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ENERGY AND MASS CONSERVATIVE AVERAGING LOCAL DISCONTINUOUS GALERKIN METHOD FOR SCHRöDINGER EQUATION

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Abstract. In this article, we develop the semi-discrete and fully discrete averaging local discontinuous Galerkin method to solve the well-known Schrödinger equation, in which space is discretized by the averaging local discontinuous Galerkin (ADG) method, and the time is discretized by Crank-Nicolson approach. Energy and mass conservative property of both schemes are proved. These schemes are shown to be unconditionally energy stable, and the error estimates are rigorously proved. Some numerical examples are performed to demonstrate the accuracy numerically.

Key words. Averaging local discontinuous Galerkin method, Schrödinger equation, energy conservative, mass conservative, error analysis.

1. Introduction

In this paper, we study the local discontinuous Galerkin method with averaging flux [27] for the nonlinear Schrödinger equation. According to the differential definition of the energy potential, the nonlinear Schrödinger equation can be divided into two types: one is called linear Schrödinger equation, i.e., the energy potential $v(x,u)$ equals to some given function, the other is nonlinear Schrödinger equation, e.g., $v(x,u) = c|u|^2$. The Schrödinger equation is the fundamental equation used to describe quantum mechanical behavior. It is often called the Schrödinger wave equation. Energy conservation and mass conservation are two important concepts in the theory of Schrödinger equation. The presence of nonlinearity is the main cause for stiffness which in turn involves many challenges for the algorithm developments. Therefore, an efficient and accurate numerical solution of this equation is needed to understand its dynamics. Concerning the temporal and spatial discretizations, various numerical approaches had been developed to solve it, including finite difference method [3, 16], finite element method [14, 23], spectral method [21], and discontinuous Galerkin method [15, 19, 25, 30]. The conservation law structure of many PDEs is considered to be fundamental in their discretization since numerical methods that can preserve the required invariants always have some advantages, e.g., the high accuracy of numerical solutions, unconditional stability properties after long-time numerical integration, etc.

The discontinuous Galerkin (DG) method was first introduced by the pioneering work of Reed and Hill for solving the neutron transport problem, see [22]. After that, Lesaint and Raviant provide the first theoretical analysis of this DG method in [17]. After this method was generalized to the local discontinuous Galerkin (LDG) method by Cockburn and Shu to solve the convection-diffusion equation in [5], the DG method has been widely used to solve various hyperbolic and parabolic problems. Using a completely discontinuous piece-wise polynomial space for the numerical solution and the test function within the finite element framework, the DG method has the advantage of flexibility for unstructured meshes, easily

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to handle complex boundary conditions and interface problems. We refer to the interested readers to the reviews [1, 6] or books [4, 10, 12, 24] and references therein.

We recall that some recent attempts have been made to apply the DG discretization to solve the Schrödinger equation [19, 25, 28, 29]. Here we give a brief review of those work. In [25], Xu and Shu developed an LDG method to solve the nonlinear Schrödinger equation. For linearized Schrödinger equation, they obtained an error estimate of order $k + 1/2$ for polynomials of degree k. The optimal error estimate was further obtained in [26] by using special local projections. In [19], Lu, Cai, and Zhang presented a mass conservative LDG method to solve one-dimensional linear Schrödinger, but the theoretical analysis is missing. Zhang, Yu, and Feng presented a mass preserving direct discontinuous Galerkin (DDG) method for the one-dimensional coupled nonlinear Schrödinger (CNLS) equation [28], and in [29] for both one and two-dimensional CNLS equation. In [29] the conservation property is verified and further validated by some long time simulation results. In [11], Guo and Xu developed energy conservation fully discrete LDG method to solve multi-dimensional Schrödinger equation with wave operator. For linearized Schrödinger equation, they obtained the optimal error estimate for the semi-discrete scheme. The mass conservative DDG method to solve the Schrödinger equations is constructed in [20]. The optimal error estimate for the semi-discrete scheme is obtained. Conservative local discontinuous Galerkin method based on upwinding flux for nonlinear Schrödinger equation is introduced by Hong, Ji, and Liu in [13]. However, all the effort on the LDG method for Schrödinger equation is about the upwind flux. According to [27], we know the averaging flux has some advantage, e.g., the $2k + 2$ superconvergent order. Hence, in this paper, we present a fully discrete averaging local discontinuous Galerkin (ALDG) method with the Crank-Nicolson time discretization to solve the linear and nonlinear Schrödinger equation. This scheme can preserve both the energy and the mass at the discrete level. An optimal error estimate of even order and suboptimal error estimate of odd order are obtained for both the semi-discrete ALDG scheme and the fully discrete ALDG scheme.

The rest of this paper is organized as follows. In section 2, the model problem and the semi-discrete is presented. Meanwhile, the energy and mass conservation property of the semi-discrete scheme is proved. An energy and mass conservative fully discrete scheme will be introduced in section 3. In section 4, we present the error analysis for the semi-discrete scheme and fully discrete scheme. Section 5 contains numerical results for both linear and nonlinear problem to demonstrate the accuracy and capability of the methods. Concluding remarks are given in section 6.

2. Model problem and semi-discrete scheme

2.1. semi-discrete scheme. In this paper, we mainly focus on the following one dimension linear or nonlinear Schrödinger problem:

$$\mathrm{i}u_t + \frac{1}{2}u_{xx} - \phi(u)u = 0, \tag{1}$$

subject to an initial data

$$u(x, 0) = u_0(x), \tag{2}$$

and periodic boundary condition or zero Dirichlet boundary condition.

We first introduce the usual notations of the ALDG method [27]. Let $\mathcal{T}_h$ be a partition of the interval $I = [a, b]$ of the form $a = x_{\frac{1}{2}} < x_{\frac{3}{2}} < \cdots < x_{M+\frac{1}{2}} = b$ with $x_{j+\frac{1}{2}} = a + (j - 1)h, h = (b - a)/M$. The points $x_{j+\frac{1}{2}}$ are called nodes, while $I_j=[x_{j-\frac{1}{2}},x_{j+\frac{1}{2}}]$ will be referred to an element and $x_j=\frac{x_{j-\frac{1}{2}}+x_{j+\frac{1}{2}}}{2}$ be the center of the element. we also denote by $u^-_{j+\frac{1}{2}}$ and $u^+_{j+\frac{1}{2}}$ be the values of u at the discontinuity point $x_{j+\frac{1}{2}}$, from the left of the element I_j and the right of the element I_{j+1}, respectively. The jump $[\![u]\!]_{j+\frac{1}{2}}$ of u at $x_{j+\frac{1}{2}}$ is defined as $u^+_{j+\frac{1}{2}}-u^-_{j+\frac{1}{2}}$, and the average $\{\!\{u\}\!\}_{j+\frac{1}{2}}$ is defined as $\frac{u^+_{j+\frac{1}{2}}+u^-_{j+\frac{1}{2}}}{2}$.

We denote $\|u\|_{0,I_j}$ and $\|u\|_{\infty,I_j}$ to be the standard L^2 and L^∞ norm of u defined on the element I_j. For any $p>0$ and integer $k\geq 1$, the norms of the Sobolev space $W^{k,p}(I_j)$ is given by

$$||u||_{k,p,I_j}=||u||_{W^{k,p}(I_j)},\ \text{and}\ ||u||_{W^{k,\infty}(I_j)}=\max_{0\leq\alpha\leq k}||D^\alpha u||_{L^\infty(I_j)}.$$

When $p=2$, we simply denote $||u||_{k,I_j}=||u||_{k,2,I_j}$. In this paper, C always denotes a constant which is independent on the mesh size h, time-steps Δt and differential from each other.

