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# Klein-Gordon-Schrödinger 方程的 几种差分格式及比较

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**摘要:** 探究在特定的初值和边界条件下一维 Klein-Gordon-Schrödinger 方程的几种差分格式并进行比较。利用经典的向前差分算子、中心差分算子、Crank-Nicolson 方法和紧差分算子分别为 Klein-Gordon-Schrödinger 方程构造向前 Euler 式、Crank-Nicolson 格式及紧差分格式。结果表明: Crank-Nicolson 格式及紧差分格式能够精确地保持离散电荷和能量守恒。数值实验验证了理论结果的正确性。

**关键词:** Klein-Gordon-Schrödinger 方程; 向前 Euler 格式; Crank-Nicolson 格式; 紧差分格式; 电荷守恒; 能量守恒

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## Several Difference Schemes and Comparisons for Klein-Gordon-Schrödinger Equation

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**Abstract:** Several difference schemes of one-dimensional Klein-Gordon-Schrödinger equation under specific initial value and boundary conditions are investigated and contrasted. The classical forward difference operator, central difference operator, Crank-Nicolson method and compact difference operator are used to construct forward Euler scheme, Crank-Nicolson scheme and compact difference scheme respectively. Results show that Crank-Nicolson scheme and the compact difference scheme can accurately conserve the discrete charge and energy conservation. The correctness of the theoretical result has been verified by numerical experiments.

**Keywords:** Klein-Gordon-Schrödinger equation; forward Euler scheme; Crank-Nicolson scheme; compact difference scheme; charge conservation; energy conservation

Klein-Gordon-Schrödinger(KGS)方程是薛定谔方程的狭义相对论形式,该系统于 1970 年被 Yukawa 首次提出。1975 年,由 Fukuda 和 Tsutsumi 提出了带有 Yukawa 作用的 KGS 系统模型<sup>[1]</sup>,被用来描述量子场理论中守恒复标量核子场与实标量介子场之间相互作用,是相对论量子力学和量子场论中的最基本方程。随着学术科研的发展与科学技术的创新,KGS 方程的研究越来越受到国内外学者的重视。在过去的二十年中,许多学者们针对 KGS 方程的解析解和数值解进行了一系列的研究。

在数学方面,Fukuda 等<sup>[1]</sup>讨论了三维空间中耦合的 KGS 方程的初边值问题,建立了初边值问题整体解的存在唯一性定理。Baillon 等<sup>[2]</sup>讨论了耦合的 KGS 方程的柯西问题,并且证明了 KGS 方程柯西问题的唯一整体解的存在性。Darwish 等<sup>[3]</sup>设计了一种代数方法来统一构造 KGS 耦合方程的一系列

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显式精确解。Wang 等<sup>[4]</sup>用雅可比椭圆函数展开法的推广得到 KGS 方程的周期波解。文献[5-10]也在数学上对 KGS 方程展开研究。

然而,该方程的解析解很难得到,大多数情形只能靠数值方法进行求解。因此,对于如何得到能够长时间地保持系统解的行为的 KGS 方程的数值解就显得尤为重要。在数值方面,学者们利用许多不同的数值方法对 KGS 方程进行了数值计算<sup>[11-17]</sup>。Wang<sup>[11]</sup>提出一个紧差分格式来计算具有齐次 Dirichlet 边界条件的 KGS 方程。通过连接合适的辛 Runge-Kutta-type 方法和辛 Runge-Kutta-Nyström-type 方法,Hong 等<sup>[12]</sup>提出了 KGS 方程的显式多辛格式,并证明用该方法构造的方法是多辛的,可在适当的边界条件下精确地保持离散电荷守恒定律。Wang 等<sup>[13]</sup>提出用傅里叶谱方法求解具有周期边界条件的空间分数阶 KGS 方程,并且表明该格式可以保持离散电荷和能量守恒。

基于此,本文在一定的初值和边值条件下,利用不同的差分格式求解一维 KGS 方程并进行比较。

## 1 数值格式的构造

在区域  $\Omega=[a,b]\times[0,T]$  上考虑一维 KGS 方程,即

$$i\varphi_t+\frac{1}{2}\varphi_{xx}+\varphi u=0,\quad x\in[a,b],\quad 0< t\leq T,\tag{1}$$

$$u_{tt}-u_{xx}+u-|\varphi|^2=0,\quad x\in[a,b],\quad 0< t\leq T.\tag{2}$$

选取初值条件

$$\varphi(x,0)=\varphi_0(x),\quad u(x,0)=u_0(x),\quad u_t(x,0)=u_1(x),\quad x\in[a,b]\tag{3}$$

