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非齐次 Schrödinger 方程的交替隐式格式

符莉丹[1],孔令华[1*],王 兰[1],符芳芳[2],黄晓梅[1]

(1. 江西师范大学数学与信息科学学院,江西 南昌 330022;
2. 南昌工学院基础部,江西 南昌 330108)

摘要: 以 Taylor 展开为基本工具,研究了非齐次多维 Schrödinger 方程的交替方向隐格式. 此格式在时空方向均具有 2 阶精度,而且所需求解的代数方程组的阶数与 1 维问题一样,具有经济、实用、易于模块化编程实现等优点. 数值实验主要检验了数值格式长时间的模拟能力、离散电荷随时间演化关系等.

关键词: Schrödinger 方程; 交替方向法; Taylor 展开

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0 引言

Schrödinger 方程是一类重要的物理方程,在自然科学以及科学技术的很多分支都有重要的应用,如量子力学、等离子物理学等[1-3]. 对于 Schrödinger 方程数值方法有很多研究,如有限差分法等[4-12]. 然而,这些文献考虑的大多数是齐次方程,对非齐次方程的数值格式,尤其是高效率的数值格式的研究比较少. 交替方向格式是求解多维偏微分方程非常有效的数值格式[13-24],其基本思想是把多维问题分解成若干步来求解,而每一步对于待求函数只有一个空间方向的导数,其余空间方向的导数用已知函数离散. 它克服了通常隐式差分格式需要求解巨大代数方程组计算效率不高的局限性. 此方法得到的代数方程组的阶数与 1 维问题相当,从而减少了内存消耗和计算时间,同时较大地提高计算效率. 本文主要考虑如下的 2 维非齐次线性 Schrödinger 方程的交替方向隐式格式:

$$\begin{cases} \mathrm{i}u_t = -0.5\Delta u + \sigma(x,y,t)u + f(x,y,t), \\ (x,y) \in \Omega, 0 < t \leqslant T, & (1) \\ u(x,y,0) = \varphi(x,y), (x,y) \in \Gamma, & (2) \\ u(x,y,t) \text{ 在边界 } \Gamma \text{ 上是周期函数}, & (3) \end{cases}$$

其中 $u(x,y,t)$ 是复值函数,它是充分光滑的,$\Omega = (0,a)^2$,Γ 为 Ω 的边界,$\mathrm{i} = \sqrt{-1}$,$\Delta = \dfrac{\partial^2}{\partial x^2} + \dfrac{\partial^2}{\partial y^2}$ 为 Laplace 算子. $\sigma(x,y,t)$,源项 $f(x,y,t)$,初始值 $\varphi(x,y)$ 是已知的光滑函数. 经计算分析得到周期初边值问题(1)~(3)的电荷 $Q(t)$ 与源项 $f(x,y,t)$ 之间有如下关系:

$$Q(t) - Q(0) = \int_\Omega |u(x,y,t)|^2 \mathrm{d}x\mathrm{d}y - \int_\Omega |u(x,y,0)|^2 \mathrm{d}x\mathrm{d}y = -\mathrm{i}\int_0^t \int_\Omega [f(x,y,\tau)\bar{u}(x,y,\tau) - \bar{f}(x,y,\tau)u(x,y,\tau)]\,\mathrm{d}x\mathrm{d}y\mathrm{d}\tau. \quad (4)$$

由(4)式可知,若源函数 $f(x,y,t)$ 是周期函数,则电荷 $Q(t)$ 将呈现周期性的波动.

为便于构造数值格式,引进以下记号: 首先对时空区域进行剖分,为简单起见,取 x,y 方向的步长均为 $h = a/M$,时间步长为 $\tau = T/N$,其中 M,N 为正整数. 记 $x_j = jh, y_k = kh, 0 \leqslant j,k \leqslant M, t_l = l\tau, 0 \leqslant l \leqslant N$. $\Omega_h = \{(x_j,y_k) | 0 \leqslant j,k \leqslant M\}$,$\Omega_\tau = \{t_l | 0 \leqslant l \leqslant N\}$,$\gamma = \{(0,k),(M,k) | 0 \leqslant k \leqslant M\} \cup \{(j,0),(j,M) | 1 \leqslant j \leqslant M-1\}$.

