = (-\Delta_h)P^n \tau e_h^u(t_{n-1})\) in (4.73) and taking the imaginary part yield

\[ J_{u1} = \text{Im} \int_{I_n} \left( i \partial_t e_h^u(t), (-\Delta_h)P^n \tau e_h^u(t_{n-1}) \right) dt \]
\[ = -\text{Im} \int_{I_n} \left( \nabla P^n \tau e_h^u(t), (-\Delta_h)P^n \tau e_h^u(t_{n-1}) \right) dt \]
\[ + \frac{\theta \tau}{2} \sum_{j=1}^k w_j \text{Im} \left( e_{n_j}^\phi g(u_{n_j}^\phi) u_{n_j}^\phi, (-\Delta_h)P^n \tau e_h^u(t_{n-1}) \right) \]
\[ + \tau \sum_{j=1}^k w_j \text{Im} \left( r_{n_j}^* (g(u_{n_j}^\phi) u_{n_j}^\phi - g(u_{n_j}^*) u_{n_j}^*), (-\Delta_h)P^n \tau e_h^u(t_{n-1}) \right) \]
\[ - \int_{I_n} \text{Im} \left( P^n d^n \tau, (-\Delta_h)P^n \tau e_h^u(t_{n-1}) \right) dt =: \sum_{m=1}^4 J_{u1}^m, \]

where

\[ J_{u1}^1 = -\text{Im} \int_{I_n} \left( \Delta_h P^n \tau e_h^u(t), \Delta_h P^n \tau e_h^u(t_{n-1}) \right) dt \]
\[ = -\text{Im} \int_{I_n} \|\Delta_h P^n \tau e_h^u(t)\|^2 (t_n - t) dt = 0. \]

From identity (3.17) and inequality (3.22), we have

\[ J_{u1}^2 = \frac{\tau \theta}{2} \sum_{j=1}^k w_j \text{Im} \left( \nabla P_h [e_{n_j}^\phi g(u_{n_j}^\phi) u_{n_j}^\phi], P^n \tau e_{n_j}^u(t_{n-1}) \right) \]

20
Substituting (4.79) and the estimates of $J_{\tau}$ we obtain

$$
\int u \leq 1 = \leq \sum_{j=1}^{k} w_j |e_{nj}^r|||P_\tau^n[\nabla P_\tau^n e_{nj}(t_n - t_{n_j})]||
$$

$$
\leq C\tau \sum_{j=1}^{k} w_j |e_{nj}^r|||P_\tau^n[\nabla P_\tau^n e_{nj}(t_n - t_{n_j})]||
$$

(here (2.9b) is used)

$$
\leq C\tau \sum_{j=1}^{k} \frac{\tau}{8\tau^2} w_j \|P_\tau^n[\nabla P_\tau^n e_{nj}(t_n - t_{n_j})]\|^2 + C\tau^3 \sum_{j=1}^{k} w_j |e_{nj}^r|^2
$$

$$
\leq \frac{1}{4\tau^2} \int_{I_n} \|P_\tau^n[\nabla P_\tau^n e_{h}^n(t_n - t)]\|^2 dt + 2C\tau^2 \int_{I_n} |e_{h}^r|^2 dt
$$

$$
\leq \frac{1}{4} \int_{I_n} \|P_\tau^n e_{h}^n\|^2 dt + 2C\tau^2 \int_{I_n} |e_{h}^r|^2 dt,
$$

$$
J_{u1}^3 = \frac{\tau}{2} \sum_{j=1}^{k} w_j \text{Im}(r_{nj}^* \nabla P_\tau [(g(u_{nj}^\phi)u_{nj}^\phi - g(u_{nj}^{*})u_{nj}^{*})], P_\tau^n[\nabla P_\tau^n e_{nj}(t_n - t_{n_j})])
$$

$$
\leq \frac{\tau}{2} \sum_{j=1}^{k} w_j |r_{nj}^*|||\nabla P_\tau [(g(P_\tau^n u_{nj}^\phi)P_\tau^n u_{nj}^\phi - g(P_\tau^n u_{nj}^{*})P_\tau^n u_{nj}^{*})]| |
$$

$$
\times \|P_\tau^n[\nabla P_\tau^n e_{nj}(t_n - t_{n_j})]\| \text{ (here } u_{nj}^\phi = P_\tau^n u_{nj}^\phi \text{ is used)}
$$

$$
\leq C\tau \sum_{j=1}^{k} w_j \|\nabla P_\tau^n e_{nj}\|||P_\tau^n[\nabla P_\tau^n e_{nj}(t_n - t_{n_j})]||
$$

(here (4.75) is used)

$$
\leq C\tau \int_{I_n} \|P_\tau^n e_{h}^n\|^2 dt + C\tau^{-1} \int_{I_n} \|P_\tau^n[\nabla P_\tau^n e_{nj}(t_n - t_{n_j})]\|^2 dt
$$

$$
\leq C\tau \int_{I_n} \|\nabla P_\tau^n e_{h}^n\|^2 dt,
$$

$$
J_{u1}^4 = - \int_{I_n} \text{Im}(\nabla P_\tau P_\tau^n d_{u}, P_\tau^n[\nabla P_\tau^n e_{h}^n(t_n - t)]) dt
$$

$$
\leq C\tau^2 \int_{I_n} \|\nabla P_\tau P_\tau^n d_{u}\|^2 dt + \frac{1}{4\tau^2} \int_{I_n} \|P_\tau^n[\nabla P_\tau^n e_{nj}(t_n - t_{n_j})]\|^2 dt
$$

$$
\leq C\tau^3 \max_{t \in I_n} \|d_{u}\|^2_{H^1} + \frac{1}{4} \int_{I_n} \|\nabla P_\tau^n e_{h}^n\|^2 dt.
$$

