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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

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

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

$L^2(-L,L)$. Set

$$u(t,x)=\phi+i\psi=\sum_{j=1}^{\infty}(q_j(t)+ip_j(t))\xi_j(x),$$

then

$$H(u)=H(p,q)=\frac{1}{2}\sum_{j=1}^{\infty}\mu_j(p_j^2+q_j^2)+b(p,q),$$

where

$$b(p,q)=\frac{1}{2}\int_{-\infty}^{+\infty}(\phi^2+\psi^2)^2dx.$$

Thus, (1.2) is reduced to

$$\begin{cases}\dfrac{dq_j}{dt}=\mu_jp_j+\dfrac{\partial b}{\partial p_j}=\dfrac{\partial H}{\partial p_j}\\ \dfrac{dp_j}{dt}=-\mu_jq_j-\dfrac{\partial b}{\partial q_j}=-\dfrac{\partial H}{\partial q_j},\end{cases}\quad j=1,2,\cdots \tag{2.1}$$

In this way, the Schrödinger equation (1.1) can be viewed as an infinite-dimensional Hamiltonian system. To set up a finite-dimensional approximation of (2.1), let

$$H_N(p,q)=\frac{1}{2}\sum_{j=1}^{N}\mu_j(p_j^2+q_j^2)+b_N(p,q),$$

where

$$b_N(p,q)=b(u_N),\quad u_N=\sum_{j=1}^{N}(q_j(t)+ip_j(t))\xi_j(x)=\phi_N+i\psi_N,$$

and we use the Hamiltonian system defined by function $H_N(p,q)$

$$\begin{cases}\dfrac{dq_j}{dt}=\dfrac{\partial H_N}{\partial p_j}=\mu_jp_j+\dfrac{\partial b_N}{\partial p_j}\\ \dfrac{dp_j}{dt}=-\dfrac{\partial H_N}{\partial q_j}=-\mu_jq_j-\dfrac{\partial b_N}{\partial q_j},\end{cases}\quad j=1,2,\cdots,N \tag{2.2}$$

as a semidiscrete approximation of (1.1). This approximation not only preserves the Hamiltonian structure but also maintains the conservation properties of the original equation.

We shall get fully discrete scheme from (2.2) by carrying further discretization in time variable. Let $\tau>0$ be the time step, $t_n=n\tau$, $n=0,1,2,\cdots$, and denote

$$p_j^{n+\frac{1}{2}}=\frac{p_j^{n+1}+p_j^n}{2},\quad q_j^{n+\frac{1}{2}}=\frac{q_j^{n+1}+q_j^n}{2},$$

then the simplist difference scheme with second order accuracy for the numerical integration of (2.2) should be the midpoint scheme:

$$\begin{cases}\dfrac{q_j^{n+1}-q_j^n}{\tau}=\mu_jp_j^{n+\frac{1}{2}}+\dfrac{\partial b_N}{\partial p_j}(p^{n+\frac{1}{2}},q^{n+\frac{1}{2}})\\ \dfrac{p_j^{n+1}-p_j^n}{\tau}=-\mu_jq_j^{n+\frac{1}{2}}-\dfrac{\partial b_N}{\partial q_j}(p^{n+\frac{1}{2}},q^{n+\frac{1}{2}}),\end{cases}\quad j=1,2,\cdots,N. \tag{2.3}$$

From the geometry theory of ODEs, we know that the evolution operators of Hamiltonian systems are cannonical mappings in the phase space. It has been point out in [1] that the midpoint scheme (2.3) maintains the symplectic structure of Hamiltonian systems, i.e. (2.3) is a symplectic scheme.