此外记 $t_{l+1/2} = (t_l + t_{l+1})/2$,$f_{jk}^{l+1/2} = f(x_j,y_k,t_{l+1/2})$. 设 $V_{h,\tau} = \{v_{jk}^l | 0 \leqslant j,k \leqslant M, 0 \leqslant l \leqslant N\}$ 为 $\Omega_h \times \Omega_\tau$ 上的网格函数,引进如下记号:

$$v_{jk}^{l+1/2} = (v_{jk}^l + v_{jk}^{l+1})/2, \delta_t v_{jk}^{l+1/2} = (v_{jk}^{l+1} - v_{jk}^l)/\tau,$$
$$\delta_x v_{j+1/2,k}^l = (v_{j+1,k}^l - v_{jk}^l)/h, \delta_y v_{j,k+1/2}^l = (v_{j,k+1}^l - v_{jk}^l)/h,$$
$$\delta_x^2 v_{jk}^l = (\delta_x v_{j+1/2,k}^l - \delta_x v_{j-1/2,k}^l)/h,$$
$$\delta_y^2 v_{jk}^l = (\delta_y v_{j,k+1/2}^l - \delta_y v_{j,k-1/2}^l)/h.$$

1 格式的建立

定义 $\Omega_h \times \Omega_\tau$ 上的网格函数 $U = \{U_{jk}^l | 0 \leqslant j,k \leqslant$

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通信作者: 孔令华(1977-),男,江西石城人,副教授,博士,主要从事偏微分方程数值解法的研究.

$M,0 \leqslant l \leqslant N\}$,其中 $U_{jk}^{l} = u(x_j,y_k,t_l)$,$0 \leqslant j,k \leqslant M$,$0 \leqslant l \leqslant N$. 在点$(x_j,y_k,t_{l+1/2})$处考虑微分方程(1)有

$$\mathrm{i}\frac{\partial u(x_j,y_k,t_{l+1/2})}{\partial t} = -\frac{1}{2}\left[\frac{\partial^2 u(x_j,y_k,t_{l+1/2})}{\partial x^2} + \frac{\partial^2 u(x_j,y_k,t_{l+1/2})}{\partial y^2}\right] + \sigma_{jk}^{l+1/2}u(x_j,y_k,t_{l+1/2}) + f(x_j,y_k,t_{l+1/2}), \tag{5}$$

由 Taylor 展开有

$$\frac{\partial u(x_j,y_k,t_{l+1/2})}{\partial t} = \delta_t U_{jk}^{l+1/2} - \frac{\tau^2}{24}\cdot\frac{\partial^3 u(x_j,y_k,\eta_{jk}^{l})}{\partial t^3},$$

$\eta_{jk}^{l} \in (t_l,t_{l+1})$,

$$u(x_j,y_k,t_{l+1/2}) = \frac{1}{2}(U_{jk}^{l} + U_{jk}^{l+1}) - \frac{\tau^2}{8}\cdot\frac{\partial^2 u(x_j,y_k,\acute{\eta}_{jk}^{l})}{\partial t^2},$$

$\acute{\eta}_{jk}^{l} \in (t_l,t_{l+1})$,

$$\frac{\partial^2 u(x_j,y_k,t_{l+1/2})}{\partial x^2} = \frac{1}{2}\left[\frac{\partial^2 u(x_j,y_k,t_l)}{\partial x^2} + \frac{\partial^2 u(x_j,y_k,t_{l+1})}{\partial x^2}\right] - \frac{\tau^2}{8}\cdot\frac{\partial^4 u(x_j,y_k,\tilde{\eta}_{jk}^{l})}{\partial x^2\partial t^2} =$$

$$\frac{1}{2}\left[\left(\delta_x^2 U_{jk}^{l} - \frac{h^2}{12}\frac{\partial^4 u(\tilde{\xi}_{jk}^{l},y_k,t_l)}{\partial x^4}\right) + \left(\delta_x^2 U_{jk}^{l+1} - \frac{h^2}{12}\cdot\frac{\partial^4 u(\tilde{\xi}_{jk}^{l+1},y_k,t_{l+1})}{\partial x^4}\right)\right] - \frac{\tau^2}{8}\cdot\frac{\partial^4 u(x_j,y_k,\tilde{\eta}_{jk}^{l})}{\partial x^2\partial t^2},$$

