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Structure-Preserving Exponential Schemes with High Accuracy for the 2D/3D Nonlinear Schrödinger Type Equation

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Abstract. The paper proposes a family of novel arbitrary high-order structure-preserving exponential schemes for the nonlinear Schrödinger equation. First, we introduce a quadratic auxiliary variable to reformulate the original nonlinear Schrödinger equation into an equivalent equation with modified energy. With that, the Lawson transformation technique is applied to the equation and deduces a conservative exponential system. Then, the symplectic Runge-Kutta method approximates the exponential system in the time direction and leads to a semi-discrete conservative scheme. Subsequently, the Fourier pseudo-spectral method is applied to approximate the space of the semi-discrete to obtain a class of fully-discrete schemes. The constructed schemes are proved to inherit quadratic invariants and are stable. Some numerical examples are given to confirm the accuracy and conservation of the developed schemes at last.

AMS subject classifications: 65M06, 65M70

Key words: Nonlinear Schrödinger equation, structure-preserving, exponential integrators, quadratic auxiliary variable, symplectic Runge-Kutta methods.

1 Introduction

In the microphysical world, especially quantum mechanics, the fundamental law of matter movement can be revealed by the following the nonlinear Schrödinger (NLS) type

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equation [18,43]

$$\mathrm{i}\frac{\partial\phi(\mathbf{x},t)}{\partial t}=-\frac{1}{2}\nabla^2\phi(\mathbf{x},t)+V(\mathbf{x})\phi(\mathbf{x},t)+\beta|\phi(\mathbf{x},t)|^2\phi(\mathbf{x},t),\quad \mathbf{x}\in\Omega\subset\mathbb{R}^d,\quad t\in(0,T],\tag{1.1}$$

with

$$\phi(\mathbf{x},0)=\phi_0(\mathbf{x}),\quad \mathbf{x}\in[-L,L]^d\subset\mathbb{R}^d,\tag{1.2}$$

where $\mathrm{i}^2=-1$, $V(\mathbf{x})$ is the potential function, $\phi(\mathbf{x},t)$ is a complex-valued wave function with a period of $2L$ in d (d=2 or 3) dimensional case. The equation describes the behavior of a single quantum particle, is a fundamental equation in quantum mechanics, and has been widely used in the fields of the atom, molecule, solid-state physics, nuclear physics, and chemistry [37,39]. Its ability to describe the wave-like behavior of particles has revolutionized our understanding of the microscopic world and has paved the way for technological advancements across various scientific disciplines. For the past few decades, various numerical methods have been presented to solve the NLS equation, such as finite difference methods [1,3,43,45], mesh-less method [32], spectral methods [2,4,14,35], finite element methods [27] and so on.

Under appropriate boundary conditions, Eq. (1.1) has the mass conservation

$$\mathcal{M}(t):=\int_\Omega|\phi(\mathbf{x},t)|^2d\mathbf{x}\equiv\mathcal{M}(0),\quad t\geq0,\tag{1.3}$$

and the energy conservation

$$\mathcal{H}(t):=\int_\Omega\Big(\frac{1}{2}|\nabla\phi(\mathbf{x},t)|^2+V(\mathbf{x})|\phi(\mathbf{x},t)|^2+\frac{\beta}{2}|\phi(\mathbf{x},t)|^4\Big)d\mathbf{x}\equiv\mathcal{H}(0),\quad t\geq0.\tag{1.4}$$

By setting $\phi=u+\mathrm{i}v$, system (1.1) can be written as a pair of real-valued equations

$$u_t=-\frac{1}{2}\nabla^2v+Vv+\beta(u^2+v^2)v,\tag{1.5a}$$

$$v_t=\frac{1}{2}\nabla^2u-Vp-\beta(u^2+v^2)u.\tag{1.5b}$$

Then system further can be rewritten as an Hamiltonian system, namely

$$\frac{d}{dt}(u,v)^T=\mathcal{J}^{-1}\Big(\frac{\delta\mathcal{H}}{\delta u},\frac{\delta\mathcal{H}}{\delta v}\Big)^T\quad\text{with}\quad\mathcal{J}=\begin{pmatrix}0&1\\-1&0\end{pmatrix}.$$

As we all know, it is necessary to maintain the internal symmetry, conservation, and other physical characteristics of the original system as much as possible when constructing the numerical algorithms for many mathematical models in aeromechanics, quantum mechanics, electromagnetism, and other disciplines. However, traditional algorithms