Let $P^k(I_j)$ denote the set of polynomials of degree no more than k defined on the element I_j. Then the discontinuous Galerkin finite element space can be chosen as

$$V^k=\{v\in L^2(I):v|_{I_j}\in P^k(I_j),j=1,2,\cdots,M\}.$$

We are now ready to define the averaging discontinuous Galerkin method. Firstly, we rewrite (1) as a first order system:

$$\mathrm{i}u_t+\frac{1}{2}q_x-\phi(u)u=0, \tag{3a}$$

$$q-u_x=0. \tag{3b}$$

Then, multiplying (3a) and (3b) by a smooth function v,w and integrating by parts over I_j, we obtain the following weak formulation,

$$\mathrm{i}\int_{I_j}u_t\overline{v}dx-\frac{1}{2}\int_{I_j}q\overline{v}_xdx+\frac{1}{2}(q\overline{v})^-_{j+\frac{1}{2}}-\frac{1}{2}(q\overline{v})^+_{j-\frac{1}{2}}-\int_{I_j}\phi(u)u\overline{v}dx=0, \tag{4a}$$

$$\int_{I_j}u\overline{w}_xdx+\int_{I_j}q\overline{w}dx-(u\overline{w})^-_{j+\frac{1}{2}}+(u\overline{w})^+_{j-\frac{1}{2}}=0. \tag{4b}$$

Finally, based on the above weak formulation, we define the averaging discontinuous Galerkin method: find $U,Q\in V^k$ such that

$$\mathrm{i}\int_{I_j}U_t\overline{v}dx-\frac{1}{2}\int_{I_j}Q\overline{v}_xdx+\frac{1}{2}(\hat{Q}\overline{v}^-)_{j+\frac{1}{2}}-\frac{1}{2}(\hat{Q}\overline{v}^+)_{j-\frac{1}{2}}-\int_{I_j}\phi(U)U\overline{v}dx=0, \tag{5a}$$

$$\int_{I_j}U\overline{w}_xdx+\int_{I_j}Q\overline{w}dx-(\hat{U}\overline{w}^-)_{j+\frac{1}{2}}+(\hat{U}\overline{w}^+)_{j-\frac{1}{2}}=0, \tag{5b}$$

for all $v,\ w\in V^k$ and elements I_j.

The"hat" terms in (5a) and (5b) in the cell boundary terms for integration by parts are so-called "numerical fluxes", which are single valued functions defined on the edges and should be designed to ensure the stability. We consider the so called "average flux", i.e, we choose

$$\hat{U}_{j+\frac{1}{2}} = \begin{cases} \frac{U^+_{j+\frac{1}{2}}+U^-_{j+\frac{1}{2}}}{2}, & \text{for } j=1,2,\cdots,M-1 \\ 0, & j=0,M \end{cases},$$

$$\hat{Q}_{j+\frac{1}{2}} = \begin{cases} \frac{Q^+_{j+\frac{1}{2}}+Q^-_{j+\frac{1}{2}}}{2}, & \text{for } j=1,2,\cdots,M-1 \\ Q^+_{\frac{1}{2}}, & j=0 \\ Q^-_{M+\frac{1}{2}}, & j=M \end{cases}, \tag{6}$$

for the zero Dirichlet boundary condition.

Remark 2.1. *If the boundary condition is periodic boundary condition, we can choose the numerical flux as*

$$\hat{U}_{j+\frac{1}{2}} = \frac{U^+_{j+\frac{1}{2}}+U^-_{j+\frac{1}{2}}}{2}, \quad \hat{Q}_{j+\frac{1}{2}} = \frac{Q^+_{j+\frac{1}{2}}+Q^-_{j+\frac{1}{2}}}{2}, \quad \forall j=0,1,\cdots,M, \tag{7}$$

where $U^-_{\frac{1}{2}} = U^-_{M+\frac{1}{2}}, U^+_{M+\frac{1}{2}} = U^+_{\frac{1}{2}}$ *and* $Q^-_{\frac{1}{2}} = Q^-_{M+\frac{1}{2}}, Q^+_{M+\frac{1}{2}} = Q^+_{\frac{1}{2}}$.

2.2. Mass conservation and Energy conservation for the semi-discrete form.

Lemma 2.1. *For any complex value* x, y, *we have* $x\overline{y} = \overline{\overline{x}y}$.

To simplify the notation, we define the following bilinear form

$$B(U,v) = \sum_{j=1}^{M}\Big(\int_{I_j} U\overline{v}_x dx - (\hat{U}\overline{v}^-)_{j+\frac{1}{2}} + (\hat{U}\overline{v}^+)_{j-\frac{1}{2}}\Big). \tag{8}$$

Lemma 2.2. *If we choose the numerical flux as (6) or (7), then we have*

$$B(U,Q) + \overline{B(Q,U)} = 0.$$

Proof. By the definition of $B(U,Q)$ in (8), we have

$$\begin{aligned} & B(U,Q) + \overline{B(Q,U)} \\ = & \sum_{j=1}^{M}\Big(\big(\int_{I_j} U\overline{Q}_x dx - (\hat{U}\overline{Q}^-)_{j+\frac{1}{2}} + (\hat{U}\overline{Q}^+)_{j-\frac{1}{2}}\big) \\ & + \overline{\big(\int_{I_j} Q\overline{U}_x dx - (\hat{Q}\overline{U}^-)_{j+\frac{1}{2}} + (\hat{Q}\overline{U}^+)_{j-\frac{1}{2}}\big)}\Big) \\ = & \sum_{j=1}^{M}\Big(\big(-\int_{I_j} U_x\overline{Q} dx - (\hat{U}\overline{Q}^-)_{j+\frac{1}{2}} + (\hat{U}\overline{Q}^+)_{j-\frac{1}{2}} + (U\overline{Q})^-_{j+\frac{1}{2}} - (U\overline{Q})^+_{j-\frac{1}{2}}\big) \\ & + \overline{\big(\int_{I_j} Q\overline{U}_x dx - (\hat{Q}\overline{U}^-)_{j+\frac{1}{2}} + (\hat{Q}\overline{U}^+)_{j-\frac{1}{2}}\big)}\Big). \end{aligned}$$

On the other hand, by simple calculation, we have

$$\begin{aligned} \sum_{j=1}^{M}\Big((\overline{U}Q)^-_{j+\frac{1}{2}} - (\overline{U}Q)^+_{j-\frac{1}{2}}\Big) = & (\overline{U}Q)^-_{M+\frac{1}{2}} - (\overline{U}Q)^+_{\frac{1}{2}} \\ & - \sum_{j=2}^{M}\Big(\{\!\{\overline{U}\}\!\}_{j-\frac{1}{2}}[\![Q]\!]_{j-\frac{1}{2}} + \{\!\{Q\}\!\}_{j-\frac{1}{2}}[\![\overline{U}]\!]_{j-\frac{1}{2}}\Big). \end{aligned}$$

Summing the above two equations together and using lemma 2.1, we finish the proof of this lemma. □

For the semi-discrete scheme (5a)-(5b), we can get the following mass conservation property.

