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Optimal error estimate of a compact scheme for nonlinear Schrödinger equation ☆

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ABSTRACT

It has been pointed out in literature that the symplectic scheme of a nonlinear Hamiltonian system can not preserve the total energy in the discrete sense Ge and Marsden (1988) [10]. Moreover, due to the difficulty in obtaining *a priori* estimate of the numerical solution, it is very hard to establish the optimal error bound of the symplectic scheme without any restrictions on the grid ratios. In this paper, we develop and analyze a compact scheme for solving nonlinear Schrödinger equation. We introduce a cut-off technique for proving optimal L^∞ error estimate for the compact scheme. We show that the convergence of the compact scheme is of second order in time and of fourth order in space. Meanwhile, we define a new type of energy functional by using a recursion relationship, and then prove that the compact scheme is mass and energy-conserved, symplectic-conserved, unconditionally stable and can be computed efficiently. Numerical experiments confirm well the theoretical analysis results.

1. Introduction

The nonlinear Schrödinger (NLS) equation describes many phenomena and has important applications in fluid dynamics, nonlinear optics and quantum mechanics [3,20]. Various kinds of numerical methods can be found for simulating solutions of the NLS equation. In [4,5,17], time-splitting pseudo-spectral methods are investigated. In [16,22,23], several important numerical methods are tested, analyzed and compared. The discontinuous Galerkin methods are considered in [13,27]. For a detailed description of various numerical methods for NLS equation as well as its implementation and applications, we refer the readers to the orthogonal spline collocation method [15,19] and the Runge–Kutta or Crank–Nicolson pseudo-spectral method [8,18] and the references therein.

Based on the basic rule that numerical algorithms should preserve the intrinsic properties of the original problems as much as possible, Feng [9] first presented the concept of symplectic schemes for Hamiltonian systems and developed the structure-preserving algorithms for the general conservative dynamical systems. In [6,26], the authors propose several conservative finite difference schemes for NLS equation and present that these schemes preserve the total mass and energy

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in the discrete sense. Ref. [11] firstly studied the standard Crank–Nicolson finite difference scheme which is a symplectic scheme [7,21], and obtained an error estimate of the numerical solution under an rigorous condition $\tau/h^2 \le o(1)$ with time-step τ and mesh-size h. However, the symplectic finite difference schemes for nonlinear Hamiltonian systems can not preserve the total energy in the discrete sense [10]. Furthermore, it is very difficult to obtain *a priori* estimate of the numerical solution of symplectic schemes in L^∞-norm.

To the best of our knowledge, there is no reference about symplectic and energy conservative numerical methods for NLS equation till now. In this work, we proposed a novel compact scheme for NLS equation. High-order compact technique is popular due to its high resolution, compactness and economy in scientific computation [14]. The proposed scheme can not only preserve the discrete symplectic structure, but also conserves the total mass and energy conservation laws. And the convergence result is analyzed, which shows that the compact scheme is of second order in time and of fourth order in space. Special techniques are utilized to achieve the optimal order of accuracy. Numerical experiments are shown to demonstrate the accuracy and capability of the proposed compact scheme.

The rest of this paper is organized as follows. In Section 2, we present some preliminary results and introduce several useful lemmas. In Section 3, a novel compact scheme for NLS equation is proposed and we show that the scheme preserves the discrete symplectic conservation law, discrete mass conservation law and discrete energy evolution law. The optimal error estimate in maximum norm is presented in Section 4. In Section 5, numerical experiments are performed to testify the effectiveness and accuracy of the scheme. Finally, some conclusions are addressed in Section 6.

2. Preliminary results

In order to simplify the notations, in this paper we consider one-dimensional NLS equation. The NLS equation of our interest is

$$iu_t + \alpha u_{xx} + V(x)u + f(|u|^2)u = 0, \quad x \in \Omega, \quad t \in (0, T], \tag{2.1}$$

with an initial condition

$$u(x, 0) = \varphi(x) \tag{2.2}$$

and homogeneous boundary conditions. Here, $\Omega = [a, b]$, $V(x)$ and $f(u)$ are arbitrary (smooth) nonlinear real functions and α is a real constant. It can be proved that the NLS equation (2.1) possesses the mass conservation law,

$$Q(t) := \int_a^b |u(x,t)|^2 dx = Constant, \tag{2.3}$$

and energy conservation law

$$E(t) := \int_a^b \Big(\alpha|\nabla u|^2 - V(x)|u|^2 - F(|u|^2)\Big)dx = Constant, \tag{2.4}$$

where

$$F(q) = \int_0^q f(p)dp.$$

If we set $u = r + is$, where r, s are real-valued functions, we can separate (2.1) into the following form

$$\begin{aligned} r_t + \alpha s_{xx} + V(x)s + f(r^2+s^2)s = 0,\\ -s_t + \alpha r_{xx} + V(x)r + f(r^2+s^2)r = 0. \end{aligned}$$

By introducing two additional new variables, $p = s_x$, $q = r_x$, and defining a state variable $z = (r, s, p, q)^T$, the equation above can be transformed to the Hamiltonian system

$$Kz_t + Lz_x = \nabla_z S(x, z), \tag{2.5}$$

where

$$K = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad L = \begin{pmatrix} 0 & 0 & 0 & -\alpha \\ 0 & 0 & -\alpha & 0 \\ 0 & \alpha & 0 & 0 \\ \alpha & 0 & 0 & 0 \end{pmatrix},$$

and