Remark. In the phase space R^{2N} of Hamiltonian system (2.2), the nondegenerate skew-bilinear form

$$\omega^2(\xi,\eta)=\xi^T J_{2N}\eta, \quad \xi,\eta\in R^{2N}$$
$$J_{2N}=\begin{pmatrix} 0 & -I_N \\ I_N & 0\end{pmatrix}, \quad I_N - \text{unitary matrix of order} N$$

defines a symplectic structure on R^{2N}. A linear operator S on R^{2N} is named as symplectic operator, if

$$\omega^2(S\xi,S\eta)=\omega^2(\xi,\eta), \quad \forall \xi,\eta\in R^{2N}.$$

A differentiable map $g=g(z):R^{2N}\to R^{2N}$ is called cannonical transformation, if its Jacobian $g_*=(\partial g)(z)$ is a symplectic operator for every $z\in R^{2N}$.

Denote the evolution operator of (2.2) by $g_t=g^t(z)$, $t\in R$, $z\in R^{2N}$. For any fixed t, g^t is a connonical transformation on R^{2N}, and the family g^t, $t\in R$ forms a continuous group of cannonical mappings. The single step difference schemes of (2.2) can be written in form

$$z^{n+1}=\Phi_\tau(z^n), \quad n=0,\pm 1,\cdots \tag{2.4}$$

which defines a family of mappings on R^{2N} depending on a parameter $\tau>0$. If for all $\tau>0$, $\Phi_\tau: R^{2N}\to R^{2N}$ are cannonical mappings, then we say scheme (2.4) is a symplectic scheme.

In addition to the structure preserving feature, the fully descrete appromximation (2.3) has the total mass conservation property as indicated by

Theorem 1. *Any solution* (p^n,q^n) *of the fully discrete scheme* (2.3) *satisfies*

$$I_1(p^n,q^n)=\sum_{j=1}^N((p_j^n)^2+(q_j^n)^2)=I_1(p^0,q^0) \ \textit{conservation of the total mass of particles}$$

Proof. Multiplying the first and the second equation of (2.3) by $q^{n+\frac12}$ and $p^{n+\frac12}$ respectively and taking sum over j we obtain

$$\sum_{j=1}^N(q_j^{n+1})^2-\sum_{j=1}^N(q_j^n)^2=2\tau\sum_{j=1}^N\mu_j p_j^{n+\frac12}q_j^{n+\frac12}+2\tau\sum_{j=1}^N q_j^{n+\frac12}\frac{\partial b_N}{\partial p_j}(p^{n+\frac12},q^{n+\frac12}),$$
$$\sum_{j=1}^N(p_j^{n+1})^2-\sum_{j=1}^N(p_j^n)^2=-2\tau\sum_{j=1}^N\mu_j p_j^{n+\frac12}q_j^{n+\frac12}-2\tau\sum_{j=1}^N p_j^{n+\frac12}\frac{\partial b_N}{\partial q_j}(p^{n+\frac12},q^{n+\frac12}).$$

Since

$$\sum_{j=1}^N q_j\frac{\partial b_N}{\partial p_j}(p,q)=\sum_{j=1}^N p_j\frac{\partial b_N}{\partial q_j}(p,q)=2\int_{-L}^{+L}(\phi_N^2+\psi_N^2)\phi_N\psi_N dx,$$

then from above two equalities we see

$$\sum_{j=1}^{N}\Big((p_j^{n+1})^2+(q_j^{n+1})^2\Big)=\sum_{j=1}^{N}\Big((p_j^{n})^2+(q_j^{2})^2\Big)$$

which shows the conclusion of the theorem.