Substituting (4.79) and the estimates of $J_{u1}^m$, $m = 1, 2, 3, 4$, into (4.78), for sufficiently small step size $\tau$ we obtain

$$
\int_{I_n} \|\nabla P_\tau^n e_{h}^n\|^2 dt
$$

$$
\leq C\tau \|\nabla e_{h}^n(t_{n-1})\|, \|\nabla P_\tau^n e_{h}^n(t_{n-1})\| + C\tau^2 \int_{I_n} |e_{h}^r|^2 dt + C\tau^3 \max_{t \in I_n} \|d_{u}\|^2_{H^1}
$$

$$
\leq C\tau \|\nabla e_{h}^n(t_{n-1})\|, \|\nabla P_\tau^n e_{h}^n(t_{n-1})\| + C\tau^2 \int_{I_n} |e_{h}^r|^2 dt + C\tau^3 \max_{t \in I_n} \|d_{u}\|^2_{H^1}
$$
\[ C\tau \| \nabla e_h^u(t_{n-1}) \| \left( \frac{1}{\tau} \int_{I_n} \| \nabla P^n e_h^u \|^2 dt \right)^{\frac{1}{2}} + C\tau^2 \int_{I_n} |e_h^r|^2 dt + C\tau^3 \max_{t \in I_n} \| d_u^n \|^2_{H^1}, \]

which then implies
\[
\int_{I_n} \| \nabla P^n e_h^u \|^2 dt \leq C\tau \| \nabla e_h^u(t_{n-1}) \|^2 + C\tau^2 \int_{I_n} |e_h^r|^2 dt + C\tau^3 \max_{t \in I_n} \| d_u^n \|^2_{H^1}.
\]

By using inequality (3.21), we can remove the operator \( P^n \) in the above inequality (meanwhile replace the \( H^1 \) seminorm by the full norm), i.e.,
\[
\int_{I_n} \| e_h^u \|^2_{H^1} dt \leq C\tau \| e_h^u(t_{n-1}) \|^2_{H^1} + C\tau^2 \int_{I_n} |e_h^r|^2 dt + C\tau^3 \max_{t \in I_n} \| d_u^n \|^2_{H^1}. \tag{4.81}
\]

**Step 2: Estimation of \( \| e_h^r \|_{L^2(I_n)} \)**: To estimate the second term on the right-hand side of (4.81), we proceed similarly as (4.76), that is,
\[
\int_{I_n} |P^n e_h^r|^2 dt = \int_{I_n} e_h^r(t) P^n e_h^r(t) dt = \int_{I_n} \left[ e_h^r(t_{n-1}) P^n e_h^r(t_{n-1}) + \int_{t_{n-1}}^t \partial_s (e_h^r(s) P^n e_h^r(s)) ds \right] dt \leq \tau e_h^r(t_{n-1}) P^n e_h^r(t_{n-1}) + \int_{I_n} \partial_t e_h^r(t) P^n [P^n e_h^r(t)(t_{n}-t)] dt + \int_{I_n} e_h^r(t)(t_{n}-t) \partial_t P^n e_h^r(t)dt \leq \tau e_h^r(t_{n-1}) P^n e_h^r(t_{n-1}) + \int_{I_n} \partial_t e_h^r(t) P^n [P^n e_h^r(t)(t_{n}-t)] dt + \int_{I_n} P^n e_h^r(t)(t_{n}-t) \partial_t P^n e_h^r(t)dt = : \tau e_h^r(t_{n-1}) P^n e_h^r(t_{n-1}) + J_{1} + J_{2},
\]

where we have changed the order of integration in the third equality, and used the following identity in the second to last equality:
\[
\int_{I_n} e_h^r(t)(t_{n}-t) \partial_t P^n e_h^r(t) dt = \int_{I_n} P^n e_h^r(t)(t_{n}-t) \partial_t P^n e_h^r(t) dt,
\]
which holds because \((t_{n}-t) \partial_t P^n e_h^r(t)\) is a polynomial of degree \(k - 1\) in time.

Using integration by parts, we have
\[
J_{2} = \int_{I_n} \frac{1}{2} \frac{d}{dt} |P^n e_h^r(t)|^2 (t_{n}-t) dt \tag{4.83}
\leq -\frac{1}{2} |P^n e_h^r(t_{n-1})|^2 + \int_{I_n} \frac{1}{2} |P^n e_h^r(t)|^2 dt \leq \frac{1}{2} \int_{I_n} |P^n e_h^r(t)|^2 dt.
\]

Then substituting (4.83) into (4.82) yields
\[
\int_{I_n} |P^n e_h^r|^2 dt \leq 2\tau (e_h^r(t_{n-1}), P^n e_h^r(t_{n-1})) + 2J_{1}
\]
\[
\begin{align*}
&\leq C \tau |e_h^n(t_{n-1})| \left\| P^n \tau e_h^n \right\|_{L^\infty(I_n)} + 2 J_{r1} \\
&\leq C \tau |e_h^n(t_{n-1})| \left( \frac{1}{\tau} \int_{I_n} |P^n \tau e_h^n|^2 \, dt \right)^{\frac{1}{2}} + 2 J_{r1} \\
&\leq C \tau |e_h^n(t_{n-1})|^2 + \frac{1}{2} \int_{I_n} |P^n \tau e_h^n|^2 \, dt + 2 J_{r1},
\end{align*}
\]
which then implies
\[
\int_{I_n} |P^n \tau e_h^n|^2 \, dt \leq C \tau |e_h^n(t_{n-1})|^2 + 4 J_{r1},
\]
(4.84)

In order to estimate \( J_{r1} \), we choose \( q_h = P^n \tau [P^n \tau e_h^n(t)(t_n - t)] \) in (4.74), which yields the following identity:
\[
J_{r1} = \int_{I_n} \partial_t e_h^n(t) P^n \tau [P^n \tau e_h^n(t)(t_n - t)] \, dt
\]
(4.85)
\[
= -\tau \frac{1}{4} \sum_{j=1}^{K} w_j \Re \left( P^n \tau [P^n \tau e_{nj}(t_n - t_{nj})] (g(u_{nj}) u_{nj}^\phi - g(u_{nj}) u_{nj}^*), \partial_t u_h^n(t_{nj}) \right)
\]
\[
+ \tau \frac{\phi}{4} \sum_{j=1}^{K} w_j \Re \left( P^n \tau [P^n \tau e_{nj}(t_n - t_{nj})] g(u_{nj}) u_{nj}^\phi, \partial_t e_h^n(t_{nj}) \right)
\]
\[
- \int_{I_n} P^n \tau d^n \tau P^n \tau [P^n \tau e_h^n(t)(t_n - t)] \, dt = \sum_{m=1}^{3} J_{r1}^m.
\]

