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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,