Theorem 2.1. *The solution to (5a)-(5b) with the numerical flux (6) satisfies the following mass conservation property*

$$\frac{d}{dt}\int_I \|U\|^2 dx = 0. \tag{9}$$

Proof. Firstly, taking $v = U, w = Q$ in (5a) and (5b), we have

$$\begin{aligned} \mathrm{i}\int_{I_j} U_t\overline{U}dx - \frac{1}{2}\int_{I_j} Q\overline{U}_x dx + \frac{1}{2}(\hat{Q}\overline{U}^-)_{j+\frac{1}{2}} \\ -\frac{1}{2}(\hat{Q}\overline{U}^+)_{j-\frac{1}{2}} - \int_{I_j}\phi(U)U\overline{U}dx = 0, \end{aligned} \tag{10a}$$

$$\int_{I_j} U\overline{Q}_x dx + \int_{I_j} Q\overline{Q}dx - (\hat{U}\overline{Q}^-)_{j+\frac{1}{2}} + (\hat{U}\overline{Q}^+)_{j-\frac{1}{2}} = 0. \tag{10b}$$

Then, summing the above equation for $j = 1$ to M, and using the notation define in (8), we obtain

$$\mathrm{i}\int_I U_t\overline{U}dx - \frac{1}{2}B(U,Q) - \int_I \phi(U)U\overline{U}dx = 0, \tag{11a}$$

$$\int_I Q\overline{Q}dx + B(Q,U) = 0. \tag{11b}$$

Moreover, multiplying (11b) by $\frac{1}{2}$ and taking the conjugate of it, we have

$$\frac{1}{2}\int_I Q\overline{Q}dx + \frac{1}{2}\overline{B(Q,U)} = 0. \tag{12}$$

Subtracting (11a) from (12), and using lemma 2.2, we have

$$\mathrm{i}\int_I U_t\overline{U}dx - \frac{1}{2}\int_{I_j} Q\overline{Q}dx - \int_{I_j}\phi(U)U\overline{U}dx = 0. \tag{13}$$

Hence, taking the image part of (13), we arrive at

$$\frac{d}{dt}\int_I \|U\|^2 dx = 0,$$

which is actually the mass conservation property of the Schrödinger equation. □

Moreover, the semi-discrete scheme (5a)-(5b) conserves the discrete energy as follows.

Theorem 2.2. *The solution to (5a)-(5b) with the numerical flux (6) or (7) satisfies*

(1) if $\phi(u) = c$,

$$\frac{d}{dt}\int_I c\|U\|^2 + \frac{1}{2}\|Q\|^2 dx = 0, \tag{14}$$

(2) if $\phi(u) = c|u|^2$,

$$\frac{d}{dt}\int_I c\|U\|^4 + \|Q\|^2 dx = 0. \tag{15}$$

Proof. Taking the time derivative in (5b), and choosing the test function $w = Q$, we obtain

$$\int_{I_j} U_t\overline{Q}_x dx + \int_{I_j} Q_t\overline{Q}dx - (\hat{U}_t\overline{Q}^-)_{j+\frac{1}{2}} + (\hat{U}_t\overline{Q}^+)_{j-\frac{1}{2}} = 0. \tag{16}$$

Summing (16) for $j = 1$ to M and taking the conjugate of the obtained equation, we have

$$\frac{1}{2}\int_I Q_t\overline{Q}dx + \frac{1}{2}\overline{B(U_t, Q)} = 0. \tag{17}$$

Then, taking $v = U_t$ in (5a), we get

$$\mathrm{i}\int_{I_j} U_t\overline{U}_t dx - \frac{1}{2}\int_{I_j} Q\overline{U}_{tx}dx + \frac{1}{2}(\hat{Q}\overline{U}_t^-)_{j+\frac{1}{2}} - \frac{1}{2}(\hat{Q}\overline{U}_t^+)_{j-\frac{1}{2}} - \int_{I_j}\phi(U)U\overline{U}_t dx = 0.$$

By summing the above equation for $j = 1$ to M, we arrive at

$$\mathrm{i}\int_I U_t\overline{U}_t dx - \frac{1}{2}B(Q, U_t) - \int_I \phi(U)U\overline{U}_t dx = 0. \tag{18}$$

Subtracting (17) from (18), and using lemma 2.2, we have

$$-\frac{1}{2}\int_I Q_t\overline{Q}dx + \mathrm{i}\int_I U_t\overline{U}_t dx - \int_I \phi(U)U\overline{U}_t dx = 0. \tag{19}$$

Finally, taking the real part of (19), we obtain

(1) if $\phi(u) = c$,

$$\frac{d}{dt}\int_I c\|U\|^2 + \frac{1}{2}\|Q\|^2 dx = 0,$$

(2) if $\phi(u) = c|u|^2$,

$$\frac{d}{dt}\int_I c\|U\|^4 + \|Q\|^2 dx = 0,$$

which is actually the energy conservation property of the semi-discrete form for both the linear and nonlinear Schrödinger equation. □

3. Analysis of the fully discrete scheme

In order to develop a fully-discrete ALDG scheme to discretize the Schrödinger equation, we divide the time interval $[0, T]$ into N uniform subintervals by points $0 = t_0 < t_1 < \cdots < t_N = T$, where $t_k = k\tau$. Moreover, we denote $I_k = [t_{k-1}, t_k]$, $\psi^k = \psi(\cdot, t_k)$, and

$$\delta_t^k\psi = \frac{\psi^{k+1} - \psi^k}{\Delta t}, \bar{\psi}^k = \frac{\psi^{k+1} + \psi^k}{2}.$$

Based on the semi-discrete scheme (5a)-(5b), we can define a fully discrete form as

$$\begin{aligned}&\mathrm{i}\sum_{j=1}^M\int_{I_j}\delta_t^n U\overline{v} - \frac{1}{2}\sum_{j=1}^M \bar{Q}^n\overline{v}_x dx + \frac{1}{2}\sum_{j=1}^M(\widehat{\bar{Q}}^n\overline{v}^-)_{j+\frac{1}{2}}\\ &-\frac{1}{2}\sum_{j=1}^M(\widehat{\bar{Q}}^n\overline{v}^+)_{j-\frac{1}{2}} - \sum_{j=1}^M\int_{I_j}\overline{\phi(U)U}^n\overline{v}dx = 0,\end{aligned} \tag{20a}$$

$$\sum_{j=1}^M\int_{I_j} U^{n+1}\overline{w}_x + Q^{n+1}w dx - \sum_{j=1}^M(\widehat{U}^{n+1}\overline{w}^-)_{j+\frac{1}{2}} + \sum_{j=1}^M(\widehat{U}^{n+1}\overline{w}^+)_{j-\frac{1}{2}} = 0, \tag{20b}$$

$$\sum_{j=1}^M\int_{I_j} U^n\overline{w}_x + Q^n\overline{w}dx - \sum_{j=1}^M(\widehat{U}^n\overline{w}^-)_{j+\frac{1}{2}} + \sum_{j=1}^M(\widehat{U}^n\overline{w}^+)_{j-\frac{1}{2}} = 0, \tag{20c}$$

where $\hat{U}^n, \hat{Q}^n$ denote the numerical flux, and

- if $\phi(u) = c$, then $\overline{\phi(U)U}^n = \dfrac{U^n + U^{n-1}}{2}$,

- if $\phi(u) = c|u|^2$, then $\overline{\phi(U)U}^n = \dfrac{c(|U^n|^2 + |U^{n-1}|^2)}{2}\dfrac{U^n + U^{n-1}}{2}$.

