文章编号:1674-7070(2012)06-0569-04

非线性 Schrödinger 方程的一个线性化紧致差分格式

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摘要

对非线性 Schrödinger 方程给出了一个线性化紧致差分格式,运用不动点定理和能量方法证明了格式的唯一可解性,还运用能量方法和数学归纳法,避开困难的先验估计,证明格式在空间方向和时间方向分别具有四阶和二阶精度,数值算例验证了格式的精度和数值稳定性.

关键词

非线性 Schrödinger 方程;紧致差分格式;存在唯一性;收敛性

中图分类号 O241.8

文献标志码 A

收稿日期 2012-04-21

资助项目 国家自然科学基金(41174165;11126292)

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0 引言

非线性 Schrödinger 方程

$$i\partial_t u + \partial_{xx} u + \alpha |u|^2 u = 0, \tag{1}$$

在量子物理学中具有极为广泛的应用[1-3],已有大量文献对它的初值问题或初边值问题进行了数值研究,包括有限差分法[4-9]、有限元方法[10]以及多项式近似方法[11-13]. 当前,构造非线性偏微分方程的高精度算法是国际上的一个研究热点[14-19],高精度算法能更为精准地捕捉高频振荡的波函数,因此具有非常广泛的应用前景.

本文研究非线性 Schrödinger 方程(1)带有如下初边值条件

$$u(x_l,t) = u(x_r,t) = 0,\quad t\in[0,T], \tag{2}$$

$$u(x,0) = \varphi(x),\quad x\in[x_l,x_r] \tag{3}$$

的初边值问题,其中 α 是一个非零常数,$u(x,t)$ 和 $\varphi(x)$ 分别为未知和已知的复值函数.

1 差分格式及其解的存在唯一性

取正整数 J 和 N,记 $h=\dfrac{x_r-x_l}{J}$,$\tau=\dfrac{T}{N}$分别为空间方向和时间方向的网格步长,记 $x_j=x_l+jh, j=0,1,2,\cdots,J$;$t_n=n\tau, n=0,1,2,\cdots,N$ 分别为空间方向和时间方向的网格点. 引入指标集

$$T_J=\{j\mid j=0,1,2,\cdots,J\},\quad T_J^o=\{j\mid j=1,2,\cdots,J-1\},$$

$$T_N=\{n\mid n=0,1,2,\cdots,N\},\quad T_N^o=\{j\mid j=1,2,\cdots,N-1\}.$$

令 U_j^n 和 u_j^n 分别表示函数 $u(x,t)$ 在点 (x_j,t_n) 上的近似解和精确解. 定义网格函数空间

$$X_J \triangleq \{v=(v_j)_{j\in T_J}\mid v_0=v_J=0\}\subseteq C^{J+1}.$$

任给 $v\in X_J$,并引入如下算符:

$$\delta_x^+ v_j^n=\frac{v_{j+1}^n-v_j^n}{h},\quad \delta_x^- v_j^n=\frac{v_j^n-v_{j-1}^n}{h},\quad \delta_t v_j^n=\frac{v_j^{n+1}-v_j^{n-1}}{2\tau},$$

$$\delta_x^2 v_j^n=\delta_x^+\delta_x^- v_j^n,\quad A_h v_j^n=\left(1+\frac{h^2}{12}\right)\delta_x^+\delta_x^- v_j^n.$$

任给 $u,v\in X_J$,并引入离散内积和半范数如下:

$$\|u\|_p^p = h\sum_{j=1}^{J-1}|u_j|^p,\quad 0<p<\infty,$$

$$\|u\|_\infty = \max_{j\in T_J}|u_j|,\quad (u,v)=h\sum_{j=1}^{J-1}u_j\bar{v}_j.$$

为了书写方便,本文记 $\|\cdot\|_2$ 为 $\|\cdot\|$,并引入记号"$\lesssim$":对两数 p,q,若存在广义常数 C(即与离散参数无关)使得 $p\leqslant Cq$,则记 $p\lesssim q$. 关于 $\partial_{xx}u$ 在点 (x_j,t_n) 处的差分离散,注意到

$$\delta_x^2 u_j^n=\left[\left(1+\frac{h^2}{12}\delta_x^2\right)\partial_{xx}u\right]_j^n+O(h^4),$$