By using (3.22), we have
\[
J_{r1}^1 \leq \tau \frac{1}{4} \sum_{j=1}^{K} w_j |P^n \tau [P^n \tau e_{nj}(t_n - t_{nj})]| g(u_{nj}) u_{nj}^\phi - g(u_{nj}) u_{nj}^* \left\| \partial_t u_h^n(t_{nj}) \right\|
\]
(4.86)
\[
\leq C \tau \sum_{j=1}^{K} w_j |P^n \tau [P^n \tau e_{nj}(t_n - t_{nj})]| e_{nj}^u
\]
\[
\leq \frac{1}{8 \tau^2} \int_{I_n} \sum_{j=1}^{K} w_j |P^n \tau [P^n \tau e_{nj}(t_n - t_{nj})]|^2 \, dt + C \tau^2 \int_{I_n} \left\| P^n \tau e_h^n \right\|^2 \, dt
\]
\[
\leq \frac{1}{8 \tau^2} \int_{I_n} \left\| P^n \tau e_h^n(t)(t_n - t) \right\|^2 \, dt + C \tau^2 \int_{I_n} \left\| P^n \tau e_h^n \right\|^2 \, dt
\]
\[
\leq \frac{1}{8 \tau^2} \int_{I_n} \left\| P^n \tau e_h^n \right\|^2 \, dt + C \tau^2 \int_{I_n} \left\| e_h^n \right\|^2 \, dt,
\]
\[
J_{r1}^2 \leq \frac{\tau}{4} \sum_{j=1}^{K} w_j |P^n \tau [P^n \tau e_{nj}(t_n - t_{nj})]| \left\| g(u_{nj}) u_{nj}^\phi \right\| \left\| \partial_t u_h^n(t_{nj}) \right\|
\]\n(4.87)
\[
\leq \frac{1}{8 \tau^2} \int_{I_n} \sum_{j=1}^{K} w_j |P^n \tau [P^n \tau e_{nj}(t_n - t_{nj})]|^2 \, dt + C \tau^2 \int_{I_n} \left\| \partial_t e_h^n(t_{nj}) \right\|^2 \, dt
\]
Substituting (4.86)–(4.88) into (4.84)–(4.85), and using (3.21), we get

\[ v_n(t) \leq C \tau^2 \int I_n \| \nabla e_h^n(t) \|^2 dt + C \tau^3 \max_{t \in I_n} \| P_n \tau e_h^n(t) \|^2. \] (4.89)

Then, combining (4.81) and (4.89), we obtain (for sufficiently small \( \tau \))

\[ \int I_n \| e_h^n(t) \|^2 dt \leq C \tau \left[ \| e_h^n(t_{n-1}) \|^2_{H^1} + \| e_h^n(t_{n-1}) \|^2 \right] \]

\[ + \tau^2 \max_{t \in I_n} \left( \| d_n \|^2_{H^1} + \| d_n \|^2 \right), \]

\[ \int I_n \| e_h^n(t) \|^2 dt \leq C \tau \left[ \| e_h^n(t_{n-1}) \|^2_{H^1} + \| e_h^n(t_{n-1}) \|^2 + \tau^2 \max_{t \in I_n} \left( \| d_n \|^2_{H^1} + \| d_n \|^2 \right) \right]. \] (4.91)

**Step 3: Estimation of \( \| \nabla e_h^n(t) \| \) and \( \| e_h^n(t) \| \)**. Setting \( v_n = \partial_t e_h^n \) in (4.73) and taking the real part, we get

\[ \frac{1}{2} \| \nabla e_h^n(t) \|^2 - \frac{1}{2} \| \nabla e_h^n(t_{n-1}) \|^2 = \frac{\theta \tau}{2} \sum_{j=1}^k w_j Re \left( \epsilon_{r_{n_j}}^n g(u_{n_j})u_{n_j}^\phi, \partial_t e_h^n(t_{n_j}) \right) \] (4.92)

\[ + \frac{\tau}{2} \sum_{j=1}^k w_j \Re \left( r_{r_{n_j}}^* \left[ g(u_{n_j})^\phi u_{n_j}^\phi - g(u_{n_j})^\phi u_{n_j}^\phi \right], \partial_t e_h^n(t_{n_j}) \right) - \int I_n \Re (d_n, \partial_t e_h^n) dt \]

\[ \leq C \tau \sum_{j=1}^k w_j (\| e_h^n(t_{n_j}) \| + \| \nabla e_h^n(t_{n_j}) \|) \| \partial_t e_h^n(t_{n_j}) \|_{H^1} + C \int I_n \| d_n \|^2_{H^1} \| \partial_t e_h^n \|^2_{H^{-1}} dt \]

\[ \leq C \int I_n \left( \| e_h^n(t) \|^2_{H^1} + \| e_h^n(t) \| \right)^2 + \| d_n \|^2_{H^1} dt + \frac{1}{2} \int I_n \| \partial_t e_h^n \|^2_{H^{-1}} dt. \]

In order to estimate the last term \( \int I_n \| \partial_t e_h^n \|^2_{H^{-1}} dt \) above, we consider (4.73), from which we can derive the following estimate for any test function \( v \in L^2(I_n; H^1_0) \):

\[ \int I_n (\partial_t e_h^n, v) dt = i \int I_n (\nabla e_h^n, \nabla P_n \tau v) dt \]

\[ - \frac{i \tau}{2} \sum_{j=1}^k w_j \left( \epsilon_{r_{n_j}}^n g(u_{n_j})u_{n_j}^\phi, P_n \tau v(t_{n_j}) \right) \]

\[ - \frac{i}{2} \sum_{j=1}^k w_j \left( r_{r_{n_j}}^* \left[ g(u_{n_j})^\phi u_{n_j}^\phi - g(u_{n_j})^\phi u_{n_j}^\phi \right], P_n \tau v(t_{n_j}) \right) \]
\[ + 1 \int_{I_n} \left( d^n u, P_n P^n v \right) dt \]
\[ \leq C \left( \| e^n \|_{L^2(I_n; H^1)} + \| e^n_h \|_{L^2(I_n)} + \| d^n u \|_{L^2(I_n; H^1)} \right) \]
\[ \leq C \left( \| e^n \|_{L^2(I_n; H^1)} + \| e^n_h \|_{L^2(I_n)} + \| d^n u \|_{L^2(I_n; H^1)} \right) \| v \|_{L^2(I_n; H^1)}. \]