$\tilde{\eta}_{jk}^{l} \in (t_l,t_{l+1})$,$\tilde{\xi}_{jk}^{l},\tilde{\xi}_{jk}^{l+1} \in (x_{j-1},x_{j+1})$.

$$\frac{\partial^2 u(x_j,y_k,t_{l+1/2})}{\partial y^2} = \frac{1}{2}\left[\frac{\partial^2 u(x_j,y_k,t_l)}{\partial y^2} + \frac{\partial^2 u(x_j,y_k,t_{l+1})}{\partial y^2}\right] - \frac{\tau^2}{8}\cdot\frac{\partial^4 u(x_j,y_k,\bar{\eta}_{jk}^{l})}{\partial y^2\partial t^2} =$$

$$\frac{1}{2}\left[\left(\delta_y^2 U_{jk}^{l} - \frac{h^2}{12}\cdot\frac{\partial^4 u(x_j,\bar{\xi}_{jk}^{l},t_l)}{\partial y^4}\right) + \left(\delta_y^2 U_{jk}^{l+1} - \frac{h^2}{12}\cdot\frac{\partial^4 u(x_j,\bar{\xi}_{jk}^{l+1},t_{l+1})}{\partial y^4}\right)\right] - \frac{\tau^2}{8}\frac{\partial^4 u(x_j,y_k,\bar{\eta}_{jk}^{l})}{\partial y^2\partial t^2},$$

$\bar{\eta}_{jk}^{l} \in (t_l,t_{l+1})$,$\bar{\xi}_{jk}^{l},\bar{\xi}_{jk}^{l+1} \in (y_{j-1},y_{j+1})$.

将上述各式代入(5)式得

$$\mathrm{i}\delta_t U_{jk}^{l+1/2} - \frac{\mathrm{i}\tau^2}{24}\cdot\frac{\partial^3 u(x_j,y_k,\eta_{jk}^{l})}{\partial t^3} = -\frac{1}{4}\left[\delta_x^2 U_{jk}^{l} - \frac{h^2}{12}\cdot\frac{\partial^4 u(\tilde{\xi}_{jk}^{l},y_k,t_l)}{\partial x^4} + \delta_x^2 U_{jk}^{l+1} - \frac{h^2}{12}\cdot\frac{\partial^4 u(\tilde{\xi}_{jk}^{l+1},y_k,t_{l+1})}{\partial x^4} - \frac{\tau^2}{4}\cdot\frac{\partial^4 u(x_j,y_k,\tilde{\eta}_{jk}^{l})}{\partial x^2\partial t^2} + \delta_y^2 U_{jk}^{l} - \frac{h^2}{12}\cdot\frac{\partial^4 u(x_j,\bar{\xi}_{jk}^{l},t_l)}{\partial y^4} + \delta_y^2 U_{jk}^{l+1} - \frac{h^2}{12}\cdot\frac{\partial^4 u(x_j,\bar{\xi}_{jk}^{l+1},t_{l+1})}{\partial y^4} - \frac{\tau^2}{4}\cdot\frac{\partial^4 u(x_j,y_k,\bar{\eta}_{jk}^{l})}{\partial x^2\partial t^2}\right] + \frac{\sigma_{jk}^{l+1/2}}{2}(U_{jk}^{l} + U_{jk}^{l+1}) - \frac{\sigma_{jk}^{l+1/2}}{8}\cdot\frac{\tau^2\partial^2 u(x_j,y_k,\acute{\eta}_{jk}^{l})}{\partial t^2} + f_{jk}^{l+1/2},$$

其中 $\sigma_{jk}^{l+1/2} = \sigma(x_j,y_k,t_{l+1/2})$,$f_{jk}^{l+1/2} = f(x_j,y_k,t_{l+1/2})$.