和对称正定算子 $\mathscr{A}_h$ 的有界性,有

$$(\mathscr{A}_h)^{-1}\delta_x^2 u_j^n=(\partial_{xx}u)_j^n+O(h^4).$$

给出如下线性化紧致差分格式:

$$i\delta_t\mathscr{A}_hU_j^n+\frac{1}{2}\delta_x^2(U_j^{n-1}+U_j^{n+1})+\alpha\mathscr{A}_h(|U_j^n|^2U_j^n)=0,$$
$$(j,n)\in\mathscr{T}_J^o\times\mathscr{T}_N^o,\tag{4}$$
$$U_0^n=U_0^n=0,\quad n\in\mathscr{T}_N,\tag{5}$$
$$U_j^0=\phi(x_j),\quad j\in\mathscr{T}_J.\tag{6}$$

其中 U^1 可由任何一个四阶精度的两层格式得到(如文献[19]中的两层紧格式). 固定 n,格式(4)可写为

$$\mathscr{A}_hU_j^{n+1}-i\tau\delta_x^2U_j^{n+1}+P_j^n=0,\quad j\in\mathscr{T}_J^o,\tag{7}$$

其中 $P_j^n=-\mathscr{A}_hU_j^n-i\tau\delta_x^2U_j^{n-1}-2i\alpha\tau\mathscr{A}_h(|U_j^n|^2U_j^n)$.

定义映射 $\mathscr{F}:w\in X_J\to\mathscr{F}(w)\in X_J$ 如下:

$$(\mathscr{F}(w))_j=\mathscr{A}_hw_j-i\tau\delta_x^2w_j+P_j^n,j\in\mathscr{T}_J^o.\tag{8}$$

易知 $\mathscr{F}$ 是 X_J 到 X_J 连续映射,而且注意到 $\mathscr{R}(\mathscr{A}_hw,w)\geqslant\frac{2}{3}\|w\|^2$,有

$$\mathscr{R}(\mathscr{F}(w),w)=\mathscr{R}(\mathscr{A}_hw,w)+\mathscr{R}(P^n,w)\geqslant\|w\|\left(\frac{2}{3}\|w\|-\|P^n\|\right).\tag{9}$$

则由(9)立得 $\lim\limits_{\|w\|\to\infty}\frac{\mathscr{R}(\mathscr{F}(w),w)}{\|w\|}=\infty$. 从而由 Brouwer 不动点定理可知存在一个解 w^* 使得 $\mathscr{F}(w^*)=0$,从而 $U^{n+1}=w^*$ 即为差分格式的一个解. 若 $w^{(1)}$ 和 $w^{(2)}$ 都是差分格式的解,记 $w=w^{(1)}-w^{(2)}$,则由(7)可得

$$\mathscr{A}_hw-\frac{i\tau}{2}\delta_x^2w=0,\quad j\in\mathscr{T}_J^o.\tag{10}$$

将(10)与 w 做内积并取实部得

$$0=R(A_hw,w)\geqslant\frac{2}{3}\|w\|^2\geqslant0.\tag{11}$$

于是有 $\|w\|=0$,进而可得 $w^{(1)}=w^{(2)}$,即差分格式的解存在唯一.

2 差分解的收敛性分析

定义格式的截断误差 $\sigma^n\in X_J$ 如下:

$$i\delta_t\mathscr{A}_hu_j^n+\frac{1}{2}\delta_x^2(u_j^{n+1}+u_j^{n-1})+\alpha\mathscr{A}_h(|u_j^n|^2u_j^n)=\sigma_j^n,$$
$$(j,n)\in\mathscr{T}_J^o\times\mathscr{T}_N^o,\tag{12}$$
$$u_0^n=u_0^n=0,\quad n\in\mathscr{T}_N,\tag{13}$$
$$u_j^0=\phi(x_j),\quad j\in\mathscr{T}_J.\tag{14}$$