However, we failed to prove scheme (2.3) satisfying the conservation property of energy. After careful observation, we find that the following modified midpoint scheme

$$\begin{cases}\dfrac{q_j^{n+1}-q_j^n}{\tau}=\mu_j p_j^{n+\frac{1}{2}}+\left(\dfrac{\partial b_N}{\partial p_j}\right)^{n+\frac{1}{2}}\\[2ex] \dfrac{p_j^{n+1}-p_j^n}{\tau}=-\mu_j q_j^{n+\frac{1}{2}}-\left(\dfrac{\partial b_N}{\partial q_j}\right)^{n+\frac{1}{2}}\end{cases}\tag{2.5}$$

simultaneously satisfies the total mass and the energy conservation law, where

$$\Big(\frac{\partial b_N}{\partial p_j}\Big)^{n+\frac{1}{2}}=2\int_{-L}^{+L}[(\phi_N^2)^{n+\frac{1}{2}}+(\psi_N^2)^{n+\frac{1}{2}}]\psi_N^{n+\frac{1}{2}}\xi_j dx,$$
$$\Big(\frac{\partial b_N}{\partial q_j}\Big)^{n+\frac{1}{2}}=2\int_{-L}^{+L}[(\phi_N^2)^{n+\frac{1}{2}}+(\psi_N^2)^{n+\frac{1}{2}}]\phi_N^{n+\frac{1}{2}}\xi_j dx,$$

In fact, we have

Theorem 2. *The solution (p^n,q^n) of scheme (2.5) satisfies*

$$I_1(p^n,q^n)=\sum_{j=1}^{N}((p_j^n)^2+(q_j^n)^2)=I_1(p^0,q^0)$$

and

$$H_N(p^n,q^n)=\sum_{j=1}^{N}\frac{\mu_j}{2}((p_j^n)^2+(q_j^n)^2)+b_N(p^n,q^n)=H_N(p^0,q^0).$$

Proof. The first conclusion is proved in the same way as Th.1. To prove the second conclusion, we multiply the first and second equation of (2.5) by $(p_j^{n+1}-p_j^n)$ and $(q_j^{n+1}-q_j^n)$ respectively to obtain

$$\begin{aligned}\frac{1}{\tau}\sum_{j=1}^{N}(q_j^{j+1}-q_j^n)(p_j^{n+1}-p_j^n)=&\frac{1}{2}\sum_{j=1}^{N}((p_j^{n+1})^2-(p_j^n)^2)^2\mu_j\\&+\sum_{j=1}^{N}\Big(\frac{\partial b_N}{\partial p_j}\Big)^{n+\frac{1}{2}}(p_j^{n+1}-p_j^n)\end{aligned}$$

and

$$\frac{1}{\tau}\sum_{j=1}^{N}(p_j^{j+1}-p_j^n)(q_j^{n+1}-q_j^n)=-\frac{1}{2}\sum_{j=1}^{N}((q_j^{n+1})^2-(q_j^n)^2)^2\mu_j-\sum_{j=1}^{N}\Big(\frac{\partial b_N}{\partial q_j}\Big)^{n+\frac{1}{2}}(q_j^{n+1}-q_j^n).$$

Notice that

$$
\begin{aligned}
\sum_{j=1}^{N}\Big(\frac{\partial b_N}{\partial p_j}\Big)^{n+\frac12}(p_j^{n+1}-p_j^n)&+\sum_{j=1}^{N}\Big(\frac{\partial b_N}{\partial q_j}\Big)^{n+\frac12}(q_j^{n+1}-q_j^n)\\
=&\frac12\int_{-L}^{+L}[(\phi_N^{n+1})^2+(\psi_N^{n+1})^2+(\phi_N^n)^2+(\psi_N^n)^2]\\
&\cdot[(\phi_N^{n+1})^2+(\psi_N^{n+1})^2-(\phi_N^n)^2-(\psi_N^n)^2]dx\\
=&\frac12\int_{-L}^{+L}[(\phi_N^{n+1})^2+(\psi_N^{n+1})^2]^2dx-\frac12\int_{-L}^{+L}[(\phi_N^n)^2+(\psi_N^n)^2]^2dx,
\end{aligned}
$$

then combining above equalities, we get

$$
\frac12\sum_{j=1}^{N}\mu_j((p_j^{n+1})^2+(q_j^{n+1})^2)+b_N(p^{n+1},q^{n+1})=\frac12\sum_{j=1}^{N}\mu_j((p_j^n)^2+(q_j^n)^2)+b_N(p^n,q^n)
$$

which shows the second conclusion of the theorem.

