Commun. Comput. Phys.
doi: 10.4208/cicp.2019.js60.05

Vol. **26**, No. 5, pp. 1365-1396
November 2019

Mass- and Energy-Conserved Numerical Schemes for Nonlinear Schrödinger Equations

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Received 28 February 2019; Accepted (in revised version) 19 April 2019

Abstract. In this paper, we propose a family of time-stepping schemes for approximating general nonlinear Schrödinger equations. The proposed schemes all satisfy both mass and energy conservation (in a modified form for the latter). Truncation and dispersion error analyses are provided for four proposed schemes. Efficient fixed-point iterative solvers are also constructed to solve the resulting nonlinear discrete problems. As a byproduct, an efficient one-step implementation of the BDF schemes is obtained as well. Extensive numerical experiments are presented to demonstrate the convergence and the capability of capturing the blow-up time of the proposed schemes.

AMS subject classifications: 65M06, 65M12

Key words: Nonlinear Schrödinger equations, mass conservation and energy conservation, BDF schemes, finite element methods, finite time blow-ups.

1 Introduction

In this paper we consider the following nonlinear Schrödinger (NLS) equation:

$$iu_t = -\Delta u + \lambda f(|u|^2)u \qquad \text{in } \mathcal{D}_T := \mathcal{D}\times(0,T), \tag{1.1}$$

$$u(0) = u_0 \qquad \text{in } \mathcal{D}, \tag{1.2}$$

where $\mathcal{D}\subset\mathbf{R}^d\,(d=1,2,3)$ is a bounded domain, $\lambda=\pm1$, $T>0$ and $i=\sqrt{-1}$ stands for the imaginary unit. $u=u(x,t):\mathcal{D}_T\to\mathbb{C}$ is a complex-valued function. $f:\mathbf{R}_+\to\mathbf{R}_+$ is a given real-valued function, which could be different in different applications, e.g., see [15, 16]

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and the references therein. The best known f is $f(s)=s$, which leads to the well-known nonlinear Schrödinger equation with cubic nonlinearity. To close the system, we also need to specify a boundary condition for u. In this paper we consider both homogeneous Dirichlet and periodic boundary conditions (see Sections 7 and 8), although most of our derivations and proofs are independent of the boundary condition.

The above Schrödinger equation describes many physical phenomena in optics, mechanics, and plasma physics. Mathematically, the NLS equation is a prototypical dispersive wave equation and its solutions exhibit some intriguing properties such as energy conservation, soliton wave, and possible blow-ups [5,20]. In particular, the equation preserves both the mass and the Hamiltonian energy, that is, the following quantities are constants in time:

$$\mathcal{M}(u)(t):=\|u(t)\|_{L^2}^2=\int_{\mathcal{D}}|u(t)|^2dx, \tag{1.3}$$

$$\mathcal{H}(u)(t):=\int_{\mathcal{D}}\Big(|\nabla u(t)|^2+\lambda F(|u(t)|^2)\Big)dx,\quad F(s)=\int_0^s f(\mu)d\mu. \tag{1.4}$$

Here the dependence of u on x variable is suppressed for notational brevity. The case with positive λ is called defocusing and with negative λ is called focusing which allows for bright soliton solutions as well as breather solutions.

Dispersion and nonlinearity can interact to produce permanent and localized wave forms in nonlinear dispersive wave equations such as the Korteweg-de Vries (KdV) equation [8,14,23] and the cubic Schrödinger equation [6,24]. A distinct feature of these equations is the infinite many conservation laws (conserved integrals as invariants), allowing for soliton solutions which emerge from collision unchanged over time. The quality of the numerical approximation hence hinges on how well the conserved integrals can be preserved at the discrete level. Numerical methods without this property may result in substantial phase and shape errors after long time integration. Indeed for some wave equations the invariant preserving high order numerical methods have been shown more accurate than non-conservative methods after long-time numerical integration (see [4,11]).

For the nonlinear Schrödinger equation considered in this paper, a natural question is whether it is possible to design numerical schemes which conserve the mass and energy simultaneously. A lot of effort has been made to preserve the mass by high order spatial discretization such as spectral methods [1–3], and discontinuous Galerkin methods [12]. A modified numerical energy may be preserved approximately by the corresponding spatial discretization (see [10]). However, since those methods are based on a time-splitting technique [3], except the Crank-Nicolson scheme, they are only mass-conserved. The objective of this work is to provide an attempt to address the above question. Specifically, in this paper we develop and analyze a family of mass- and energy-conserved time-stepping schemes for approximating the cubic and general nonlinear Schrödinger equations. It should be noted that the energy conservation is also achieved for a modified energy, instead of the original energy.

The rest of this paper is organized as follows. In Section 2 we present a general framework involving two sequences of time-stepping schemes, which is shown to preserve