和 Dirichlet 零边界条件

$$\varphi(a,t)=\varphi(b,t)=0,\quad u(a,t)=u(b,t)=0,\quad t\in(0,T].\tag{4}$$

式(3)中: $\varphi_0(x)$ 是给定的具有足够光滑性的复值函数; $u_0(x)$ 和  $u_1(x)$ 是两个给定的具有足够光滑性的实值函数,这 3 个函数充当求解过程中的初始解。

式(1)~(4)具有电荷守恒律和能量守恒律,即

$$Q(t)=\int_a^b|\varphi|^2dx=Q(0),\tag{5}$$

$$E(t)=\frac{1}{2}\int_a^b(u^2+u_t^2+u_x^2+|\varphi_x|^2-2u|\varphi|^2)dx=E(0).\tag{6}$$

对区域  $\Omega=[a,b]\times[0,T]$  进行网格剖分,设  $J$  和  $N$  是正整数,取空间步长为  $h=\frac{b-a}{J}$ ,时间步长为  $\tau=T/N$ ,则定义网格点集合为

$$\Omega_h=\{x_j=a+jh,j=1,\cdots,J-1\},\quad \Omega_\tau=\{t_n=n\tau,n=1,\cdots,N-1\},$$

$$\overline{\Omega}_h=\{x_j=a+jh,j=0,1,\cdots,J\},\quad \overline{\Omega}_\tau=\{t_n=n\tau,n=0,1,\cdots,N\}.$$

设  $\{v_j^n|0\leq n\leq N,0\leq j\leq J\}$  为  $\overline{\Omega}_h\times\overline{\Omega}_\tau$  上的网格函数,引入差分算子

$$\delta_x^+v_j^n=\frac{v_{j+1}^n-v_j^n}{h},\quad j\neq J,$$

$$\delta_x^2v_j^n=\frac{v_{j+1}^n-2v_j^n+v_{j-1}^n}{h^2},\quad j\neq 0,J,$$

$$\delta_t^+v_j^n=\frac{v_j^{n+1}-v_j^n}{\tau},\quad n\neq N,$$

$$\delta_t^2v_j^n=\frac{v_j^{n+1}-2v_j^n+v_j^{n-1}}{\tau^2},\quad n\neq 0,N,$$

$$\delta_tv_j^n=\frac{v_j^{n+1}-v_j^{n-1}}{2\tau},\quad n\neq 0,N,$$

$$A_hv_j^n=\left(1+\frac{h^2}{12}\delta_x^2\right)v_j^n=\frac{1}{12}(v_{j+1}^n+10v_j^n+v_{j-1}^n),\quad j\neq 0,J.$$

定义空间

$$V_h=\{\widetilde{\boldsymbol{v}}|\widetilde{\boldsymbol{v}}=(v_1,v_2,\cdots,v_{J-1})\},$$

$$V_h^0=\{\boldsymbol{v}|\boldsymbol{v}=\{v_j|0\leqslant j\leqslant J\}\in V_h,v_0=v_J=0\}$$

和三对角矩阵

$$\boldsymbol{A}=\frac{1}{h^2}\begin{pmatrix}-2&1&0&0&\cdots&0\\1&-2&1&0&\cdots&0\\0&1&-2&1&\cdots&0\\\vdots&\vdots&\vdots&\vdots&\vdots&\vdots\\0&\cdots&0&1&-2&1\\0&\cdots&0&0&1&-2\end{pmatrix}_{(J-1)\times(J-1)},$$
$$\boldsymbol{B}=\frac{1}{12}\begin{pmatrix}10&1&0&0&\cdots&0\\1&10&1&0&\cdots&0\\0&1&10&1&\cdots&0\\\vdots&\vdots&\vdots&\vdots&\vdots&\vdots\\0&\cdots&0&1&10&1\\0&\cdots&0&0&1&10\end{pmatrix}_{(J-1)\times(J-1)}.$$