Theorem 2 tells us that for given initial functions $\phi^0(x)$, $\psi^0(x)\in H^1(R)$, the solution (ϕ_N^n,ψ_N^n) of (2.5) will be uniformly bounded not only in $L^2(R)$ but also in $H^1(R)$ even as $t\to\infty$. The results of Theorem 2 indicate that the modified midpoint scheme (2.5) has a better stability property than (2.3), and it is easy to see, scheme (2.5) also has the accuracy of second order in τ. Moreover, due to

$$
[(\phi_N^2)^{n+\frac12}+(\psi_N^2)^{n+\frac12}]-[(\phi_N^{n+\frac12})^2+(\psi_N^{n+\frac12})^2]=\Big(\frac{\phi_N^{n+1}-\phi_N^n}{2}\Big)^2+\Big(\frac{\psi_N^{n+1}-\phi_N^n}{2}\Big)^2,
$$

we see that scheme (2.5) differs from the midpoint scheme (2.3) only in a perturbation term $o(\tau^2)$.

Denote $U=(\phi,\psi)^T$ and define S_N to be the subspace spanded by eigenfunctions $\{\xi_j(x),\ j=1,2,\cdots,N\}$. Let P_N be the projection operator from $L^2(R)\times L^2(R)$ onto $S_N\times S_N$. Thus scheme (2.5) can be rewritten in operator form

$$
\frac{U_N^{n+1}-U_N^n}{\tau}=-J_2\partial_{xx}U_N^{n+\frac12}+P_N(|U_N^{n+1}|^2+|U_N^n|^2)J_2U_N^{n+\frac12}, \tag{2.6}
$$

where

$$
J_2=\begin{pmatrix}0&-1\\1&0\end{pmatrix},\quad (v^TJ_2v=0,\forall v\in R^2).
$$

This formulation will fit the need to carry the convergence analysis and error estimation of the discrete method. Based on the uniform boundedness of the approximate solutions guaranteed by Theorem 2, by a conventional argument similar to finite element analysis we easily prove

Theorem 3. *For given initial data $U^0=(\phi^0,\psi^0)$, assume that the solution $U=(\phi,\psi)$ of (1.2) exists and is smooth. Then when $\tau>0$ sufficiently small, the discrete problem (2.6) has an unique solution $U_N^n=(\phi_N^n,\psi_N^n)$, and the following error estimate holds*

$$
\|U_N^n-U(t_n,x_j)\|\le e^{Ct_n}\{\|U_0^N-U(0,x)\|+O(N^{-s}+\tau^2)\}
$$

where C is a constant independent of N and τ, s is an integer determined by the smoothness of the exact solution U.

4. Numerical Experiment

As an example, we consider the following periodic boundary value problem of the nonlinear Schrödinger equation

$$\begin{aligned}
&i\frac{\partial u}{\partial t}+\frac{\partial^2 u}{\partial x^2}-2|u|^2u=0, \quad 0<x<1, t>0\\
&u(0,t)=u(1,t)\\
&u(x,0)=\sin 2\pi x
\end{aligned} \tag{3.1}$$

and use schemes (2.3) and (2.5) proposed in Section 2 to compute the approximate solution of this problem. In the Fourier expansion with respect to space variable we choose $N=10$, and for the further discretization of time variable we take $\tau=0.01$. All the Fourier coefficients are computed by exact formula. Since (2.3) and (2.5) are implicit schemes, we make use of iteration method in each time step to compute the solution.

Table 1 records the total mass and total energy values of the approximate solution of (2.3) and (2.5) for the first 182 steps. The experimental results show that the scheme (2.5) and scheme (2.3) preserve not only the mass conservation but also the energy conservation law prety well. Figs.1 and 2 are the pictures of the approximate solutions ϕ_N^n and ψ_N^n computed by scheme (2.3) for time $t=0.0,0.1,\cdots,0.5$.