In our fully discrete scheme, we take

$$\hat{U}^n_{j+\frac{1}{2}} = \begin{cases} \frac{(U^n_{j+\frac{1}{2}})^+ + (U^n_{j+\frac{1}{2}})^-}{2}, & \text{for } j = 1, 2, \cdots, M-1 \\ 0, & j = 0, M \end{cases}$$

$$\hat{Q}^n_{j+\frac{1}{2}} = \begin{cases} \frac{(Q^n_{j+\frac{1}{2}})^+ + (Q^n_{j+\frac{1}{2}})^-}{2}, & \text{for } j = 1, 2, \cdots, M-1 \\ (Q^n_{\frac{1}{2}})^+, & j = 0 \\ (Q^n_{M+\frac{1}{2}})^-, & j = M \end{cases} \tag{21}$$

for zero dirichlet boundary condition, and

$$\hat{U}^n_{j+\frac{1}{2}} = \frac{(U^n_{j+\frac{1}{2}})^+ + (U^n_{j+\frac{1}{2}})^-}{2}, \quad \hat{Q}^n_{j+\frac{1}{2}} = \frac{(Q^n_{j+\frac{1}{2}})^+ + (Q^n_{j+\frac{1}{2}})^-}{2}, \quad \forall j = 0, 1, \cdots, M, \tag{22}$$

for periodic boundary condition, with $(U^n_{\frac{1}{2}})^- = (U^n_{M+\frac{1}{2}})^-, (U^n_{M+\frac{1}{2}})^+ = (U^n_{\frac{1}{2}})^+$ and $(Q^n_{\frac{1}{2}})^- = (Q^n_{M+\frac{1}{2}})^-, (Q^n_{M+\frac{1}{2}})^+ = (Q^n_{\frac{1}{2}})^+$.

Then, we will show our fully discrete scheme (20a)–(20c) not only conserve the mass, but also conserve the energy.

Theorem 3.1. *The solution to (20a)-(20c) with the numerical flux (21) or (22) satisfies the following mass conservation property*

$$\int_I |U^{n+1}|^2 dx = \int_I |U^n|^2 dx, \quad \forall n = 1, 2, \cdots, N. \tag{23}$$

Proof. On the one hand, taking $w = \bar{Q}^n$ in (20b) and (20c), and summing them for $j = 1$ to M, we obtain

$$\sum_{j=1}^{M} \int_{I_j} \bar{U}^n \overline{\bar{Q}^n}_x + \bar{Q}^n \overline{\bar{Q}^n} dx - \sum_{j=1}^{M} (\hat{\bar{U}}^n \overline{\bar{Q}^n}^-)_{j+\frac{1}{2}} + \sum_{j=1}^{M} (\hat{\bar{U}}^n \overline{\bar{Q}^n}^+)_{j-\frac{1}{2}} = 0. \tag{24}$$

Then, multiplying (24) by $\frac{1}{2}$ and taking the conjugate, we get

$$\frac{1}{2} \int_I \bar{Q}^n \overline{\bar{Q}^n} dx + \frac{1}{2} \overline{B(\bar{U}^n, \bar{Q}^n)} = 0. \tag{25}$$

On the other hand, taking $w = \bar{U}^n$ in (20a) and summing them for $j = 1$ to M, we have

$$\mathrm{i} \int_I \delta_t^n U \overline{\bar{U}^n} dx - \frac{1}{2} B(\bar{Q}^n, \bar{U}^n) - \int_I \overline{\phi(U)U}^n \bar{U}^n dx = 0. \tag{26}$$

Therefore, subtracting (26) from (25), we obtain

$$\mathrm{i} \int_I \delta_t^n U \overline{\bar{U}^n} dx - \int_I \overline{\phi(U)U}^n \bar{U}^n dx - \frac{1}{2} \int_I \bar{Q}^n \overline{\bar{Q}^n} dx = 0. \tag{27}$$

Finally, taking the image part of (27) leads to

$$\int_I \|U^{n+1}\|^2 dx = \int_I \|U^n\|^2 dx,$$

which is (23). □

Theorem 3.2. *The solution to (20a)-(20c) with the numerical flux (21) or (22) satisfies the following energy conservation property*

(1) if $\phi(u) = c$, then

$$\int_I c\|U^{n+1}\|^2 + \frac{1}{2}\|Q^{n+1}\|^2 dx = \int_I c\|U^n\|^2 + \frac{1}{2}\|Q^n\|^2 dx, \tag{28}$$

(2) if $\phi(u) = c|u|^2$, then

$$\int_I c\|U^{n+1}\|^4 + \|Q^{n+1}\|^2 dx = \int_I c\|U^n\|^4 + \|Q^n\|^2 dx. \tag{29}$$

Proof. On one hand, by subtracting (20c) from (20b), we have

$$\int_{I_j} (U^{n+1} - U^n)\overline{w}_x + (Q^{n+1} - Q^n)\overline{w} dx$$
$$-\Big((\widehat{U}^{n+1} - \widehat{U}^n)\overline{w}^-\Big)_{j+\frac{1}{2}} + \Big((\widehat{U}^{n+1} - \widehat{U}^n)\overline{w}^+\Big)_{j-\frac{1}{2}} = 0.$$

Taking $w = \dfrac{Q^{n+1} + Q^n}{2}$ in the above equation and summing for $j = 1$ to M, we arrive at

$$\int_I (Q^{n+1} - Q^n)\frac{\overline{Q^{n+1} + Q^n}}{2} dx + B(U^{n+1} - U^n, \frac{Q^{n+1} + Q^n}{2}) = 0. \tag{30}$$

On the other hand, taking $v = U^{n+1} - U^n$ in (20a) and summing for $j = 1$ to M, we obtain

(31)

$$\mathrm{i}\int_I \delta_t^n U(\overline{U^{n+1} - U^n})dx - \frac{1}{2}B(\overline{Q}^n, U^{n+1} - U^n) - \int_I \overline{\phi(U)U}^n(\overline{U^{n+1} - U^n})dx = 0.$$

Subtracting (31) from (30), and using lemma 2.2, we get

$$\mathrm{i}\int_I \delta_t^n U(\overline{U^{n+1} - U^n})dx - \int_I \overline{\phi(U)U}^n(\overline{U^{n+1} - U^n})dx$$
$$- \frac{1}{2}\int_I (Q^{n+1} - Q^n)\frac{\overline{Q^{n+1} + Q^n}}{2} dx = 0. \tag{32}$$

Finally, by taking the real part of (32), we arrive at

$$\begin{cases} \int_I c\|U^{n+1}\|^2 + \frac{1}{2}\|Q^{n+1}\|^2 dx = \int_I c\|U^n\|^2 + \frac{1}{2}\|Q^n\|^2 dx, & \text{if } \phi(u) = c; \\ \int_I c\|U^{n+1}\|^4 + \|Q^{n+1}\|^2 dx = \int_I c\|U^n\|^4 + \|Q^n\|^2 dx, & \text{if } \phi(u) = c|u|^2. \end{cases} \tag{33}$$

It finishes the proof of this theorem. □

4. Error analysis for the linear case

In this section, we derive the optimal error estimates for the conserving ALDG method proposed in the above sections of the linear Schrödinger equation, i.e., we assume $\phi(u) = c$.

4.1. The semi-discrete scheme. To prove the L^2 error analysis of the semi-discrete scheme, we need the following notations and lemmas.

let l_i be i-th order Legendre polynomial on the reference interval $E = [-1, 1]$, i.e., $l_i(s) = \gamma_i \partial_s^i (s^2 - 1)^i$, $\gamma_i = \dfrac{1}{2^i i!}$, $i = 0, 1, 2, \cdots$. Any function defined on E can be expanded as

$$u(s) = \sum_{i=0}^{\infty} b_i l_i(s), \quad b_i = (i + \frac{1}{2})(u,\ l_i)_E. \tag{34}$$

Let the k-th order partial sum of u in (34) and its remainder be u_L^k and R_u, respectively. In other words,

$$u_L^k = \sum_{i=0}^{k} b_i l_i(s),\ R_u = u - u_L^k = \sum_{i=k+1}^{\infty} b_i l_i(s). \tag{35}$$

It is easy to see that R_u is orthogonal to any polynomials $P^i(s)$ whose degree is less than k.