其中:矩阵  $\boldsymbol{A}$  根据二阶中心差分算子可得,矩阵  $\boldsymbol{B}$  为对角占优矩阵,因此是可逆矩阵。

设  $\boldsymbol{u},\boldsymbol{v}\in V_h$ ,定义离散内积和离散范数,即

$$\begin{cases}\langle \boldsymbol{u},\boldsymbol{v}\rangle_J=h\sum_{j=1}^{J-1}u_j\bar{v}_j, & \|\boldsymbol{v}\|_J=\langle \boldsymbol{v},\boldsymbol{v}\rangle_J^{\frac{1}{2}}, & \|\boldsymbol{v}\|_\infty=\max_{0\leqslant j\leqslant J}|v_j|, \\ \|\delta_x\boldsymbol{v}\|_J=(h\sum_{j=0}^J|\delta_x v_j|^2)^{\frac{1}{2}}, & \|\delta_x\boldsymbol{v}\|_J=\langle -\boldsymbol{B}^{-1}\boldsymbol{A}\boldsymbol{v},\boldsymbol{v}\rangle_J^{\frac{1}{2}}.\end{cases}$$

上式中: $\bar{v}$  为  $v$  的共轭复数。

经过简单计算,可得  $\|\delta_x\boldsymbol{v}\|_J=\langle -\boldsymbol{A}\boldsymbol{v},\boldsymbol{v}\rangle_J^{\frac{1}{2}}$ 。

2 几种差分格式

2.1 向前 Euler 格式

令  $\Phi_j^n=\varphi(x_j,t_n),U_j^n=u(x_j,t_n)$ 。在节点  $(x_j,t_n)$  处考虑 KGS 方程(1)~(2),有

$$\mathrm{i}\frac{\partial \varphi}{\partial t}(x_j,t_n)+\frac{1}{2}\frac{\partial^2 \varphi}{\partial x^2}(x_j,t_n)+u(x_j,t_n)\varphi(x_j,t_n)=0, \tag{7}$$

$$\frac{\partial^2 u}{\partial t^2}(x_j,t_n)-\frac{\partial^2 u}{\partial x^2}(x_j,t_n)+u(x_j,t_n)-|\varphi(x_j,t_n)|^2=0. \tag{8}$$

式(7),(8)中: $0\leqslant n\leqslant N-1;1\leqslant j\leqslant J-1$ 。

由向前差分算子及二阶中心差分算子,有

$$\begin{aligned}\frac{\partial^2 \varphi}{\partial x^2}(x_j,t_n)&=\frac{1}{h^2}[\varphi(x_{j-1},t_n)-2\varphi(x_j,t_n)+\varphi(x_{j+1},t_n)]-\frac{h^2}{12}\frac{\partial^4 \varphi}{\partial x^4}(\zeta_{j,n},t_n)=\\&\delta_x^2\Phi_j^n-\frac{h^2}{12}\frac{\partial^4 \varphi}{\partial x^4}(\zeta_{j,n},t_n),\quad x_{j-1}<\zeta_{j,n}<x_{j+1},\end{aligned} \tag{9}$$

$$\begin{aligned}\frac{\partial \varphi}{\partial t}(x_j,t_n)&=\frac{1}{\tau}[\varphi(x_j,t_{n+1})-\varphi(x_j,t_n)]-\frac{\tau}{2}\frac{\partial^2 \varphi}{\partial t^2}(x_j,\eta_{j,n})=\\&\delta_t^+\Phi_j^n-\frac{\tau}{2}\frac{\partial^2 \varphi}{\partial t^2}(x_j,\eta_{j,n}),\quad t_n<\eta_{j,n}<t_{n+1},\end{aligned} \tag{10}$$

$$\begin{aligned}\frac{\partial^2 u}{\partial t^2}(x_j,t_n)&=\frac{1}{\tau^2}[u(x_j,t_{n+1})-2u(x_j,t_n)+u(x_j,t_{n-1})]-\frac{\tau^2}{12}\frac{\partial^4 u}{\partial t^4}(x_j,\Theta_{j,n})=\\&\delta_t^2U_j^n-\frac{\tau^2}{12}\frac{\partial^4 u}{\partial t^4}(x_j,\Theta_{j,n}),\quad t_{n-1}<\Theta_{j,n}<t_{n+1},\end{aligned} \tag{11}$$

$$\frac{\partial^2 u}{\partial x^2}(x_j,t_n)=\frac{1}{h^2}[u(x_{j-1},t_n)-2u(x_j,t_n)+u(x_{j+1},t_n)]-\frac{h^2}{12}\frac{\partial^4 u}{\partial x^4}(\theta_{j,n},t_n)=$$

$$\delta_x^2 U_j^n - \frac{h^2}{12} \frac{\partial^4 u}{\partial x^4}(\theta_{j,n}, t_n), \quad x_{j-1} < \theta_{j,n} < x_{j+1}. \quad (12)$$

