Journal of Computational Mathematics, Vol.25, No.1, 2007, 31–48.

MULTISYMPLECTIC FOURIER PSEUDOSPECTRAL METHOD FOR THE NONLINEAR SCHRÖDINGER EQUATIONS WITH WAVE OPERATOR *1)

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Abstract

In this paper, the multisymplectic Fourier pseudospectral scheme for initial-boundary value problems of nonlinear Schrödinger equations with wave operator is considered. We investigate the local and global conservation properties of the multisymplectic discretization based on Fourier pseudospectral approximations. The local and global spatial conservation of energy is proved. The error estimates of local energy conservation law are also derived. Numerical experiments are presented to verify the theoretical predications.

Mathematics subject classification: 35Q55, 65M70, 65P10
Key words: Multisymplecticity, Fourier pseudospectral method, Local conservation laws.

1. Introduction

The nonlinear Schrödinger equations with wave operator (NSEW)

$$\frac{\partial^2\psi}{\partial t^2} - \frac{\partial^2\psi}{\partial x^2} + i\frac{\partial\psi}{\partial t} + g(|\psi|^2)\psi = 0, \tag{1.1}$$

is one of the most important models of mathematical physics, with applications in different fields such as plasma physics, nonlinear optics, water waves and biomolecular dynamics. In this work, we will concentrate on equation (1.1) subject to initial-boundary conditions

$$\begin{aligned} &\psi(0,t) = \psi(L,t), \\ &\psi(x,0) = \psi_0, \quad \psi_t(x,0) = \psi_1. \end{aligned} \tag{1.2}$$

The important feature of problem (1.1)-(1.2) is the following energy conservation law

$$\|\psi_t\|^2 + \|\psi_x\|^2 + \int_0^L Q(|\psi|^2)dx = const., \tag{1.3}$$

where Q is a primitive function of g, defined by

$$Q(s) = \int_0^s g(x)dx.$$

Several numerical methods have been investigated for solving equation (1.1), such as finite difference methods with conservative type [1, 2].

Bridge and Reich presented a multisymplectic integrator based on a multisymplectic structure of some Hamiltonian PDEs, such as Schrödinger equations and Klein-Gordon equations [3, 4]. The theoretical results indicated that significant features of the multisymplectic integrator are excellent for local invariant properties. Many numerical experiments demonstrated

* Received March 10, 2005; final revised December 18, 2005; accepted March 24, 2006.
1) This work was supported by E-Institutes of Shanghai Municipal Education Commission N.E03004.

that the multisymplectic-preserving methods can preserve local and global conservation properties for long time computations [3, 4, 6, 9, 10, 11, 12, 13]. Moreover, when the Hamiltonian function is quadratic, the multisymplectic integrators preserve discrete local energy and local momentum exactly. However, error estimates of energy and momentum conservation laws for the multisymplectic integrator in the literature remain very limited. Recently, Hong and Li [10] used Runge-Kutta methods to construct multisymplectic schemes for the nonlinear Dirac equations and presented the error estimates of local and global conservation laws of energy and momentum.

Fourier pseudospectral methods have been proven very powerful for periodic initial value problems with constant coefficients. The well known results include spectral accuracy for smooth solutions and dispersion free. These properties are important in the numerical simulation of some physical phenomena.

The NSEW admits a multisymplectic Hamiltonian formulation. It is our objective in this paper to apply the multisymplectic Fourier pseudospectral method [9] to the equation and discuss properties of energy conservation law.

This paper is structured as follows. In Section 2, the multisymplectic Hamiltonian formulation for NSEW is established and some conservation properties are obtained. Section 3 is concerned with multisymplectic Fourier pseudospectral discretizations and spatial conservation laws of energy. Section 4 involves the construction of fully discretizations scheme and error estimates of energy conservation law. Numerical experiments are given in Section 5. Finally, Section 6 contains concluding remarks.

2. Multisymplecticity and Local Conservation Law

A Hamiltonian differential equation is said to be multisymplectic if it can be written as

$$\mathbf{M}\partial_t \mathbf{z} + \mathbf{K}\partial_x \mathbf{z} = \nabla_z S(\mathbf{z}), \tag{2.1}$$

where ∂_t and ∂_x are the operators of total differentiation with respect to t and x, respectively; $\mathbf{M}$, $\mathbf{K} \in R^{d\times d}$ are skew-symmetric; $\mathbf{z}(x,t)$ is the vector of state variables and $S\colon R^d \to R^1$ is a smooth function; $\nabla_z S(\mathbf{z})$ denotes the gradient of the function $S = S(\mathbf{z})$ with respect to variable $\mathbf{z}$.

According to [3, 4], an important consequence of multisymplecticity is that the system (2.1) has a multisymplectic conservation law (MSCL):

$$\partial_t \omega + \partial_x \kappa = 0, \tag{2.2}$$

where ω and κ are pre-symplectic forms

$$\omega = dz \wedge \mathbf{M}_+ dz, \quad \kappa = dz \wedge \mathbf{K}_+ dz, \tag{2.3}$$

which define a symplectic space-time structure. Here $\wedge$ is the exterior multiplication of the two vectors, and $\mathbf{M}_+$ and $\mathbf{K}_+$ satisfy

$$\mathbf{M} = \mathbf{M}_+ + \mathbf{M}_- \quad \textit{and} \quad \mathbf{K} = \mathbf{K}_+ + \mathbf{K}_-,$$

with

$$\mathbf{M}_+^T = -\mathbf{M}_- \quad \textit{and} \quad \mathbf{K}_+^T = -\mathbf{K}_-.$$

For example, $\mathbf{M}_+$ and $\mathbf{K}_+$ can be taken as the upper triangular part of matrix $\mathbf{M}$ and $\mathbf{K}$, respectively [8].

The MSCL (2.2) is a local property which indicates that symplecticity for Hamiltonian PDEs can be vary locally over the spatial domain.

The system (2.1) has local energy conservation law (LECL)

$$\partial_t E + \partial_x F = 0, \tag{2.4}$$