By the duality between \( L^2(I_n; H^{-1}) \) and \( L^2(I_n; H^1) \), we obtain
\[ \int_{I_n} \| \partial_t e^n_h \|_{H^{-1}} dt \leq C \int_{I_n} \left( \| e^n \|_{H^1}^2 + \| e^n_h \|_{H^{-1}}^2 \right) dt. \tag{4.93} \]

Then, summing up (4.92) and (4.93), we have
\[ \| \nabla e^n_{t_n} \|_{H^1}^2 - \| \nabla e^n_{t_{n-1}} \|_{H^1}^2 + \int_{I_n} \| \partial_t e^n_{t} \|_{H^{-1}} dt \]
\[ \leq C \int_{I_n} \left( \| e^n \|_{H^1}^2 + \| e^n_h \|_{H^{-1}}^2 \right) dt. \tag{4.94} \]

Setting \( q_h = 2e^n_h \) in (4.74) yields
\[ | e^n_{t_n} |^2 - | e^n_{t_{n-1}} |^2 = \frac{7}{2} \sum_{j=1}^k w_j \text{Re} \left( e^n_{n_j} \left( g(u^n_{n_j}) u^n_{n_j} - g(u^n_{n_j}) u^n_{n_j} \right), \partial_t u^n_{n_j} \right) \]
\[ + \frac{\theta \tau}{2} \sum_{j=1}^k w_j \text{Re} \left( e^n_{n_j} g(u^n_{n_j}) u^n_{n_j}, \partial_t e^n_{n_j} \right) \]
\[ - \int_{I_n} P^n d^n \| 2 e^n \| dt \tag{4.95} \]
\[ \leq C \tau \sum_{j=1}^k w_j | e^n_{n_j} | | e^n_{n_j} | + C \tau \sum_{j=1}^k w_j | e^n_{n_j} | \| \partial_t e^n_{n_j} \|_{H^1} \]
\[ + C \int_{I_n} | P^n d^n \| \| e^n \| dt \]
\[ \leq C \int_{I_n} \left( \| e^n \|_{H^1}^2 + \| e^n_h \|_{H^1}^2 + \| \partial_t e^n_{n_j} \|_{H^{-1}}^2 \right) dt + C \int_{I_n} \| P^n d^n \| ^2 dt \]
\[ \leq C \int_{I_n} \left( \| e^n \|_{H^1}^2 + \| e^n_h \|_{H^1}^2 \right) dt + C \int_{I_n} \left( d^n u \| ^2 + | P^n d^n \| ^2 \right) dt, \]

where we have used (4.93) to obtain the last inequality.

**Step 4: Completion of the proof.** Summing up (4.94) and (4.95) yields
\[ \| \nabla e^n_{t_n} \|_{H^1}^2 - \| \nabla e^n_{t_{n-1}} \|_{H^1}^2 + \int_{I_n} \| \partial_t e^n_{n_j} \|_{H^{-1}}^2 dt \]
\[ \leq C \int_{I_n} \left( \| e^n \|_{H^1}^2 + \| e^n_h \|_{H^1}^2 \right) dt + C \int_{I_n} \left( d^n u \| ^2 + | P^n d^n \| ^2 \right) dt. \tag{4.96} \]

Then, substituting (4.90)–(4.91) into the inequality above, we obtain
\[ \left( \| \nabla e^n_{t_n} \|_{H^1}^2 + \| e^n_{t_n} \|_{H^1}^2 \right) - \left( \| \nabla e^n_{t_{n-1}} \|_{H^1}^2 + | e^n_{t_{n-1}} \|_{H^1}^2 \right) + \int_{I_n} \| \partial_t e^n_{n_j} \|_{H^{-1}}^2 dt \tag{4.97} \]
\[ \leq C\tau (\|\nabla e_h^{u}(t_{n-1})\|^2 + |e_h^{r}(t_{n-1})|^2) + C \int_{I_n} (\|d_n^{u}\|_{H^1}^2 + |P^{nu}d_n^{r}|^2) dt. \]

It follows from Gronwall’s inequality that
\[
\max_{1 \leq n \leq N} (\|\nabla e_h^{u}(t_n)\|^2 + |e_h^{r}(t_n)|^2) + C \int_0^T \|\partial_t e_h^{u}\|_{H^{-1}}^2 dt
\leq C (\|e_h^{u}(0)\|_{H^1}^2 + |e_h^{r}(0)|^2) + C \sum_{n=1}^N \int_{I_n} (\|d_n^{u}\|_{H^1}^2 + |P^{nu}d_n^{r}|^2) dt. \tag{4.98} \]

Then, substituting this inequality into (4.90)–(4.91) and using temporal inverse inequality, we obtain
\[
\max_{t \in [0,T]} (\|e_h^{u}(t)\|_{H^1}^2 + |e_h^{r}(t)|^2)
\leq C \left[ \|e_h^{u}(0)\|_{H^1}^2 + |e_h^{r}(0)|^2 + \max_{1 \leq n \leq N} \max_{t \in I_n} (\|d_n^{u}\|_{H^1}^2 + |P^{nu}d_n^{r}|^2) \right]. \tag{4.99} \]

Hence, (4.70) holds.