将式(9)~(12)代入式(7), (8), 得到

$$i\delta_t^+ \Phi_j^n + \frac{1}{2} \delta_x^2 \Phi_j^n + U_j^n \Phi_j^n = \frac{i\tau}{2} \frac{\partial^2 \varphi}{\partial t^2}(x_j, \eta_{j,n}) + \frac{h^2}{24} \frac{\partial^4 \varphi}{\partial x^4}(\zeta_{j,n}, t_n), \quad 1 \leq j \leq J-1, \quad 0 \leq n \leq N-1, \quad (13)$$

$$\delta_t^2 U_j^n - \delta_x^2 U_j^n + U_j^n - |\Phi_j^n|^2 = \frac{\tau^2}{12} \frac{\partial^4 u}{\partial t^4}(x_j, \Theta_{j,n}) - \frac{h^2}{12} \frac{\partial^4 u}{\partial x^4}(\theta_{j,n}, t_n), \quad 1 \leq j \leq J-1, \quad 1 \leq n \leq N-1. \quad (14)$$

结合式(3), (4), 可得

$$\begin{cases} \Phi_j^0 = \varphi_0(x_j), & U_j^0 = u_0(x_j), & U_j^1 = u_0(x_j) + \tau u_1(x_j), & 0 \leq j \leq J, \\ \Phi_j^n = \Phi_j^n = 0, & U_j^n = U_j^n = 0, & & 1 \leq n \leq N. \end{cases}$$

忽略式(13), (14)的小量项, 则有

$$R_{j,n}^{(1)} = \frac{i\tau}{2} \frac{\partial^2 \varphi}{\partial t^2}(x_j, \eta_{j,n}) + \frac{h^2}{24} \frac{\partial^4 \varphi}{\partial x^4}(\zeta_{j,n}, t_n), \quad R_{j,n}^{(2)} = \frac{\tau^2}{12} \frac{\partial^4 u}{\partial t^4}(x_j, \Theta_{j,n}) - \frac{h^2}{12} \frac{\partial^4 u}{\partial x^4}(\theta_{j,n}, t_n),$$

并用  $\varphi_j^n, u_j^n$  分别代替  $\Phi_j^n, U_j^n$ , 得到差分格式为

$$i\delta_t^+ \varphi_j^n + \frac{1}{2} \delta_x^2 \varphi_j^n + u_j^n \varphi_j^n = 0, \quad 1 \leq j \leq J-1, \quad 0 \leq n \leq N-1, \quad (15)$$

$$\delta_t^2 u_j^n - \delta_x^2 u_j^n + u_j^n - |\varphi_j^n|^2 = 0, \quad 1 \leq j \leq J-1, \quad 1 \leq n \leq N-1, \quad (16)$$

$$\varphi_j^0 = \varphi_0(x_j), \quad u_j^0 = u_0(x_j), \quad u_j^1 = u_0(x_j) + \tau u_1(x_j), \quad 0 \leq j \leq J, \quad (17)$$

$$\varphi_j^n = \varphi_j^n = 0, \quad u_j^n = u_j^n = 0, \quad 1 \leq n \leq N. \quad (18)$$

式(15)~(18)即为 KGS 方程的向前 Euler 格式。称  $R_{j,n}^{(1)}$  和  $R_{j,n}^{(2)}$  为差分格式(15)和差分格式(16)的局部截断误差。记

$$\begin{aligned} c_1 &= \max \left\{ \frac{1}{2} \max_{\substack{a \leq x \leq b \\ 0 \leq t \leq T}} \left| \frac{\partial^2 \varphi}{\partial t^2}(x, t) \right|, \frac{1}{24} \max_{\substack{a \leq x \leq b \\ 0 \leq t \leq T}} \left| \frac{\partial^4 \varphi}{\partial x^4}(x, t) \right| \right\}, \\ c_2 &= \max \left\{ \frac{1}{12} \max_{\substack{a \leq x \leq b \\ 0 \leq t \leq T}} \left| \frac{\partial^4 u}{\partial t^4}(x, t) \right|, \frac{-1}{12} \max_{\substack{a \leq x \leq b \\ 0 \leq t \leq T}} \left| \frac{\partial^4 u}{\partial x^4}(x, t) \right| \right\}, \end{aligned}$$