Table 1

Time step n	Total energy Scheme(2.3)	Total mass Scheme(2.3)	Total energy Scheme(2.5)	Total mass Scheme(2.5)
2	5.6848024770	1.0000000000	5.6848024772	1.0000000000
12	5.6848024691	0.9999999991	5.6848024575	0.9999999973
22	5.6848024464	0.9999999955	5.6848024580	0.9999999973
32	5.6848024364	0.9999999940	5.6848024637	0.9999999982
42	5.6848024571	0.9999999972	5.6848024295	0.9999999929
52	5.6848024320	0.9999999933	5.6848023984	0.9999999881
62	5.6848024391	0.9999999944	5.6848024160	0.9999999908
72	5.6848024324	0.9999999934	5.6848023942	0.9999999874
82	5.6848024198	0.9999999914	5.6848023770	0.9999999847
92	5.6848024599	0.9999999976	5.6848024093	0.9999999898
102	5.6848024644	0.9999999983	5.6848024008	0.9999999884
112	5.6848024615	0.9999999979	5.6848023891	0.9999999866
122	5.6848024332	0.9999999935	5.6848024066	0.9999999893
132	5.6848024059	0.9999999892	5.6848023798	0.9999999852
142	5.6848023818	0.9999999855	5.6848023905	0.9999999868
152	5.6848023574	0.9999999817	5.6848023820	0.9999999855
162	5.6848023854	0.9999999861	5.6848024021	0.9999999886
172	5.6848023722	0.9999999840	5.6848024024	0.9999999887
182	5.6848023937	0.9999999873	5.6848023887	0.9999999866

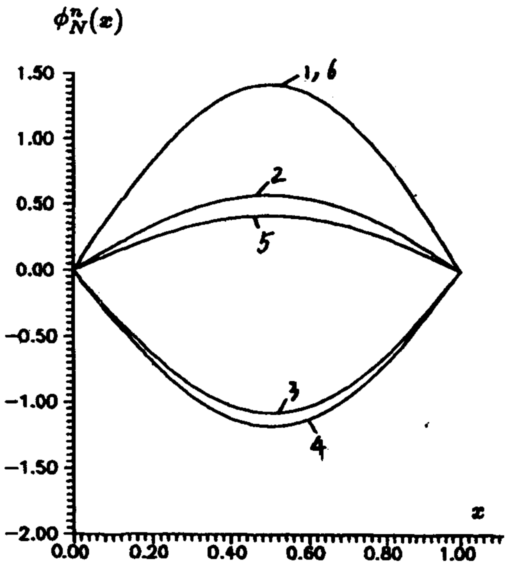

Fig. 1

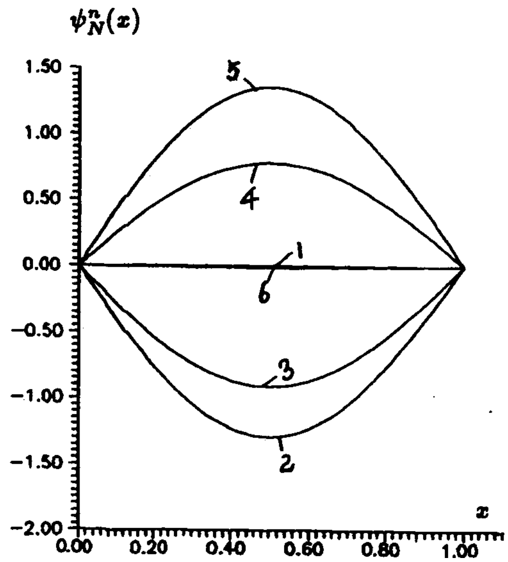

Fig. 2

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