When \(\tau\) and \(h\) are sufficiently small, inequality (4.99) implies that
\[
\max_{t \in [0,T]} \|e_h^{u}(t)\|_{H^1} \leq \frac{1}{2} \quad \text{and} \quad \max_{t \in [0,T]} |e_h^{r}(t)| \leq \frac{1}{2}. \tag{4.100} \]

On the one hand, by the inverse inequality, we have
\[
\max_{t \in [0,T]} \|e_h^{u}(t)\|_{L^\infty} \leq C \ell_h \max_{t \in [0,T]} \|e_h^{u}(t)\|_{H^1}
\leq C \ell_h \left[ \|e_h^{u}(0)\|_{H^1} + |e_h^{r}(0)| + \max_{1 \leq n \leq N} \max_{t \in I_n} (\|d_n^{u}\|_{H^1} + |P^{nu}d_n^{r}|) \right], \tag{4.101} \]

where
\[ \ell_h = \begin{cases} \frac{1}{\ln(2 + 1/h)} & \text{if } d = 2, \\ h^{-\frac{1}{2}} & \text{if } d = 3. \end{cases} \]

On the other hand, by choosing a test function \(v\) in (4.73) satisfying the properties \(v(t_{nj}) = 1\) and \(v(t_{ni}) = 0\) for \(i \neq j\), and using property (3.18), we obtain
\[
\|\Delta_h e_{nj}^{u}\| = \|i \partial_t e_{nj}^{u} - \theta P_h \left[ e_{nj}^{r} g(u_{nj}^{\phi}) u_{nj}^{\phi} \right] + P_h d_{nj}^{u} - P_h \left[ r_{nj}^{*} (g(u_{nj}^{\phi}) u_{nj}^{\phi} - g(u_{nj}^{*}) u_{nj}^{*}) \right] \| 
\leq C \tau^{-1} \left[ \|e_h^{u}(0)\|_{H^1} + |e_h^{r}(0)| + \max_{1 \leq n \leq N} \max_{t \in I_n} (\|d_n^{u}\|_{H^1} + |P^{nu}d_n^{r}|) \right], \]

where we have used (4.98)–(4.99) and an inverse inequality in time in estimating \(\partial_t e_{nj}^{u}\). By the discrete Sobolev embedding inequality, for \(1 \leq d \leq 3\) we have
\[
\|e_{nj}^{u}\|_{L^\infty} \leq C \|e_{nj}^{u}\|_{H^1}^{\frac{1}{2}} \|\Delta_h e_{nj}^{u}\|^{\frac{1}{2}}
\leq C \tau^{-\frac{1}{2}} \max_{1 \leq n \leq N} \left[ \|e_h^{u}(0)\|_{H^1} + |e_h^{r}(0)| + \max_{1 \leq n \leq N} \max_{t \in I_n} (\|d_n^{u}\|_{H^1} + |P^{nu}d_n^{r}|) \right], \tag{4.103} \]

26
where we have used (4.99) and (4.102) in the last inequality. Then, combining (4.101) and (4.103) yields

\[
\max_{1 \leq n \leq N} \max_{1 \leq j \leq k} \|e^{n}(t_{nj})\|_{L^{\infty}} \\
\leq C \min(\epsilon, \tau^{-\frac{1}{2}}) \left[\left\|e^{0}(0)\right\|_{H^{1}} + \left|e^{0}(0)\right| + \max_{1 \leq n \leq N} \max_{t \in t_{n}} \left(\|d^{n}_{t}\|_{H^{1}} + \|P^{n}_{t}d^{n}_{t}\|_{H^{1}}\right)\right] \\
\leq C(h^{p-\frac{1}{2}} + \tau^{k+\frac{1}{2}}),
\]

where we have used the consistency estimate from Theorem 3.3. When \(\tau\) and \(h\) are sufficiently small, the inequality above implies

\[
\max_{1 \leq n \leq N} \max_{1 \leq j \leq k} \|e^{n}(t_{nj})\|_{L^{\infty}} \leq \frac{1}{2}.
\]

This together with (4.100) gives (4.71).

Furthermore, since \(\phi_{h} = \theta e^{h}_{n}\) and \(\varphi_{h} = \theta e^{r}_{n}\), it follows that

\[
\max_{1 \leq n \leq N} \max_{1 \leq j \leq k} \|\phi_{h}(t_{nj})\|_{L^{\infty} \cap H^{1}} \leq \frac{1}{2} \quad \text{and} \quad \max_{1 \leq n \leq N} \max_{1 \leq j \leq k} \|\varphi_{h}(t_{nj})\| \leq \frac{1}{2},
\]

which imply \(\rho[\phi_{h}] = \rho[\varphi_{h}] = 1\) in view of the definition in (4.62). This proves (4.72). \(\square\)

We now are ready to state and prove existence, uniqueness and convergence of numerical solutions, which comprise of the second main theorem of this paper.

**Theorem 4.2** Let \(1 \leq d \leq 3\) and assume that the solution of the NLS equation (1.1) is sufficiently smooth. Then there exist positive constants \(\tau_{0}\) and \(h_{0}\) such that when \(\tau \leq \tau_{0}\) and \(h \leq h_{0}\), the numerical method (2.12) has a unique solution \((u_{h}, r_{h}) \in X^{*}_{\tau, h} \times Y^{*}_{\tau, h}\). Moreover, this solution satisfies the following error estimate:

\[
\max_{t \in [0, T]} \left(\|u_{h}(t) - u^{n}_{h}(t)\|_{H^{1}} + \|r_{h}(t) - r^{n}_{h}(t)\|_{H^{1}}\right) \leq C(h^{p} + \tau^{k+1}).
\]

**Proof.** Step 1: Existence. By the definition of \(\mathfrak{B}\), if \((\phi_{h}, \varphi_{h}) \in \mathfrak{B}\) and \((e^{u}_{h}, e^{r}_{h}) = M(\phi_{h}, \varphi_{h})\) then \(\phi_{h} = \theta e^{u}_{h}\) and \(\varphi_{h} = \theta e^{r}_{h}\). Thus (4.70) implies

\[
\|(\phi_{h}, \varphi_{h})\|_{X^{*}_{\tau, h} \times Y^{*}_{\tau, h}} = \|\phi_{h}\|_{L^{\infty}(0, T; H^{1})} + \|\varphi_{h}\|_{L^{\infty}(0, T)} \leq C,
\]

which together with Schaefer’s fixed point theorem imply the existence of a fixed point \((\phi_{h}, \varphi_{h})\) for the mapping \(M\) (corresponding to \(\theta = 1\)), with

\[
(e^{u}_{h}, e^{r}_{h}) = (\phi_{h}, \varphi_{h}), \quad u^{\phi} = u^{*}_{h} + \phi_{h} \quad \text{and} \quad r^{\phi} = r^{*}_{h} + \varphi_{h},
\]

satisfying (4.66)–(4.67), where we have used (4.72) in the expression (4.65). Consequently, \((e^{u}_{h}, e^{r}_{h})\) is a solution of (4.58) with \((u_{h}, r_{h}) = (u^{0}_{h}, r^{0}_{h}) = (u^{*}_{h} + e^{u}_{h}, r^{*}_{h} + e^{r}_{h})\). Hence, in view of the discussions in Remark 4.1, \((u_{h}, r_{h})\) is a solution of the numerical scheme (2.12), and (4.71) implies \((u_{h}, r_{h})\) is in the set \(X^{*}_{\tau, h} \times Y^{*}_{\tau, h}\) defined in (4.60)–(4.61). This proves existence of a numerical solution in \(X^{*}_{\tau, h} \times Y^{*}_{\tau, h}\).