则可知截断误差  $R_{j,n}^{(1)}, R_{j,n}^{(2)}$  满足

$$\begin{aligned} |R_{j,n}^{(1)}| &\leq c_1(\tau + h^2), \quad 0 \leq n \leq N-1, \quad 1 \leq j \leq J-1, \\ |R_{j,n}^{(2)}| &\leq c_2(\tau^2 + h^2), \quad 1 \leq n \leq N-1, \quad 1 \leq j \leq J-1. \end{aligned}$$

其中:  $c_1, c_2$  是与  $h$  和  $\tau$  无关的常数。

**注 1** 向前 Euler 格式(15)~(18)是一个非线性显性格式, 并且该格式下  $\varphi$  的数值解在时间方向和空间方向上分别具有 1 阶和 2 阶精度,  $u$  的数值解在时间方向和空间方向上都具有 2 阶精度。

## 2.2 Crank-Nicolson 格式

令  $t_{n+1/2} = \frac{1}{2}(t_n + t_{n+1})$ , 在点  $(x_j, t_{n+1/2})$  处考虑方程(1)可得

$$i \frac{\partial \varphi}{\partial t}(x_j, t_{n+1/2}) + \frac{1}{2} \frac{\partial^2 \varphi}{\partial x^2}(x_j, t_{n+1/2}) + u(x_j, t_{n+1/2}) \varphi(x_j, t_{n+1/2}) = 0.$$

其中:  $0 \leq n \leq N-1; 1 \leq j \leq J-1$ 。

应用公式

$$\frac{\partial^2 \varphi}{\partial x^2}(x_j, t_{n+1/2}) = \frac{1}{2} \left( \frac{\partial^2 \varphi}{\partial x^2}(x_j, t_n) + \frac{\partial^2 \varphi}{\partial x^2}(x_j, t_{n+1}) \right) - \frac{\tau^2}{8} \frac{\partial^4 \varphi}{\partial x^2 \partial t^2}(x_j, \xi_{j,n}), \quad t_n < \xi_{j,n} < t_{n+1} \quad (19)$$

可得到

$$\begin{aligned} i \frac{\partial \varphi}{\partial t}(x_j, t_{n+1/2}) + \frac{1}{4} \left( \frac{\partial^2 \varphi}{\partial x^2}(x_j, t_n) + \frac{\partial^2 \varphi}{\partial x^2}(x_j, t_{n+1}) \right) - \frac{\tau^2}{16} \frac{\partial^4 u}{\partial x^2 \partial t^2}(x_j, \xi_{j,n}) + \\ u(x_j, t_{n+1/2}) \varphi(x_j, t_{n+1/2}) = 0, \quad 1 \leq j \leq J-1, \quad 0 \leq n \leq N-1. \end{aligned}$$

再利用式(9)及

$$\frac{\partial \varphi}{\partial t}(x_j, t_{n+1/2}) = \delta_i^+ \Phi_j^n + o(\tau^2), \tag{20}$$

$$u(x_j, t_{n+1/2}) = \frac{1}{2}(u(x_j, t_n) + u(x_j, t_{n+1})) + \bar{c}_1 \tau^2 = U_j^{n+1/2} + \bar{c}_1 \tau^2, \tag{21}$$

$$\varphi(x_j, t_{n+1/2}) = \frac{1}{2}(\varphi(x_j, t_n) + \varphi(x_j, t_{n+1})) + \bar{c}_2 \tau^2 = \Phi_j^{n+1/2} + \bar{c}_2 \tau^2, \tag{22}$$

可以得到

$$\begin{aligned} i\delta_i^+ \Phi_j^n + \frac{1}{2} \delta_x^2 \Phi_j^{n+1/2} + U_j^{n+1/2} \Phi_j^{n+1/2} &= \frac{1}{48} \left( \frac{\partial^4 \varphi}{\partial x^4}(\zeta_{j,n}, t_n) + \frac{\partial^4 \varphi}{\partial x^4}(\zeta_{j,n+1}, t_{n+1}) \right) h^2 + \\ &\quad \left( \frac{i}{24} \frac{\partial^3 \varphi}{\partial t^3}(x_j, \tilde{\eta}_{j,n}) + \frac{1}{16} \frac{\partial^4 u}{\partial x^2 \partial t^2}(x_j, \xi_{j,n}) - \bar{c}_1 \bar{c}_2 \right) \tau^2. \end{aligned} \tag{23}$$

在  $(x_j, t_{n+1/2})$  处考虑方程(2), 即

$$\frac{\partial^2 u}{\partial t^2}(x_j, t_{n+1/2}) - \frac{\partial^2 u}{\partial x^2}(x_j, t_{n+1/2}) + u(x_j, t_{n+1/2}) - |\varphi(x_j, t_{n+1/2})|^2 = 0. \tag{24}$$

式(24)中:  $1 \leq n \leq N-1; 1 \leq j \leq J-1$ .