Then, we have the following estimate for the remainder R_u,

Lemma 4.1. [27]*Let $u \in W^{k+1,p}(I)$. The remainder of u on the element $I_j, j = 1, 2, \cdots, M$ satisfies*

$$||R_u||_{0,q,I_j} \le Ch^{k+1+(\frac{1}{q}-\frac{1}{p})}||u||_{k+1,p,I_j}.$$

In particular, when k is even and $u \in W^{k+2,p}(I)$, the average of the reminder on the nodes $x_{j+\frac{1}{2}}$ satisfies

$$|\{\!\{R_u\}\!\}(x_{j+\frac{1}{2}})| \le Ch^{k+2}||u||_{k+2,\infty,I_j+I_{j+1}}, j = 1, 2, \cdots, M-1.$$

Lemma 4.2. (Gronwall's lemma) *Suppose that ϕ is a nonnegative continuous function such that*

$$\phi(t) \le a + b\int_0^t \phi(s)ds,\ \textit{for } t > 0,$$

where a and b are nonnegative constants. Then

$$\phi(t) \le ae^{bt}.$$

In the following, we will show the convergence order of the proposed semi-discrete ALDG scheme (5a)–(5b). Denote by $e_u = u - U, e_q = q - Q$. Then, using the definition of R_u introduced above, we can decompose e_u, e_q as

$$e_u = u - U = u - R_u - (U - R_u) \equiv \rho_u - \theta_u,$$
$$e_q = q - Q = q - R_q - (Q - R_q) \equiv \rho_q - \theta_q.$$

By the definition of R_u and R_q, we have the following orthogonal property,

$$(\rho_\xi, \theta_\zeta) = 0, \quad \forall \xi, \zeta = u, q. \tag{36}$$

By the definition of the numerical flux in (6) or (7), we know that they are consistent. Hence, the combination of (4a)–(4b) and the semi-discrete scheme (5a)–(5b) leads to the following error equation on each element I_j,

$$\mathrm{i}\int_{I_j} e_{ut}\overline{v}dx - \frac{1}{2}\int_{I_j} e_q\overline{v}_x dx + \frac{1}{2}(\hat{e}_q\overline{v}^-)_{j+\frac{1}{2}} - \frac{1}{2}(\hat{e}_q\overline{v}^+)_{j-\frac{1}{2}} - \int_{I_j} ce_u v\overline{v}dx = 0,$$
$$\int_{I_j} e_u\overline{w}_x dx + \int_{I_j} e_q\overline{w}dx - (\hat{e}_u\overline{w}^-)_{j+\frac{1}{2}} + (\hat{e}_u\overline{w}^+)_{j-\frac{1}{2}} = 0.$$

Then, summing the above two equation from $j = 1$ to $j = M$, we get

$$\mathrm{i}\sum_{j=1}^{M}\int_{I_j} e_{ut}\overline{v}dx - \frac{1}{2}\sum_{j=1}^{M}\int_{I_j} e_q\overline{v}_x dx$$
$$+ \frac{1}{2}\sum_{j=1}^{M}(\hat{e}_q\overline{v}^-)_{j+\frac{1}{2}} - \frac{1}{2}\sum_{j=1}^{M}(\hat{e}_q\overline{v}^+)_{j-\frac{1}{2}} - \sum_{j=1}^{M}\int_{I_j} ce_u\overline{v}dx = 0, \tag{38a}$$

$$\sum_{j=1}^{M}\int_{I_j} e_u\overline{w}_x dx + \sum_{j=1}^{M}\int_{I_j} e_q\overline{w}dx - \sum_{j=1}^{M}(\hat{e}_u\overline{w}^-)_{j+\frac{1}{2}} + \sum_{j=1}^{M}(\hat{e}_u\overline{w}^+)_{j-\frac{1}{2}} = 0. \tag{38b}$$

Finally, we can show the following convergent result:

Theorem 4.1. *Suppose that u, q be the exact solution of (1), U, Q be the ALDG solution of (5a)-(5b). Then*

- *when k is even, we have*

$$\|q(\cdot,T)-Q(\cdot,T)\|+\|u(\cdot,T)-U(\cdot,T)\|\le Ch^{k+1}(\|u\|_{k+2}+\|Q\|_{k+2}),$$

- *when k is odd, we have*

$$\|q(\cdot,T)-Q(\cdot,T)\|+\|u(\cdot,T)-U(\cdot,T)\|\le Ch^{k}(\|u\|_{k+1}+\|Q\|_{k+1}).$$

Proof. Taking $v=\theta_u$ in (38a), $w=\theta_q$ in (38b) and using the orthogonal properties (36), we get

$$\mathrm{i}\sum_{j=1}^{M}\int_{I_j}\theta_{ut}\overline{\theta_u}dx-\frac{1}{2}B(\theta_q,\theta_u)+\frac{1}{2}B(\rho_q,\theta_u)+\sum_{j=1}^{M}\int_{I_j}c\theta_u\overline{\theta_u}dx=0, \tag{39a}$$

$$-\sum_{j=1}^{M}\int_{I_j}\theta_q\overline{\theta_q}dx+B(\theta_u,\theta_q)-B(\rho_u,\theta_q)=0. \tag{39b}$$

Then, taking the conjugate of (39b), we arrive at

$$-\frac{1}{2}\sum_{j=1}^{M}\int_{I_j}\theta_q\overline{\theta_q}dx+\frac{1}{2}\overline{B(\theta_u,\theta_q)}-\frac{1}{2}\overline{B(\rho_u,\theta_q)}=0. \tag{40}$$

Subtracting (40) from (39a), we obtain

(41)

$$\mathrm{i}\sum_{j=1}^{M}\int_{I_j}\theta_{ut}\overline{\theta_u}dx+\sum_{j=1}^{M}\int_{I_j}c\theta_u\overline{\theta_u}dx+\frac{1}{2}\sum_{j=1}^{M}\int_{I_j}\theta_q\overline{\theta_q}dx=-\frac{1}{2}B(\rho_q,\theta_u)-\frac{1}{2}\overline{B(\rho_u,\theta_q)}.$$

Therefore, taking the image part of (41), we have

$$\sum_{j=1}^{M}\int_{I_j}\theta_{ut}\overline{\theta_u}dx=-Im\{\frac{1}{2}B(\rho_q,\theta_u)+\frac{1}{2}\overline{B(\rho_u,\theta_q)}\}. \tag{42}$$

Hence, taking the real part of (41), we obtain

$$\sum_{j=1}^{M}\int_{I_j}c\theta_u\overline{\theta_u}dx+\frac{1}{2}\sum_{j=1}^{M}\int_{I_j}\theta_q\overline{\theta_q}dx=-Re\{\frac{1}{2}B(\rho_q,\theta_u)+\frac{1}{2}\overline{B(\rho_q,\theta_u)}\}. \tag{43}$$

Finally, by the combination of (40), (43), lemma 4.1 and lemma 4.2, we have

1). if k is even, then

$$\|\theta_q(\cdot,T)\|^2+\|\theta_u(\cdot,T)\|^2\le C(T)h^{2k+2}(\|u\|_{k+2}^2+\|q\|_{k+2}^2),$$

2). if k is odd, then

$$\|\theta_q(\cdot,T)\|^2+\|\theta_u(\cdot,T)\|^2\le C(T)h^{2k}(\|u\|_{k+1}^2+\|q\|_{k+1}^2).$$

Using the triangle inequality, we complete the proof of this theorem. □

4.2. The fully discrete scheme. In this subsection, we will introduce the error estimate of the fully discrete scheme for the linear Schrödinger equation.