Step 2: Uniqueness. Suppose that \((u_{h}, r_{h})\) and \((\bar{u}_{h}, \bar{r}_{h})\) in \(X^{*}_{\tau, h} \times Y^{*}_{\tau, h}\) are two pairs of numerical solutions, and set \(e^{h}_{h} = u_{h} - \bar{u}_{h}\) and \(e^{r}_{h} = r_{h} - \bar{r}_{h}\) (abusing the notation). Subtracting the
corresponding equations satisfied by \((u_h, r_h)\) and \((\tilde{u}_h, \tilde{r}_h)\) shows that \((e^u_h, e^r_h)\) satisfies equations (4.58) with \(d^u_n = d^r_n = 0\). In the meantime, the definition in (4.60)–(4.61) implies
\[
\left\| e^u_h(t_{nj}) \right\|_{L^\infty(H^1)} \leq 1 \quad \text{and} \quad \left| e^r_h(t_{nj}) \right| \leq 1.
\]
(4.107)

Accordingly, \((e^u_h, e^r_h)\) is a fixed point of the mapping \(M\) (corresponding to \(\theta = 1\) in \(\mathcal{B}\)) in the case \(e^u_h(0) = e^r_h(0) = 0\) and \(d^u_n = d^r_n = 0\). Hence, an application of (4.70) yields
\[
\left\| e^u_h \right\|_{L^\infty(0,T;H^1)} + \left\| e^r_h \right\|_{L^\infty(0,T)} \leq C \left[ \left\| e^u_h(0) \right\|_{H^1} + \left\| e^r_h(0) \right\| + \max_{1 \leq n \leq N} \max_{t \in I_n} \left( \left\| d^u_n \right\|_{H^1} + \left| P_n^\tau d^r_n \right| \right) \right] = 0.
\]

Thus, \((u_h, r_h) = (\tilde{u}_h, \tilde{r}_h)\) and the uniqueness of the numerical solution is proved.

**Step 3: Error estimate.** Since the error functions \(e^u_h = u_h - u_h^*\) and \(e^r_h = r_h - r_h^*\) satisfy (4.58) and (4.107), it follows that \((e^u_h, e^r_h)\) is a fixed point of the mapping \(M\) (corresponding to \(\theta = 1\) in \(\mathcal{B}\)). Hence, an application of (4.70) yields
\[
\left\| e^u_h \right\|_{L^\infty(0,T;H^1)} + \left\| e^r_h \right\|_{L^\infty(0,T)} \leq C \left[ \left\| e^u_h(0) \right\|_{H^1} + \left\| e^r_h(0) \right\| + \max_{1 \leq n \leq N} \max_{t \in I_n} \left( \left\| d^u_n \right\|_{H^1} + \left| P_n^\tau d^r_n \right| \right) \right] = 0.
\]

Substituting the consistency error estimates from Theorem 3.3 into the above inequality yields the desired estimate (4.105). The proof is complete. \(\square\)

**Remark 4.2** For the periodic and Neumann boundary conditions, the mass and energy conservations in Theorem 3.1 and the error estimate in Theorem 4.2 can be proved similarly.

## 5 Numerical experiments

In this section, we present some one-dimensional numerical tests to validate the theoretical results proved in Theorems 3.1 and 4.2 about the mass and energy conservations, and the convergence rates of the proposed method. All the computations are performed using the software package FEniCS (https://fenicsproject.org).

We consider the cubic nonlinear Schrödinger equation
\[
i\partial_t u - \partial_{xx} u - 2|u|^2 u = 0 \quad \text{in} \quad (-L, L) \times (0,T],
\]
\[
u|_{t=0} = u_0 \quad \text{in} \quad (-L, L), \quad \text{with} \quad L = 20,
\]
subject to the periodic boundary condition. We choose \(u_0 = \text{sech}(x) \exp(2ix)\) so that the exact solution is given by
\[
u(x,t) = \text{sech}(x + 4t) \exp(i(2x + 3t)).
\]

This example contains a soliton wave and is often used as a benchmark for measuring the effectiveness of numerical methods for the NLS equation; see [35, 39, 26].
5.1 Convergence rates

We solve problem (5.108) by the proposed method (2.12) and compare the numerical solutions with the exact solution (5.109). Newton’s iteration is used to solve the nonlinear system. The iteration is stopped when the error is below $10^{-10}$.

The time discretization errors are presented in Table 1, where we have used finite elements of degree 3 with a sufficiently spatial mesh $h = 2L/5000$ so that the error from spatial discretization is negligibly small in observing the temporal convergence rates. From Table 1 we see that the error of time discretization is $O(\tau^{k+1})$, which is consistent with the result proved in Theorem 4.2.

The spatial discretization errors are presented in Table 2, where we have chosen $k = 3$ with a sufficiently small time stepsize $\tau = 1/1000$ so that the time discretization error is negligibly small compared to the spatial error. From Table 2 we see that the spatial discretization errors are $O(h^p)$ in the $H^1$ norm. This is also consistent with the result proved in Theorem 4.2.

5.2 Mass and energy conservations

We denote the mass and SAV energy of a numerical solution by

$$M_h(t) = \int_{\Omega} |u_h(t)|^2 dx \quad \text{and} \quad E_h(t) = \frac{1}{2} \int_{\Omega} |\nabla u_h(t)|^2 dx - r_h(t)^2,$$

(5.110)

respectively. The evolution of mass and SAV energy of the numerical solutions is presented in Figure 1 with $\tau = 0.2$ and $h = 0.2$. It is shown that

$$\text{mass} = 2 + O(10^{-12}) \quad \text{and} \quad \text{SAV energy} = -3.66679024258 + O(10^{-12}),$$

which are much smaller than the error of the numerical solutions, as shown in Figure 2. This shows the effectiveness of the proposed method in preserving mass and energy (independent of the error of numerical solutions).