运用 Taylor 展开易得

引理 1 假设 $u\in C^{6,3}$,则格式(4)—(6)的截断误差满足如下估计

$$|\sigma_j^n|\lesssim\tau^2+h^4,\quad(j,n)\in\mathscr{T}_J^o\times\mathscr{T}_N^o.$$

定义误差函数 $e^n\in X_J$ 为

$$e_j^n=u_j^n-U_j^n,\quad(j,n)\in\mathscr{T}_J\times\mathscr{T}_N,\tag{15}$$

则关于 e^n 有如下定理:

定理 1 假设 $u\in C^{6,3}$,若 $\tau^2=o(h)$,则格式(4)—(6)的解 U^n 按离散 L^2 范数收敛到原问题(1)—(3)的解 u^n,收敛阶在时空方向分别为二阶和四阶,即

$$\|e^n\|\lesssim\tau^2+h^4,\quad n\in\mathscr{T}_N^o.$$

证明 将(1)—(3)与(4)—(6)相减得误差方程

$$i\delta_t\mathscr{A}_he_j^n+\frac{1}{2}\delta_x^2(e_j^{n+1}+e_j^{n-1})+\alpha\mathscr{A}_h(|u_j^n|^2u_j^n)-$$
$$\alpha\mathscr{A}_h(|U_j^n|^2U_j^n)=\sigma_j^n,\quad(j,n)\in\mathscr{T}_J^o\times\mathscr{T}_N^o,\tag{16}$$
$$e_0^n=e_0^n=0,\quad n\in\mathscr{T}_N,\tag{17}$$
$$e_j^0=0,\quad j\in\mathscr{T}_J.\tag{18}$$

显见 $\|e^0\|=0$,又由文献[19]知 $\|e^1\|\lesssim\tau^2+h^4$. 下面运用数学归纳法对定理 1 进行证明. 为此假设 $\|e^n\|\lesssim\tau^2+h^4,n=m-1\leqslant N-1$,只需证明 $\|e^{n+1}\|\lesssim\tau^2+h^4$. 由 $\|e^n\|_\infty\lesssim h^{-1}\|e^n\|\lesssim h^{-1}(\tau^2+h^4)$ 可得 $\|U^n\|_\infty\leqslant\|u^n\|_\infty+\|e^n\|_\infty\lesssim C_0+h^{-1}(\tau^2+h^4)$,其中 $C_0=\max_{(j,n)\in\mathscr{T}_J\times\mathscr{T}_N}|u_j^n|$. 若 $\tau^2=o(h)$,则对足够小的 h 和 τ,有 $\|U^n\|_\infty\leqslant C_0+1$.

将(16)与 $e^{n-1}+e^{n+1}$ 做内积然后取虚部得

$$\mathscr{R}(\delta_t\mathscr{A}_he^n,e^{n-1}+e^{n+1})+L_1=L_2,\quad n\in\mathscr{T}_N^o,\tag{19}$$

其中

$$L_1=\mathscr{I}\left\{h\sum_{j=1}^{J-1}A_h(|u_j^n|^2u_j^n-|U_j^n|^2U_j^n)(\bar{e}_j^{n-1}+\bar{e}_j^{n+1})\right\}=$$
$$\mathscr{I}\left\{h\sum_{j=1}^{J-1}(|u_j^n|^2u_j^n-|U_j^n|^2U_j^n)A_h(\bar{e}_j^{n-1}+\bar{e}_j^{n+1})\right\}\lesssim$$
$$(C_0+1)(\|e^{n-1}\|^2+\|e^n\|^2+\|e^{n+1}\|^2),\tag{20}$$
$$L_2=\mathscr{I}\left\{h\sum_{j=1}^{J-1}\sigma_j^n(\bar{e}_j^{n-1}+\bar{e}_j^{n+1})\right\}\lesssim$$
$$\|\sigma^n\|^2+\|e^{n-1}\|^2+\|e^{n+1}\|^2.\tag{21}$$

注意到 $\mathscr{A}_h$ 是一个对称正定的有界线性算子,可定义如下半范数:

$$|||e^n|||^2=h\sum_{j=1}^{J-1}\mathscr{A}_he_j^n\bar{e}_j^n,\tag{22}$$

且易证

$$\frac{2}{3}\| e^n \|^2 \leqslant ||| e^n |||^2 \leqslant \| e^n \|^2. \tag{23}$$