Denote by $e_u^n=u^n-U^n, e_q^n=q^n-Q^n$. Then, we can decompose them as

$$e_u^n=u^n-U^n=u^n-R_u^n-(U^n-R_u^n)\equiv\rho_u-\theta_u,$$
$$e_q^n=q^n-Q^n=q^n-R_q^n-(Q^n-R_q^n)\equiv\rho_q-\theta_q.$$

By the definition of R_u^n and R_q^n, we have the following orthogonal property,

$$(\rho_\xi^j,\theta_\zeta^i)=0,\quad \forall 0\le i,j\le N,\ \text{and}\ \xi,\zeta=u,q. \tag{44}$$

To prove the L^2 Error analysis of the fully discrete scheme, we need the following lemmas.

Lemma 4.3. *Denote* $u^k = u(\cdot, k\tau)$*. For any* $u \in H^2([0,T],(L^2(\Omega)))$*, we have*

$$||\Delta t\bar{u}^{k+1} - \int_{I_k} u(s)ds||_0^2 \leq \frac{\Delta t^5}{4}\int_{I_k} ||u_{tt}(s)||^2 ds.$$

Lemma 4.4. (The discrete Gronwall inequality) *Let* $\Delta t, B, C > 0, \{a_n\}_n$ *be sequence of nonnegative numbers satisfying*

$$a_n \leq B + C\Delta t\sum_{j=0}^{n} a_i, \forall n \geq 0.$$

If $C\tau \leq 1$*, then*

$$a_n \leq e^{C(n+1)\Delta t}B.$$

In the following, we are ready to introduce the error equation of the proposed ALDG method (20a)-(20c). Integrating (4a) over $[t_n, t_{n+1}]$ with respect to t on both sides of it and dividing by Δt, then subtracting (20a), we get

$$\frac{\mathrm{i}}{\Delta t}(e_u^{n+1} - e_u^n, v) - \frac{1}{2\Delta t}\int_{t_n}^{t_{n+1}} B(q,v)dt + \frac{B(Q^n + Q^{n+1}, v)}{4}$$
$$- \frac{1}{\Delta t}\int_{t_n}^{t_{n+1}}(u,v)dt + \frac{(U^n + U^{n+1}, v)}{2} = 0.$$

By inserting some intermediate term, the above equation can be rewritten as

$$\frac{\mathrm{i}}{\Delta t}(e_u^{n+1} - e_u^n, v) - \frac{1}{2\Delta t}\int_{t_n}^{t_{n+1}} B(q,v)dx + \frac{B(q^n + q^{n+1}, v)}{4}$$
$$- \frac{B(e_q^n + e_q^{n+1}, v)}{4} - \frac{(e_u^n + e_u^{n+1}, v)}{2} - \frac{1}{\Delta t}\int_{t_n}^{t_{n+1}}(u,v)dt + \frac{(u^n + u^{n+1}, v)}{2} = 0. \tag{45}$$

On the other hand, integrating (4b) over $[t_k, t_{k+1}]$ with respect to t on both sides of it and subtracting (20b) and (20c), we obtain

$$\frac{1}{\Delta t}\int_{t_n}^{t_{n+1}}(q,w)dt - \frac{(Q^n + Q^{n+1}, w)}{2}$$
$$+\frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} B(u,w)dt - \frac{B(U^n + U^{n+1}, w)}{2} = 0.$$

By inserting some intermediate term, the above equation can be rewritten as

$$\frac{1}{\Delta t}\int_{t_n}^{t_{n+1}}(q,w)dt - \frac{(q^n + q^{n+1}, w)}{2} + \frac{(e_q^n + e_q^{n+1}, w)}{2}$$
$$+\frac{B(e_u^n + e_u^{n+1}, w)}{2} + \frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} B(u,w)dt - \frac{B(u^n + u^{n+1}, w)}{2} = 0, \tag{46}$$

where $(u,v) = \sum_{j=1}^{M}(u,v)_{I_j}$.

Theorem 4.2. *Let* u, q *be the solution of (20a)-(20c) with the numerical flux (6) or (7) and* U^n, Q^n *be the solution of (1). Then*

- *if* k *is even, we have*

$$\|q^n - Q(\cdot, t_n)\| + \|u^n - U(\cdot, t_n)\| \leq C(\Delta t^2 + h^{k+1}), \forall 0 \leq n \leq N,$$

- *if k is odd, we have*

$$\|q^n - Q(\cdot,t_n)\| + \|u^n - U(\cdot,t_n)\| \le C(\Delta t^2 + h^k), \forall 0 \le n \le N.$$

Proof. Taking $v = \theta_u^{n+1} + \theta_u^n$ in (45), and using the orthogonal property (44), we have

$$\begin{aligned}
&-\frac{\mathrm{i}}{\Delta t}(\theta_u^{n+1} - \theta_u^n, \theta_u^{n+1} + \theta_u^n) - \frac{1}{2\Delta t}\int_{t_n}^{t_{n+1}} B(q, \theta_u^{n+1} + \theta_u^n)dx \\
&+\frac{B(q^n + q^{n+1}, \theta_u^{n+1} + \theta_u^n)}{4} - \frac{B(\rho_q^n + \rho_q^{n+1}, \theta_u^{n+1} + \theta_u^n)}{4} \\
&+\frac{B(\theta_q^n + \theta_q^{n+1}, \theta_u^{n+1} + \theta_u^n)}{4} + \frac{(\theta_u^n + \theta_u^{n+1}, \theta_u^{n+1} + \theta_u^n)}{2} \\
&-\frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} (u, \theta_u^{n+1} + \theta_u^n)dt + \frac{(u^n + u^{n+1}, \theta_u^{n+1} + \theta_u^n)}{2} = 0.
\end{aligned} \tag{47}$$

Meanwhile, taking $w = \theta_q^{n+1} + \theta_q^n$ in (46), we obtain

$$\begin{aligned}
&\frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} (q, \theta_q^{n+1} + \theta_q^n)dt - \frac{(q^n + q^{n+1}, \theta_q^{n+1} + \theta_q^n)}{2} \\
&- \frac{(\theta_q^n + \theta_q^{n+1}, \theta_q^{n+1} + \theta_q^n)}{2} + \frac{B(\rho_u^n + \rho_u^{n+1}, \theta_q^{n+1} + \theta_q^n)}{2} \\
&- \frac{B(\theta_u^n + \theta_u^{n+1}, \theta_q^{n+1} + \theta_q^n)}{2} + \frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} B(u, \theta_q^{n+1} + \theta_q^n)dt \\
&- \frac{B(u^n + u^{n+1}, \theta_q^{n+1} + \theta_q^n)}{2} = 0.
\end{aligned} \tag{48}$$

By subtracting the conjugate of (48) from (47), one gets

$$\begin{aligned}
&-\mathrm{i}\frac{1}{\Delta t}\Big(||\theta_u^{n+1}||^2 - ||\theta_u^n||\Big) + \frac{1}{4}\|\theta_q^{n+1} + \theta_q^n\|^2 + \frac{1}{4}\|\theta_u^{n+1} + \theta_u^n\|^2 \\
=&\frac{1}{2\Delta t}\int_{t_n}^{t_{n+1}} B(q, \theta_u^{n+1} + \theta_u^n)dx - \frac{B(q^n + q^{n+1}, \theta_u^{n+1} + \theta_u^n)}{4} \\
&+ \frac{B(\rho_q^n + \rho_q^{n+1}, \theta_u^{n+1} + \theta_u^n)}{4} + \frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} (u, \theta_u^{n+1} + \theta_u^n)dt \\
&- \frac{(u^n + u^{n+1}, \theta_u^{n+1} + \theta_u^n)}{2} + \overline{\frac{1}{2\Delta t}\int_{t_n}^{t_{n+1}} (q, \theta_q^{n+1} + \theta_q^n)dt} \\
&- \overline{\frac{(q^n + q^{n+1}, \theta_q^{n+1} + \theta_q^n)}{4}} - \overline{\frac{B(u^n + u^{n+1}, \theta_q^{n+1} + \theta_q^n)}{4}} \\
&+ \overline{\frac{B(\rho_u^n + \rho_u^{n+1}, \theta_q^{n+1} + \theta_q^n)}{4}} + \overline{\frac{1}{2\Delta t}\int_{t_n}^{t_{n+1}} B(u, \theta_q^{n+1} + \theta_q^n)dt}.
\end{aligned}$$