5.3 Comparison of different methods in preserving the shape of a soliton

The graph of $|u(x,t)|$ is a soliton propagating towards left. Its shape remains unchanged for all $t \geq 0$ as shown in Figure 3. The graphs of numerical solutions given by several different numerical methods using the same mesh sizes are presented in Figures 4 and 5. All the methods preserve mass and energy conservations. The numerical results show the effectiveness of the proposed method in preserving the shape of the soliton.

References

[1] G. D. Akrivis, V. A. Dougalis and O. A. Karakashian, On fully discrete Galerkin methods of second-order temporal accuracy for the NLS equation, Numer. Math., 59(1991), pp. 31–53.

[2] G. Akrivis, Finite difference discretization of the cubic Schrödinger equation, IMA J. Numer. Anal. 13(1993), pp. 115–124.

[3] G. Akrivis, B. Li and D. Li, Energy-decaying extrapolated RK-SAV methods for the Allen–Cahn and Cahn–Hilliard equations, SIAM J. Sci. Comput., 41(2019), pp. A3703–A3727.
Table 1: Time discretization errors of the proposed method, with $h = \frac{2L}{5000}$ and $T = 1$.

| $k$ | $\tau$ | $p = 3$ |
|-----|---------|---------|
|     |         | $\|u(x,t) - u_h(x,t)\|_{L^\infty(0,T;H^1)}$ | order |
| 1/60 | 3.7964E-05 | – |
| 1/70 | 2.3429E-05 | 3.1312 |
| 1/80 | 1.5460E-05 | 3.1132 |
| 1/90 | 1.0733E-05 | 3.0985 |
| 1/100| 7.7542E-06 | 3.0853 |

| 1/20 | 3.4019E-05 | – |
| 1/20 | 1.3821E-05 | 4.0364 |
| 1/30 | 6.6322E-06 | 4.0275 |
| 1/35 | 3.5689E-06 | 4.0200 |
| 1/40 | 2.0886E-06 | 4.0123 |

| 1/8  | 1.2291E-04 | – |
| 1/12 | 1.5120E-05 | 5.1681 |
| 1/14 | 6.8492E-06 | 5.1369 |
| 1/16 | 3.4634E-06 | 5.1067 |
| 1/20 | 1.1555E-06 | 4.9192 |

Table 2: Time discretization errors of the proposed method, with $\tau = \frac{1}{1000}$ and $T = 1$.

| $p$ | $M$ | $k = 3$ |
|-----|-----|---------|
|     |     | $\|u(x,t) - u_h(x,t)\|_{L^\infty(0,T;H^1)}$ | order |
| 2   | 1400| 5.8670E-02 |     |
| 1   | 1600| 5.1134E-02 | 1.0295 |
| 1   | 1800| 4.5330E-02 | 1.0229 |
| 1   | 2000| 4.0719E-02 | 1.0183 |
| 1   | 2200| 3.6964E-02 | 1.0149 |
|     | 240 | 1.9306E-02 | – |
|     | 260 | 1.6438E-02 | 2.0094 |
| 2   | 280 | 1.4167E-02 | 2.0062 |
| 2   | 300 | 1.2338E-02 | 2.0041 |
| 2   | 320 | 1.0842E-02 | 2.0027 |
| 3   | 90 | 1.6147E-02 | – |
| 3   | 100 | 1.1661E-02 | 3.0894 |
| 3   | 110 | 8.7112E-03 | 3.0599 |
|     | 120 | 6.6844E-03 | 3.0436 |
|     | 130 | 5.2435E-03 | 3.0334 |
Figure 1: Evolution of mass $M_h(t) - M_h(0)$ and SAV energy $E_h(t) - E_h(0)$, with $p = 3$ and $\tau = h = 0.2$.

Figure 2: Evolution of error of the numerical solution, with $p = 3$ and $\tau = h = 0.2$.

Figure 3: Soliton propagation when $t \in [0, 2]$: graph of the exact solution $|u(\cdot, t)|$. 
Figure 4: Soliton propagation when $t \in [0, 2]$: numerical solutions with $p = 1$, $M = 1200$ and $\Delta t = 0.1$.

Figure 5: Soliton propagation when $t \in [0, 2]$: numerical solutions with $p = 1$, $M = 1200$ and $\Delta t = 0.05$. 
[4] X. Antoine, W. Bao and C. Besse, Computational methods for the dynamics of the nonlinear Schrödinger/Gross–Pitaevskii equations, Comput. Phys. Commun., 184(2013), pp. 2621–2633.

[5] W. Bao and Y. Cai, Optimal error estimates of finite difference methods for the Gross–Pitaevskii equation with angular momentum rotation, Math. Comp., 82(2013), pp. 99–128.

[6] W. Bao, Q. Tang and Z. Xu, Numerical methods and comparison for computing dark and bright solitons in the NLS equation, J. Comput. Phys., 235(2013), pp. 423–445.

[7] C. Besse, A relaxation scheme for the nonlinear Schrödinger equation, SIAM J. Numer. Anal., 42(2004), pp. 934–952.

[8] J. Bourgain, Global Solutions of Nonlinear Schrödinger Equations, vol. 46, American Mathematical Society, 1999.

[9] S. C. Brenner and L. R. Scott, The Mathematical Theory of FEMs, Third edition. Texts in Applied Mathematics, Vol. 15, Springer, New York, 2008.

[10] C. Canuto, M. Y. Hussaini, A. Quarteroni and T. A. Zang, Spectral Methods: Fundamentals in Single Domains, Springer, Berlin, 2007.

[11] M. Delfour, M. Fortin and G. Payre, Finite-difference solutions of a non-linear Schrödinger equation, J. Comput. Phys., 44(1981), pp. 277–288.

[12] L. C. Evans, Partial Differential Equations, second edition, Graduate Studies in Mathematics 19, AMS, Providence, RI, 2010.

[13] X. Feng, H. Liu and S. Ma, Mass- and energy-conserved numerical schemes for nonlinear Schrödinger equations, Commun. Comput. Phys., 26(2019), pp. 1365–1396.