将(20)和(21)代入(19)并注意到(22)和(23)得

$$\frac{1}{\tau}(||| e^{n+1} |||^2 - ||| e^{n-1} |||^2) \lesssim \| \sigma^n \|^2 + (C_0+1)(||| e^{n-1} |||^2 + ||| e^n |||^2 + ||| e^{n+1} |||^2), \tag{24}$$

对式(24)运用 Gronwall 不等式,并注意到引理 1,可得

$$||| e^{n+1} ||| \lesssim \tau^2 + h^4, \tag{25}$$

进而由式(23)可得

$$\| e^{n+1} \| \lesssim \tau^2 + h^4. \tag{26}$$

注 1 上述理论结果对非线性 Schrödinger 周期初值问题也成立.

3 数值算例

在本节中,通过一个数值算例来说明所给算法的有效性. 考虑周期初值问题

$$i\partial_t u(x,t) + \partial_{xx} u(x,t) + 2|u(x,t)|^2 u(x,t) = 0, \quad (x,t)\in \mathbf{R}\times[0,T], \tag{27}$$

$$u(x,t) = u(x+\pi,t), \quad (x,t)\in \mathbf{R}\times[0,T], \tag{28}$$

$$u(x,0) = e^{2ix}, \quad x\in\mathbf{R}, \tag{29}$$

该问题的精确解为 $u(x,t) = e^{2i(x-t)}$. 记

$$误差 = \| u^N - U^N \|,$$

$$收敛阶 = \log\left(\frac{eu(4\tau,2h)}{eu(\tau,h)}\right)/\log 2.$$

取 $\tau = \frac{5h^2}{2\pi^2}$,数值结果列于表 1. 表 1 验证了格式在空间方向的四阶收敛性. 取足够小的空间网格步长 $h = \frac{\pi}{40}$,数值结果列于表 2 中,表 2 验证了格式在时间方向的二阶收敛性. 表 3 则给出大网格比 $\lambda = \frac{\tau}{h^2}$ 下的误差,由这些数据可知格式具有很好的数值稳定性.

表 1 数值解 $t=1$ 时刻的误差

Table 1 Errors of numerical solution at $t=1$

h	τ	误差	收敛阶
$\pi/5$	0.1	$1.838\,0\times10^{-1}$	—
$\pi/10$	0.025	$1.200\,0\times10^{-2}$	3.94
$\pi/20$	0.006 25	$7.498\,9\times10^{-4}$	4.00
$\pi/40$	0.001 562 5	$4.684\,3\times10^{-5}$	4.00

表 2 $h=\pi/40$ 时数值解在 $t=1$ 时刻的误差

Table 2 Errors of numerical solution with $h=\pi/40$ at $t=1$

τ	误差	收敛阶
0.1	$1.115\,0\times10^{-1}$	—
0.05	$2.913\,3\times10^{-2}$	1.94
0.025	$7.369\,5\times10^{-3}$	1.98
0.012 5	$1.861\,1\times10^{-3}$	1.99

表 3 大网格比下 $t=1$ 时刻的误差

Table 3 Errors of numerical solution with large mesh ratio at $t=1$

h	τ	$\lambda=\frac{\tau}{h^2}$	误差
$\pi/40$	0.1	$1.621\,1\times10^{1}$	$1.115\,0\times10^{-1}$
$\pi/400$	0.1	$1.621\,1\times10^{3}$	$1.114\,9\times10^{-1}$
$\pi/80$	0.05	$3.242\,3\times10^{1}$	$2.911\,7\times10^{-2}$
$\pi/800$	0.05	$3.242\,3\times10^{3}$	$2.911\,5\times10^{-2}$