进一步地,

$$\mathrm{i}\delta_t U_{jk}^{l+1/2} = -\frac{1}{4}\delta_x^2 U_{jk}^{l} - \frac{1}{4}\delta_x^2 U_{jk}^{l+1} - \frac{1}{4}\delta_y^2 U_{jk}^{l} - \frac{1}{4}\delta_y^2 U_{jk}^{l+1} + \frac{\sigma_{jk}^{l+1/2}}{2}(U_{jk}^{l} + U_{jk}^{l+1}) + f_{jk}^{l+1/2} + \frac{\mathrm{i}\tau}{8}(\delta_x^2 - \sigma_{jk}^{l+1/2})(\delta_y^2 - \sigma_{jk}^{l+1/2})(U_{jk}^{l+1} - U_{jk}^{l}) + R_{jk}^{l+1/2}, \tag{6}$$

其中

$$R_{jk}^{l+1/2} = \left[\frac{\mathrm{i}}{24}\cdot\frac{\partial^3 u(x_j,y_k,\eta_{jk}^{l})}{\partial t^3} + \frac{1}{16}\cdot\frac{\partial^4 u(x_j,y_k,\tilde{\eta}_{jk}^{l})}{\partial x^2\partial t^2} + \frac{1}{16}\cdot\frac{\partial^4 u(x_j,y_k,\bar{\eta}_{jk}^{l})}{\partial y^2\partial t^2} - \frac{\sigma_{jk}^{l+1/2}}{8}\cdot\frac{\partial^2 u(x_j,y_k,\acute{\eta}_{jk}^{l})}{\partial t^2} - \frac{\mathrm{i}}{8}(\delta_x^2 - \sigma_{jk}^{l+1/2})(\delta_y^2 - \sigma_{jk}^{l+1/2})\delta_t U_{jk}^{l+1/2}\right]\tau^2 + \left[\frac{1}{48}\cdot\frac{\partial^4 u(\tilde{\xi}_{jk}^{l},y_k,t_l)}{\partial x^4} + \frac{1}{48}\cdot\frac{\partial^4 u(\tilde{\xi}_{jk}^{l+1},y_k,t_{l+1})}{\partial x^4} + \frac{1}{48}\cdot\frac{\partial^4 u(x_j,\bar{\xi}_{jk}^{l},t_l)}{\partial y^4} + \frac{1}{48}\cdot\frac{\partial^4 u(x_j,\bar{\xi}_{jk}^{l+1},t_{l+1})}{\partial y^4}\right]h^2.$$

由初边值条件(2)和(3)得

$U_{jk}^{0} = \varphi(x_j,y_k)$,$1 \leqslant j,k \leqslant M$,

$U_{jk}^{l} = \alpha(x_j,y_k,t_l)$,$(j,k) \in \gamma$,$0 \leqslant l \leqslant N$,

在(6)式中略去小量项 $R_{jk}^{l+1/2}$,并用 u_{jk}^{l} 代替 U_{jk}^{l},可得差分格式:

$$\mathrm{i}\delta_t u_{jk}^{l+1/2} = -\frac{1}{2}\delta_x^2 u_{jk}^{l+1/2} - \frac{1}{2}\delta_y^2 u_{jk}^{l+1/2} + \sigma_{jk}^{l+1/2}u_{jk}^{l+1/2} + f_{jk}^{l+1/2} + \frac{\mathrm{i}\tau}{8}(\delta_x^2 - \sigma_{jk}^{l+1/2})(\delta_y^2 - \sigma_{jk}^{l+1/2})\delta_t u_{jk}^{l+1/2},$$

即

$$\left[I - \frac{\mathrm{i}\tau}{4}(\delta_x^2 - \sigma_{jk}^{l+1/2})\right]\left[I - \frac{\mathrm{i}\tau}{4}(\delta_y^2 - \sigma_{jk}^{l+1/2})\right]u_{jk}^{l+1} = \left[I + \frac{\mathrm{i}\tau}{4}(\delta_x^2 - \sigma_{jk}^{l+1/2})\right]\left[I + \frac{\mathrm{i}\tau}{4}(\delta_y^2 - \sigma_{jk}^{l+1/2})\right]u_{jk}^{l} - \mathrm{i}\tau f_{jk}^{l+1/2},$$

