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A STRUCTURE-PRESERVING DISCRETIZATION OF NONLINEAR SCHRÖDINGER EQUATION[*1)]

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Abstract

This paper studies the geometric structure of nonlinear Schrödinger equation and from the view-point of preserving structure a kind of fully discrete schemes is presented for the numerical simulation of this important equation in quantum. It has been shown by theoretical analysis and numerical experiments that such discrete schemes are quite satisfactory in keeping the desirable conservation properties and for simulating the long-time behaviour.

Key words: Schrödinger equation, Hamiltonian system, Discrete schemes, Structure preserving algorithm.

1. Introduction

Many important differential equations of evolution type in physics and mechanics have specific geometric structure. For instance, the Hamiltonian systems in classical mechanics, the Schrödinger equation in quantum, the Korteweg-de Vries and Klein-Gordon equations of nonlinear waves have symplectic structure, i.e. the evolutions in phase spases of these equations are canonical mappings. To simulate convincingly the dynamic behaviour of differential equations, it is very natural to look for discretized systems which preserve as much as possible the geometric structure and symmetries of the original continuous systems. Such discretization methods would be more satisfactory than the conventional methods in keeping the desirable conservation properties and simulating the long-time and global behaviour. In recent 10 years, studies on numerical methods from the view-point of geometry have become more and more popular. Since 1984, the symplectic methods initiated by Feng K.[1] for computation of Hamiltonian systems have been studied systematically by Qin M.Z.[2], Sanz-Serna J.M.[3], Channel P.J. and Scovel C.[4], etc.. Huang M.Y. in [5] and [6] discussed the structure preserving methods for nonlinear wave equation and Korteweg-de Vries equation, where the discretizations are related to the spectral or finite element approximations of partial differential equations and used to compute the time periodic solutions and the solitary waves respectively.

In this paper, we shall discuss the discrete approximation of Schrödinger equation, which preserves the geometric structure and desirable properties of the continuous

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system. As a model, here we consider the following nonlinear Schrödinger equation with one space variable

$$i\frac{\partial u}{\partial t} + \frac{\partial^2 u}{\partial^2 x} - |u|^2 u = 0, \tag{1.1}$$

where $i = \sqrt{-1}$, unknown function $u = \phi + i\psi$ is assumed to be periodic in x or rapidly decay as $x \to \pm\infty$.

To study the geometric structure of equation (1.1), we introduce the functional by integral

$$H(u) = \frac{1}{2}\int_{-L}^{+L} [\phi_x^2 + \psi_x^2 + (\phi^2 + \psi^2)^2] dx,$$

where $0 < L < +\infty$ when the periodic boundary condition with period $2L$ is considered and $L = \infty$ when the rapidly decay boundary condition is considered, then (1.1) is equivalent to the following system with unknown functions ϕ and ψ:

$$\begin{aligned} \frac{\partial \phi}{\partial t} &= -\frac{\partial^2 \psi}{\partial^2 x} + 2(\phi^2 + \psi^2)\psi = \frac{\delta H}{\delta \psi} \\ \frac{\partial \psi}{\partial t} &= \frac{\partial^2 \phi}{\partial^2 x} - 2(\phi^2 + \psi^2)\phi = -\frac{\delta H}{\delta \phi} \end{aligned} \tag{1.2}$$

where $\frac{\delta H}{\delta \psi}, \frac{\delta H}{\delta \phi}$ respresent the variations of $H(u)$ with respect to ψ and ϕ respectively.

From (1.2) we see that the equation (1.1) has a Hamiltonian (Symplectic) structure. It is easy to show that the solution $u(t) = u(t, x)$ of (1.1) or (1.2) has the following conservation properties:

$$\begin{aligned} &I_1(u(t)) = \int_{-L}^{+L} (\phi^2 + \psi^2) dx = \text{Const.} \quad \text{(Total Mass of particles)}; \\ &I_2(u(t)) = \int_{-L}^{+L} \psi\phi_x dx = \text{Const.} \quad \text{(Total momentum)}; \\ &I_3(u(t)) = H(u(t)) = \text{Const.} \quad \text{(Total energy)}. \end{aligned}$$

In long time simulation problems, to maintain these conservation properties is considered to be particularly important.

2. Discrete Approximation

In this section, a properly discretization of equation (1.1) with periodic boundary condition will be introduced based on formulation (1.2).

Assume that

$$-\frac{\partial^2}{\partial x^2}\xi_j(x) = \mu_j \xi_j(x), \quad \xi_j(-L) = \xi_j(L), \quad j = 1, 2, \cdots$$

i.e. $\xi_j(x)$, $j = 1, 2, \cdots$ are eigenfunctions of the operator $-\partial_{xx}$ and μ_j, $j = 1, 2, \cdots$ the corresponding eigenvalues, and consider $\{\xi_j(x)\}$ to be a ortho-normalized basis of