Therefore, by taking both the image and the real part of the above equation, we have

$$\begin{aligned}
&\frac{1}{\Delta t}\Big(||\theta_u^{n+1}||^2 - ||\theta_u^n||\Big) \\
=&-Im\Big\{\frac{1}{2\Delta t}\int_{t_n}^{t_{n+1}} B(q, \theta_u^{n+1} + \theta_u^n)dx - \frac{B(q^n + q^{n+1}, \theta_u^{n+1} + \theta_u^n)}{4} \\
&+ \frac{B(\rho_q^n + \rho_q^{n+1}, \theta_u^{n+1} + \theta_u^n)}{4} + \frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} (u, \theta_u^{n+1} + \theta_u^n)dt
\end{aligned}$$

$$
\begin{aligned}
&-\overline{\frac{(u^n+u^{n+1},\theta_u^{n+1}+\theta_u^n)}{2}}+\overline{\frac{1}{2\Delta t}\int_{t_n}^{t_{n+1}}(q,\theta_q^{n+1}+\theta_q^n)dt}\\
&-\overline{\frac{(q^n+q^{n+1},\theta_q^{n+1}+\theta_q^n)}{4}}-\overline{\frac{B(u^n+u^{n+1},\theta_q^{n+1}+\theta_q^n)}{4}}\\
&+\overline{\frac{B(\rho_u^n+\rho_u^{n+1},\theta_q^{n+1}+\theta_q^n)}{4}}+\overline{\frac{1}{2\Delta t}\int_{t_n}^{t_{n+1}}B(u,\theta_q^{n+1}+\theta_q^n)dt}\Big\},
\end{aligned}
$$

and

$$
\begin{aligned}
&\frac{1}{4}\|\theta_q^{n+1}+\theta_q^n\|^2+\frac{1}{2}\|\theta_u^{n+1}+\theta_u^n\|^2\\
=&Re\Big\{\frac{1}{2\Delta t}\int_{t_n}^{t_{n+1}}B(q,\theta_u^{n+1}+\theta_u^n)dx-\frac{B(q^n+q^{n+1},\theta_u^{n+1}+\theta_u^n)}{4}\\
&+\frac{B(\rho_q^n+\rho_q^{n+1},\theta_u^{n+1}+\theta_u^n)}{4}+\frac{1}{\Delta t}\int_{t_n}^{t_{n+1}}(u,\theta_u^{n+1}+\theta_u^n)dt\\
&-\frac{(u^n+u^{n+1},\theta_u^{n+1}+\theta_u^n)}{2}+\overline{\frac{1}{2\Delta t}\int_{t_n}^{t_{n+1}}(q,\theta_q^{n+1}+\theta_q^n)dt}\\
&-\overline{\frac{(q^n+q^{n+1},\theta_q^{n+1}+\theta_q^n)}{4}}-\overline{\frac{B(u^n+u^{n+1},\theta_q^{n+1}+\theta_q^n)}{4}}\\
&+\overline{\frac{B(\rho_u^n+\rho_u^{n+1},\theta_q^{n+1}+\theta_q^n)}{4}}+\overline{\frac{1}{2\Delta t}\int_{t_n}^{t_{n+1}}B(u,\theta_q^{n+1}+\theta_q^n)dt},
\end{aligned}
$$

which together with lemma 4.1, lemma 4.3, and lemma 4.4 yields

- when k is even,
$$
\begin{aligned}
&\|\theta_q^{n+1}\|^2+\|\theta_u^{n+1}\|^2\\
\le&C(T)(\Delta t^4\int_0^L||u_{tt}||^2+||q_{tt}||^2ds+h^{2k+2}||u||_{k+2,2}^2+h^{2k+2}||q||_{k+2}^2),
\end{aligned}
$$
- when k is odd,
$$
\begin{aligned}
&\|\theta_q^{n+1}\|^2+|\theta_u^{n+1}\|^2\\
\le&C(T)(\Delta t^4\int_0^L||u_{tt}||^2+||q_{tt}||^2ds+h^{2k}||u||_{k+1,2}^2+h^{2k}||q||_{k+1}^2).
\end{aligned}
$$

Finally, using the triangle inequality, we complete the proof of this theorem. □

Remark 4.1. *Although we only focus on one-dimensional case, our results can be easily extended to two-dimensional and three-dimensional cases with tensor product meshes.*

5. Numerical results

In this section, we present some numerical examples to illustrate both accuracy and capacity of the proposed ALDG method with flux (21) and (22) for both linear and nonlinear Schrödinger equations.

Example 1: Consider the numerical solution to the linear Schrödinger equation

$$
\begin{aligned}
&\mathrm{i}u_t+u_{xx}+u=f,\ t>0,\ 0\le x\le 1,\\
&u(x,0)=u_0(x),
\end{aligned}
\tag{49}
$$

with zero direct boundary conditions. Suppose the exact solution of (49) with some given source term f be

$$u(x,t)=\sin(\pi x)\exp(\mathrm{i}t).$$

The L^2 error and order of accuracy at $t = 1$ for $k = 1, 2, 3, 4$ are given in table 1. We see that the optimal $(k+1)$-th order of accuracy of even $k = 2, 4$ and suboptimal k-th order of accuracy of odd $k = 1, 3$.

TABLE 1. The convergence rate at $t = 1$.

k	N	$Error_{ur}$	$order$	$Error_{ui}$	$order$	$Error_{qr}$	$order$	$Error_{qi}$	$order$
1	4	3.7245e-2		2.4646e-2		7.6467e-2		7.2007e-2	
	8	1.7894e-2	1.0576	1.1644e-2	1.0818	4.0037e-2	0.9333	3.5681e-2	1.0130
	16	8.1576e-3	1.1333	5.9986e-3	0.9569	1.9890e-2	1.0093	1.7864e-2	0.9981
	32	4.0028e-3	1.0217	3.0684e-3	0.9671	9.7098e-3	1.0345	8.6472e-3	1.0468
2	4	5.8516e-4		9.0190e-4		7.0405e-3		1.2365e-2	
	8	7.7885e-5	2.9094	1.2222e-4	2.8835	1.0352e-3	2.7658	1.4608e-3	3.0814
	16	9.2711e-6	3.0705	1.4399e-5	3.0854	1.6677e-4	2.6340	1.4087e-4	3.3743
	32	1.1431e-6	3.0198	1.7767e-6	3.0187	1.8449e-5	3.1762	1.9969e-5	2.8185
3	4	1.4835e-4		1.1098e-4		2.2777e-3		2.5180e-3	
	8	9.6025e-6	3.9495	1.4187e-5	2.9677	1.5736e-4	3.8554	3.7809e-4	2.7355
	16	1.3160e-6	2.8673	1.8336e-6	2.9518	2.5323e-5	2.6355	4.6299e-5	3.0297
	32	1.8361e-7	2.8414	2.0829e-7	3.1380	3.8075e-6	2.7335	5.8350e-6	2.9882
4	4	2.6355e-6		2.7222e-6		6.1471e-5		2.2402e-5	
	8	8.1058e-8	5.0230	8.6180e-8	4.9813	1.9024e-6	5.0140	7.0105e-7	4.9980
	16	2.5700e-9	4.9791	2.6605e-9	5.0176	6.0034e-8	4.9859	2.1882e-8	5.0017