其中 I 是单位变换,即 $Iu_{jk}^{l} = u_{jk}^{l}$. 按如下方式引入过渡层 $\bar{u}_{jk}$,得

$$\left[I - \frac{\mathrm{i}\tau}{4}(\delta_x^2 - \sigma_{jk}^{l+1/2})\right]\bar{u}_{jk} = \left[I + \frac{\mathrm{i}\tau}{4}(\delta_y^2 - \sigma_{jk}^{l+1/2})\right]u_{jk}^{l} - \frac{\mathrm{i}\tau}{2}f_{jk}^{l+1/2}, \tag{7}$$

$$\left[I - \frac{\mathrm{i}\tau}{4}(\delta_y^2 - \sigma_{jk}^{l+1/2})\right]u_{jk}^{l+1} = \left[I + \frac{\mathrm{i}\tau}{4}(\delta_x^2 - \sigma_{jk}^{l+1/2})\right]\bar{u}_{jk} - \frac{\mathrm{i}\tau}{2}f_{jk}^{l+1/2}. \tag{8}$$

由(8)式得

$$\left[I + \frac{\mathrm{i}\tau}{4}(\delta_x^2 - \sigma_{jk}^{l+1/2})\right]\bar{u}_{jk} = \left[I - \frac{\mathrm{i}\tau}{4}(\delta_y^2 - \sigma_{jk}^{l+1/2})\right]u_{jk}^{l+1} + \frac{\mathrm{i}\tau}{2}f_{jk}^{l+1/2}, \tag{9}$$

将(9)式与(7)式相加可得

$$\bar{u}_{jk} = u_{jk}^{l+1/2} - \frac{\mathrm{i}\tau^2}{8}\delta_y^2\delta_t u_{jk}^{l+1/2} + \frac{\mathrm{i}\tau^2}{8}\sigma_{jk}^{l+1/2}\delta_t u_{jk}^{l+1/2}.$$

由于 $u_{0k}^{l+1/2}$ 和 $u_{Mk}^{l+1/2}$ 为已知的,则过渡层变量应该满足:

$$\bar{u}_{0k} = u_{0k}^{l+1/2} - \frac{\mathrm{i}\tau^2}{8}\delta_y^2\delta_t u_{0k}^{l+1/2} + \frac{\mathrm{i}\tau^2}{8}\sigma_{jk}^{l+1/2}\delta_t u_{0k}^{l+1/2},$$

$$\bar{u}_{Mk} = u_{Mk}^{l+1/2} - \frac{\mathrm{i}\tau^2}{8}\delta_y^2\delta_t u_{Mk}^{l+1/2} + \frac{\mathrm{i}\tau^2}{8}\sigma_{jk}^{l+1/2}\delta_t u_{Mk}^{l+1/2},$$

其中 $1 \leqslant k \leqslant M-1$.

由上述的推导过程可知,此格式的局部截断误差为 $O(\tau^2 + h^2)$.

2　数值例子

取空间区域为 $\bar{\Omega} = [0,\pi]^2$,在方程(1)中取 $f(x,y,t) = (1 - 4k^2 - \sin 2(x+y))\mathrm{e}^{2ik(x+y)-it}$,其中 k 是波数,在此实验中取 $k = 1$,$\sigma(x,y,t) = \sin 2(x+y)$. 在适当的初始条件下此问题有精确解 $u(x,y,t) = \mathrm{e}^{2ki(x+y)-it}$. 令 $\tau = 0.025$,$h = \pi/80$. 用格式(7)和(8)模拟此问题直到 $t = 500$. 图 1 画出了当 $t = 500$ 时数值解和精确解之间的相对误差,图 1(a)为实部误差,图 1(b)为虚部误差,从图 1 可以看出实部的误差可以达到 10^{-4} 数量级,虚部的误差可以达到 10^{-3} 数量级. 图 2(a)描述了数值解在 $t = 500$ 时刻实部与虚部之间的关系,图 2(b)描述了各个时刻实部与虚部之间关系的相图,从图 2 中可以看出解的各个时刻实部与虚部保持在单位圆上,这表明方法保持解的长时间稳定. 图 3 展示了离散电荷随时间的演化关系. 由图 3 可以看出,电荷在小范围内随时间呈周期性波动,这与理论分析完全吻合. 图 4 展示了数值解的实部与虚部的误差与空间网格数之间的关系. 同时由图 4 可以看出,格式在空间方向具有 2 阶精度,同样可以得到时间方向也具有 2 阶收敛精度.