[14] Z. Gao and S. Xie, Fourth-order alternating direction implicit compact finite difference schemes for two-dimensional Schrödinger equations, Appl. Numer. Math., 61(2011), pp. 593–614.

[15] D. Gilbarg and N. Trudinger, Elliptic Partial Differential Equations of Second Order, Springer, New York, 2001.

[16] G. H. Golub and J. H. Welsch, Calculation of Gauss quadrature rules, Math. Comput., 23(1969), pp. 221–230.

[17] Y. Gong, Q. Wang and Y. Wang, A conservative Fourier pseudo-spectral method for the nonlinear Schrödinger equation, J. Comput. Phys., 328(2017), pp. 354–370.

[18] Y. Gong and J. Zhao, Energy-stable Runge-Kutta schemes for gradient flow models using the energy quadratization approach, Appl. Math. Letters, 94(2019), pp. 224–231.

[19] Y. Gong, J. Zhao and Q. Wang, Arbitrarily high-order unconditionally energy stable schemes for thermodynamically consistent gradient flow models, SIAM J. Sci. Comput. 42(2020), pp. B135–156.
[20] P. Henning and D. Peterseim, *Crank-Nicolson Galerkin approximations to nonlinear Schrödinger equations with rough potentials*, Math. Models Meth. Appl. Sci., 27(2017), pp. 2147–2184.

[21] J. Hong, Y. Liu, H. Munthe-Kaas and A. Zanna, *Globally conservative properties and error estimation of a multi-symplectic scheme for Schrödinger equations with variable coefficients*, Appl. Numer. Math., 56(2006), pp. 814–843.

[22] O. Karakashian and C. Makridakis, *A space-time finite element method for the nonlinear Schrödinger equation: the discontinuous Galerkin method*, Math. Comp., 67(1998), pp. 479–499.

[23] O. Karakashian and C. Makridakis, *A space-time finite element method for the nonlinear Schrödinger equation: the continuous Galerkin method*, SIAM J. Numer. Anal., 36(1999), pp. 1779–1807.

[24] D. A. Kopriva, *Implementing spectral methods for partial differential equations: Algorithms for scientists and engineers*, Springer Science & Business Media, 2009.

[25] H. Liu, Y. Huang, W. Lu and N. Yi, *On accuracy of the mass-preserving DG method to multi-dimensional Schrödinger equations*, IMA J. Numer. Anal., 39(2019), pp. 760–791.

[26] W. Lu, and Y. Huang and H. Liu, *Mass preserving discontinuous Galerkin methods for Schrödinger equations*, J. Comput. Phys., 282(2015), pp. 210–226.

[27] D. E. Pelinovsky, V. V. Afanasjev and Y. S. Kivshar, *Nonlinear theory of oscillating, decaying, and collapsing solitons in the generalized nonlinear Schrödinger equation*, Phys. Rev. E, 53(1996), pp. 1940–1953.

[28] J. M. Sanz-Serna, *Methods for the numerical solution of the nonlinear Schrödinger equation*, Math. Comp., 43(1984), pp. 21–27.

[29] J. M. Sanz-Serna and V. S. Manoranjan, *A method for the integration in time of certain partial differential equations*, J. Comput. Phys., 52(1983), pp. 273–289.

[30] H. W. Schürmann, *Traveling-wave solutions of the cubic-quintic nonlinear Schrödinger equation*, Phys. Rev. E, 54 (1996), pp. 4312–4320.

[31] J. Shen, J. Xu and J. Yang, *A new class of efficient and robust energy stable schemes for gradient flows*, SIAM Rev., 61(2019), pp. 474–506.

[32] J. Shen, J. Xu and J. Yang, *The scalar auxiliary variable (SAV) approach for gradient flows*, J. Comput. Phys., 353(2018), pp. 407–416.

[33] J. Shen, T. Tang and L. L. Wang, *Spectral methods: algorithms, analysis and applications*, Springer Science & Business Media, 41(2011).

[34] W. A. Strauss and L. Vazquez, *Numerical solution of a nonlinear Klein–Gordon equation*, J. Comput. Phys., 28(1978), pp. 271–278.

[35] N. Taghizadeh, M. Mirzazadeh and F. Farahrooz, *Exact solutions of the nonlinear Schrödinger equation by the first integral method*, J. Math. Anal. Appl., 374(2011), pp. 549–553.
[36] T. Tao, Nonlinear Dispersive Equations: Local and Global Analysis, American Mathematical Society, 2006.

[37] J. Wang, A new error analysis of Crank–Nicolson Galerkin FEMs for a generalized nonlinear Schrödinger equation, J. Sci. Comput., 60(2014), pp. 390–407.

[38] T. Wang, B. Guo and Q. Xu, Fourth-order compact and energy conservative difference schemes for the nonlinear Schrödinger equation in two dimensions, J. Comput. Phys., 243(2013), pp. 382–399.

[39] Y. Xu and C. W. Shu, Local discontinuous Galerkin methods for nonlinear Schrödinger equations, J. Comput. Phys., 205(2005), pp. 72–97.

[40] X. Yang, Linear, first and second-order, unconditionally energy stable numerical schemes for the phase field model of homopolymer blends, J. Comput. Phys. 327(2016), pp. 294–316.

[41] X. Yang and L. Ju, Efficient linear schemes with unconditional energy stability for the phase field elastic bending energy model, Comput. Meth. Appl. Mech. Engrg., 315(2017), pp. 691–712.

[42] X. Yang and L. Ju, Linear and unconditionally energy stable schemes for the binary fluid-surfactant phase field model, Comput. Meth. Appl. Mech. Engrg., 318(2017), pp. 1005–1029.

[43] X. Yang, J. Zhao, Q. Wang and J. Shen, Numerical approximations for a three components Cahn–Hilliard phase-field model based on the invariant energy quadratization method, Math. Models Methods Appl. Sci., 27(2017), pp. 1993–2030.

[44] N. J. Zabusky and M. D. Kruskal, Interaction of ”solitons” in a collisionless plasma and the recurrence of initial states, Phys. Rev. Lett., 15(1965), pp. 240–243.

[45] F. Zhang, V. M. Pérez-Garcia and L. Vázquez, Numerical simulation of nonlinear Schrödinger systems: a new conservative scheme, Appl. Math. Comput., 71(1995), pp.165–177.