TABLE 2. The convergence rate at $t = 1$.

k	N	$Error_{ur}$	$order$	$Error_{ui}$	$order$	$Error_{qr}$	$order$	$Error_{qi}$	$order$
1	200	8.9065e-2		9.6784e-2		4.9018e-1		5.7761e-1	
	400	4.6701e-2	0.9314	4.9801e-2	0.9586	2.4987e-1	0.9721	2.8709e-1	1.0086
	800	2.3287e-2	1.0039	2.4098e-2	1.0473	1.2086e-1	1.0478	1.3910e-1	1.0454
2	100	4.8936e-2		5.0141e-2		2.0162e-1		2.0062e-1	
	200	9.4797e-4	5.6899	9.2703e-4	5.7572	8.9153e-3	4.4922	8.9073e-3	4.4933
	400	8.8805e-5	3.4161	8.8291e-5	3.3923	1.0145e-3	3.1355	1.0155e-3	3.1328
	800	1.1076e-5	3.0032	1.2234e-5	2.9744	1.2516e-4	3.0189	1.2520e-4	3.0199
3	100	1.7313e-3		1.7234e-3		1.2284e-2		1.2281e-2	
	200	1.4897e-4	3.5388	1.4906e-4	3.5313	1.9547e-3	2.6518	1.9523e-3	2.6532
	400	1.6783e-5	3.1499	1.6802e-5	3.1492	2.5630e-4	2.9310	2.5628e-4	2.9294
	800	1.8020e-6	3.2193	1.8030e-6	3.2202	3.3254e-5	2.9462	3.3279e-5	2.9450
4	100	1.6035e-4		1.8971e-4		3.0087e-3		2.9836e-3	
	200	5.0084e-6	5.0007	5.8918e-6	5.0089	9.2019e-5	5.0311	9.5109e-5	4.9713
	400	1.5697e-7	4.9958	1.8719e-7	4.9761	2.9379e-6	4.9691	2.9138e-6	5.0286

Example 2: Consider the numerical solution to the nonlinear Schrödinger equation

$$\begin{aligned} &\mathrm{i}u_t + u_{xx} + 2|u|^2 u = 0, \;\; t > 0, \;\; -25 \le x \le 25, \\ &u(x, 0) = u_0(x), \end{aligned} \tag{50}$$

with periodic boundary conditions and initial condition $u_0(x) = \operatorname{sech}(x)\exp(2\mathrm{i}x)$, and the exact solution to be

$$u(x, t) = \operatorname{sech}(x - 4t)\exp(\mathrm{i}(2x - 3t)).$$

The L^2 error and order of accuracy at $T = 1$ for $k = 1, 2, 3, 4$ are given in table 2. We see that the optimal $(k+1)$-th order of accuracy of even $k = 2, 4$ and suboptimal k-th order of accuracy of odd $k = 1, 3$. Further, Fig. 1 shows the discrete mass

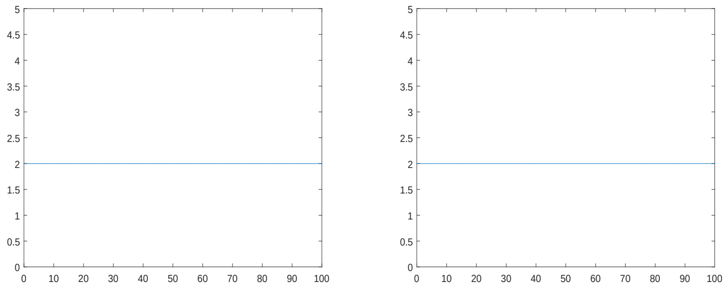

FIGURE 1. The numerical mass of Example 2. $k = 2$(Left), $k = 3$(Right).

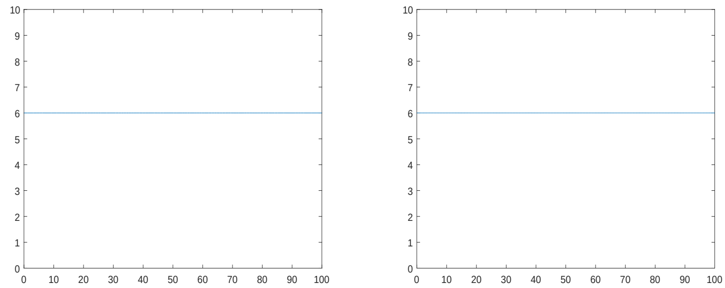

FIGURE 2. The numerical energy of Example 2. $k = 2$(Left), $k = 3$(Right).

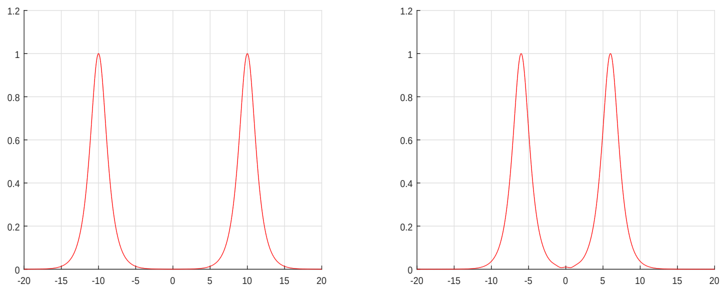

FIGURE 3. The soliton propagation of Eq. (51) with initial condition (52). $c_1 = 4, x_1 = -10, c_2 = -4, x_2 = 10$. $T = 0$(Left), $T = 1$(Right).

conserve all the time, Fig. 2 shows the discrete energy conserve. This means our theoretical predictions are true.

Example 3: Consider the numerical solution to the nonlinear Schrödinger equation

$$\begin{aligned} &\mathrm{i}u_t + u_{xx} + 2|u|^2 u = 0,\ t > 0,\ -20 \le x \le 20, \\ &u(x,0) = u_0(x), \end{aligned} \tag{51}$$

with periodic boundary conditions and the initial condition to be

$$u(x,0) = \sum_{j=1}^{2} \operatorname{sech}(x - x_j)\exp(\frac{1}{2}\mathrm{i}c_j(x - x_j)). \tag{52}$$

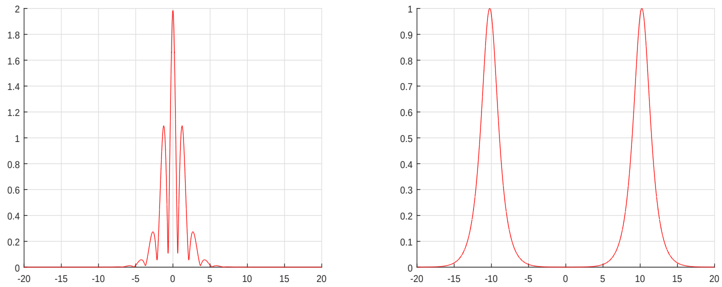

FIGURE 4. The soliton propagation of Eq. (51) with initial condition (52). $c_1 = 4, x_1 = -10, c_2 = -4, x_2 = 10$. $T = 2.5$(Left), $T = 5$(Right).

In this example, we show the process of the two solitons when they meet, collide and separate by displaying $|U(x,t)|$ in Figs. 3-4 with P^2 element and $M = 100$.

6. Concluding Remarks

In this paper, we developed the energy and mass conservative local discontinuous Galerkin method to solve the linear and nonlinear Schrödinger equation. In our ALDG method, we choose the average flux rather than the up-winding flux or alternating flux. This method conserves both energy and mass. An optimal error estimate of even order and suboptimal error estimate of odd order are obtained for the linear case. Finally, numerical results demonstrate that in most cases, our error estimates are optimal, i.e., the error bounds are sharp.

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