参考文献
References

[1] Griffiths D J. Introduction to Quantum mechanics[M]. Englewood Cliffs, NJ: Prentice-Hall, 1995
[2] Menyuk C R. Stability of solitons in birefringent optical fibers Ⅱ. Arbitrary amplitudes[J]. J Opt Soc Am B, 1998, 5(2): 392-402
[3] Wadati M, Iizuka T, Hisakado M. A coupled nonlinear Schrödirnger equation and optical solitons[J]. J Phys Soc Jpn, 1992, 61(7): 2241-2245
[4] Chang Q S, Jia E H, Sun W. Difference schemes for solving the generalized nonlinear Schrödinger equation[J]. J Comput Phys, 1999, 148(2): 397-415
[5] Dai W. An unconditionally stable three-level explicit difference scheme for the Schrödinger equation with a variable coefficient[J]. SIAM J Numer Anal, 1992, 29(1): 174-181
[6] Ivanauskas F, Radziunas M. On convergence and stability of the explicit difference method for solution of nonlinear Schrödinger equations[J]. SIAM J Numer Anal, 1999, 36(5): 1466-1481
[7] Nash P L, Chen L Y. Efficient finite difference solutions to the time-dependent Schrödinger equation[J]. J Comput Phys, 1997, 130(2): 266-268
[8] Sun Z Z, Wu X. The stability and convergence of a difference scheme for the Schrödinger equation on an infinite domain by using artificial boundary conditions[J]. J Comput Phys, 2006, 214(1): 209-223
[9] Fei Z, Pérez-García V M, Vázquez L. Numerical simulation of nonlinear Schrödinger systems: A new conservative scheme[J]. Appl Math Comput, 1995, 71(2/3): 165-177
[10] Karakashian O A, Akrivis G D, Dougalis V A. On optimal order error estimates for the nonlinear Schrödinger equation[J]. SIAM J Numer Anal, 1993, 30(2): 377-400

[11] Bao W Z, Jaksch D. An explicit unconditionally stable numerical method for solving damped nonlinear Schrödinger equations with a focusing nonlinearity[J]. SIAM J Numer Anal, 2003, 41(4): 1406-1426
[12] Li B K, Fairweather G, Bialecki B. Discrete-time orthogonal spline collocation methods for Schrödinger equations in two space variables[J]. SIAM J Numer Anal, 1998, 35(2): 453-477
[13] Robinson M P, Fairweather G. Orthogonal spline collocation methods for Schrödinger-type equations in one space variable[J]. Numer Math, 1994, 68(3): 355-376
[14] Berikelashvili G, Gupta M M, Mirianashvili M. Convergence of fourth order compact difference schemes for three-dimensional convection-diffusion equations[J]. SIAM J Numer Anal, 2007, 45(1): 443-455
[15] Gopaul A, Bhuruth M. Analysis of a fourth-order scheme for a three-dimensional convection-diffusion model problem[J]. SIAM J Sci Comput, 2006, 28(6): 2075-2094
[16] Liao H L, Sun Z Z. Maximum norm error bounds of ADI and compact ADI methods for solving parabolic equations[J]. Numerical Methods for Partial Differential Equations, 2010, 26(1): 37-60
[17] Liao H L, Sun Z Z, Shi H S. Error estimate of fourth-order compact scheme for linear Schrödinger equations[J]. SIAM J Numer Anal, 2010, 47(6): 4381-4401
[18] Xie S S, Li G X, Yi S. Compact finite difference schemes with high accuracy for one-dimensional nonlinear Schröinger equation[J]. Comput Meths Appl Mech Engrg, 2009, 198(9/10/11/12): 1052-1060
[19] Wang T C, Guo B L. Unconditional convergence of two conservative compact difference schemes for nonlinear Schrödinger equation in one dimension[J]. Scientia Sinica Mathematica, 2011, 41(3): 207-233

A linearized compact difference scheme for nonlinear Schrödinger equation

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Abstract We propose a linearized compact difference scheme for the nonlinear Schrödinger equation. The existence of the difference solution is proved by Brouwer fixed point theorem. It is proved by the discrete energy method and the method of mathematical induction that the new scheme is uniquely solvable and convergent with fourth-order in x-direction and second-order in t-direction. Numerical results verify the precision and numerical stability of the proposed scheme.

Key words nonlinear Schrödinger equation; compact difference scheme; unique solvability; convergence