由图 1 ~ 图 4 可以观察到,本文所构造的交替方向隐式格式能够很好地模拟原问题. 格式的误差控制在 1‰ 左右的范围. 与精确解一样,数值解的相图始终保持在单位圆上. 数值格式在时空间方向均具有 2 阶收敛精度. 以上的模拟结果与理论部分的分析结论是一致的.

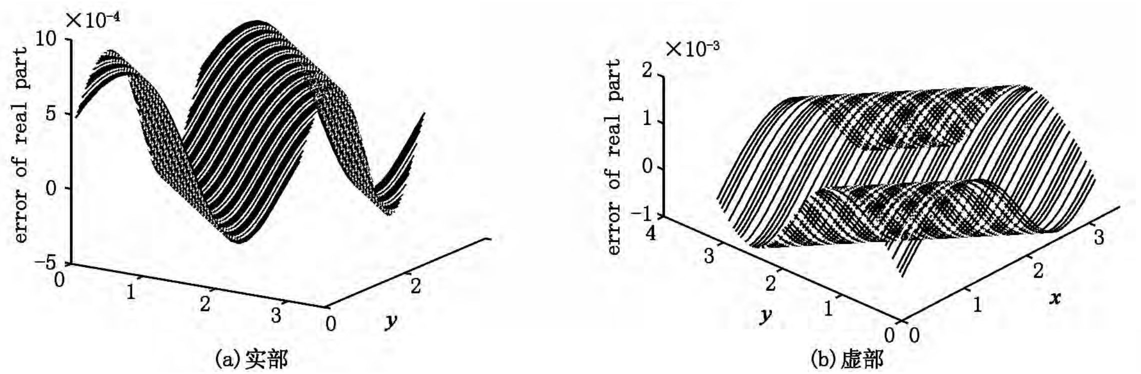

图 1　数值解在 $t = 500$ 时刻的误差

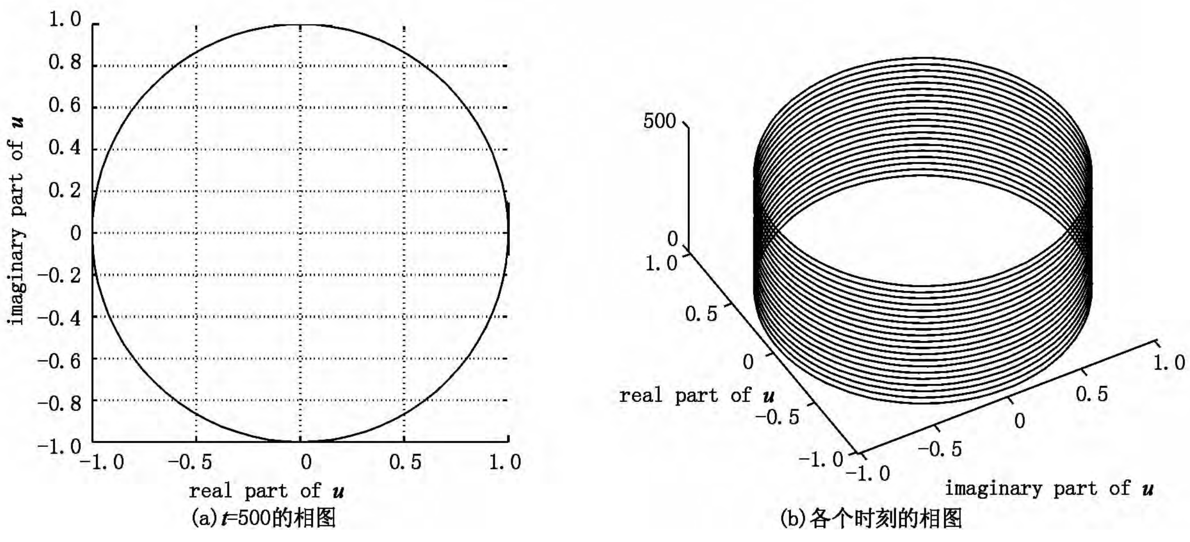

图 2　数值解的实部与虚部之间的相图

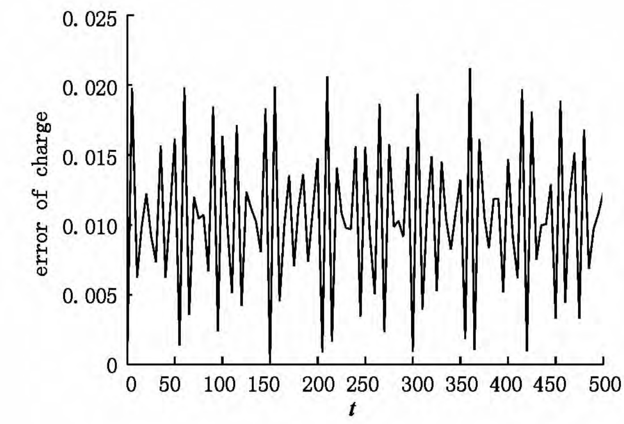

图3 电荷误差随时间的演化关系

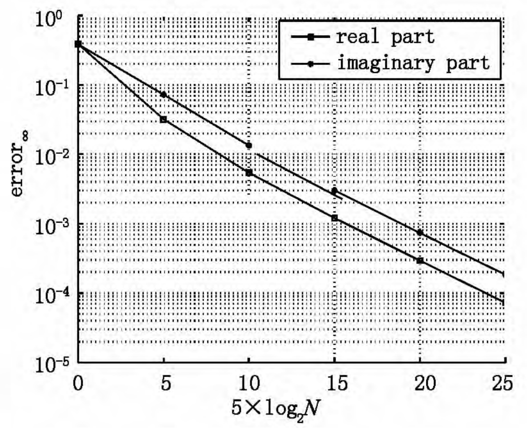

图4 数值解的误差与空间网格数之间的关系

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Premium Estimator under Stein Loss

YU Jun[1], ZHANG Yi[2], WEN Li-min[1,3*]

(1. College of Mathematics and Informatics, Jiangxi Normal University, Nanchang Jiangxi 330022, China;
2. School of Computer Science, Jiangxi Normal University, Nanchang Jiangxi 330022, China;
3. College of Information Management, Jiangxi University of Finance and Economics, Nanchang Jiangxi 330013)

Abstract: The premium estimate under a typical asymmetric Stein loss function is studied by the credibility theory. The three type of estimator including Bayes estimator, credibility estimator and hierarchical Bayes estimator under Stein loss function are discussed. Finally, by numerical simulation method the quality of three estimates are compared. The results show that, under Stein loss function, when the sample size n tends to infinity, all the three premium estimator convergence to risk premiums respectively. In addition, the robustness of hierarchical Bayes estimator is better than that of two other estimator.

Key words: Bayes estimator; credibility estimator; hierarchical Bayes estimator; robustness

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The Alternative Direction Implicit Scheme for Inhomogeneous Schrödinger Equation

FU Li-dan[1], KONG Ling-hua[1*], WANG Lan[1], FU Fang-fang[2], HUANG Xiao-mei[1]

(1. College of Mathematics and Informatics, Jiangxi Normal University, Nanchang Jiangxi 330022, China;
2. Department of Basic Teaching, Nanchang Institute of Science and Technology, Nanchang Jiangxi 330108, China)

Abstract: Based on Taylor's expansion, an alternative direction implicit scheme was proposed for multidimensional Schrödinger equation. The scheme is of second order both in time and space. Moreover, the scale of the algebraic equations resulting from the scheme is the same with a one-dimensional problem. It is economic, practical and can be coded modularly. Numerical experiments verify the long-term simulation of the developed scheme to original problem and the evolution of discrete charge against time.

Key words: Schrödinger equation; alternative direction implicit scheme; Taylor's expansion

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