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A Conservative SAV-RRK Finite Element Method for the Nonlinear Schrödinger Equation

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Abstract. In this paper, we propose, analyze and numerically validate a conservative finite element method for the nonlinear Schrödinger equation. A scalar auxiliary variable (SAV) is introduced to reformulate the nonlinear Schrödinger equation into an equivalent system and to transform the energy into a quadratic form. We use the standard continuous finite element method for the spatial discretization, and the relaxation Runge-Kutta method for the time discretization. Both mass and energy conservation laws are shown for the semi-discrete finite element scheme, and also preserved for the full-discrete scheme with suitable relaxation coefficient in the relaxation Runge-Kutta method. Numerical examples are presented to demonstrate the accuracy of the proposed method, and the conservation of mass and energy in long time simulations.

AMS subject classifications: 65M15, 65M60

Key words: Schrödinger equation, mass conservation, energy conservation, finite element method, relaxation Runge-Kutta, scalar auxiliary variable.

1 Introduction

This paper focuses on developing structure-preserving numerical method for the initial boundary value problem of the nonlinear Schrödinger (NLS) equation defined by

$$\begin{cases} \mathrm{i}u_t - \alpha\Delta u + (V+\beta|u|^2)u = 0 & \text{in } \Omega\times(0,T], \\ u = u_0 & \text{in } \Omega\times\{0\}, \end{cases} \tag{1.1}$$

where $i=\sqrt{-1}$, u is an unknown complex function with homogeneous Dirichlet boundary or periodic boundary conditions, α and β are real constants. The nonlinear

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Schrödinger equation (1.1) arises from many applications in physics and engineering and is one of the fundamental equations in mathematical physics.

It is well known that the solution of Eq. (1.1) satisfies the following conservation laws

$$\frac{d}{dt}\int_\Omega |u|^2 dx = 0, \qquad \text{(mass conservation)},$$
$$\frac{d}{dt}\int_\Omega \left(\frac{\alpha}{2}|\nabla u|^2 + \frac{1}{2}V|u|^2 + \frac{\beta}{4}|u|^4\right) dx = 0 \qquad \text{(energy conservation)}.$$

The development of numerical methods that preserve these conservation properties is important for long time numerical simulation, and therefore has been one of the research hotspots for the numerical approximation of the nonlinear Schrödinger equation. Inspired by the work of Strauss and Vazquez [21] for the Klein-Gordon equation, Delfour et al. [4] proposed a second-order modified Crank-Nicolson scheme for solving the NLS equation, which could maintain the conservation of both mass and energy. Later, Sanz-Serna [17] generalized the modified Crank-Nicolson time-stepping scheme to the nonlinear Schrödinger equation with more general nonlinear terms and established the optimal error estimates for the fully-discrete scheme. Yi and Liu [26] constructed and analyzed a conservative discontinuous Galerkin (DG) method for the Schrödinger-Poisson equation.

Recently, two energy quadratic methods have been proposed for constructing structure-preserving numerical schemes that inherit the PDE properties. One quadratic technique is the invariant energy quadratic (IEQ) method initialed by Yang et al. [23–25]. The basic idea of the IEQ method is to modify the original system into an equivalent system by introducing a new variable. This equivalent system maintains the corresponding conservation law for the new variables. The advantage of this method is that the nonlinear terms can be explicitly processed in discretization, which avoids the computational cost of nonlinear iteration. The IEQ method is also successfully applied to many other problems, such as the sine-Gordon equation [11], the Lorentz force system [13] etc. The other quadratic technique is the scalar auxiliary variable (SAV) method [18, 19], in which an auxiliary variable is introduced and defined as the square root of the integral of the shifted potential energy integral. SAV method is an improvement of the IEQ method, which inherits the advantages of the IEQ method, and eliminates the need to assume the below-bound limit of the nonlinear free energy potential as a limit. Both IEQ and SAV methods have been widely used in many models to develop unconditional energy stable schemes [3, 15]. Interested readers are referred to [18–20] and references therein.

As we all know, most of the structure-preserving time-discrete methods are implicit. The implicit high-order symplectic structure of the Hamiltonian system is already well known. Li et al. [14] developed a family of linear implicit high-order energy conservation schemes for solving nonlinear wave equations by using SAV method and combining the classical high-order Gaussian method with the extrapolation approximation. Using IEQ technique, Zhang et al. [27] proposed a kind of diagonal implicit RK scheme for solving nonlinear Hamiltonian equations. It is proved that the proposed scheme can preserve a modified quadratic energy conservation law. Based on the scalar auxiliary variable