结合式(11), (12), (21)及

$$\frac{\partial^2 u}{\partial x^2}(x_j, t_{n+1/2}) = \frac{1}{2} \left[ \frac{\partial^2 u}{\partial x^2}(x_j, t_n) + \frac{\partial^2 u}{\partial x^2}(x_j, t_{n+1}) \right] - \frac{\tau^2}{8} \frac{\partial^4 u}{\partial x^2 \partial t^2}(x_j, \tilde{\theta}_{j,n}), \quad t_n < \tilde{\theta}_{j,n} < t_{n+1}, \tag{25}$$

$$\frac{\partial^2 u}{\partial t^2}(x_j, t_{n+1/2}) = \frac{1}{2} \left[ \frac{\partial^2 u}{\partial t^2}(x_j, t_n) + \frac{\partial^2 u}{\partial t^2}(x_j, t_{n+1}) \right] - \frac{\tau^2}{8} \frac{\partial^4 u}{\partial t^4}(x_j, \tilde{\Theta}_{j,n}), \quad t_n < \tilde{\Theta}_{j,n} < t_{n+1}, \tag{26}$$

$$|\varphi(x_j, t_{n+1/2})|^2 = \frac{1}{2} (|\varphi(x_j, t_n)|^2 + |\varphi(x_j, t_{n+1})|^2) + \bar{c}_3 \tau^2, \tag{27}$$

可将式(24)改写为

$$\begin{aligned} \delta_i^2 U_j^{n+1/2} - \delta_x^2 U_j^{n+1/2} + U_j^{n+1/2} - \frac{1}{2} (|\Phi_j^n|^2 + |\Phi_j^{n+1}|^2) &= \\ &\quad \left( \frac{1}{8} \left( \frac{\partial^4 u}{\partial t^4}(x_j, \tilde{\Theta}_{j,n}) - \frac{\partial^4 u}{\partial x^2 \partial t^2}(x_j, \tilde{\theta}_{j,n}) \right) + \frac{1}{24} \left( \frac{\partial^4 u}{\partial t^4}(x_j, \Theta_{j,n}) + \frac{\partial^4 u}{\partial t^4}(x_j, \Theta_{j,n+1}) \right) + \bar{c}_3 - \bar{c}_1 \right) \tau^2 - \\ &\quad \frac{1}{24} \left( \frac{\partial^2 u}{\partial x^2}(\theta_{j,n}, t_n) + \frac{\partial^2 u}{\partial x^2}(\theta_{j,n+1}, t_n) \right) h^2, \quad 1 \leq n \leq N-1, \quad 1 \leq j \leq J-1. \end{aligned} \tag{28}$$

略去式(23)和式(28)的小量项, 则有

$$\begin{aligned} R_{j,n}^{(3)} &= \frac{1}{48} \left( \frac{\partial^4 \varphi}{\partial x^4}(\zeta_{j,n}, t_n) + \frac{\partial^4 \varphi}{\partial x^4}(\zeta_{j,n+1}, t_{n+1}) \right) h^2 + \left( \frac{i}{24} \frac{\partial^3 \varphi}{\partial t^3}(x_j, \tilde{\eta}_{j,n}) + \frac{1}{16} \frac{\partial^4 u}{\partial x^2 \partial t^2}(x_j, \xi_{j,n}) - \bar{c}_1 \bar{c}_2 \right) \tau^2, \\ R_{j,n}^{(4)} &= -\frac{1}{24} \left( \frac{\partial^2 u}{\partial x^2}(\theta_{j,n}, t_n) + \frac{\partial^2 u}{\partial x^2}(\theta_{j,n+1}, t_n) \right) h^2 + \\ &\quad \left( \frac{1}{8} \left( \frac{\partial^4 u}{\partial t^4}(x_j, \tilde{\Theta}_{j,n}) - \frac{\partial^4 u}{\partial x^2 \partial t^2}(x_j, \tilde{\theta}_{j,n}) \right) + \frac{1}{24} \left( \frac{\partial^4 u}{\partial t^4}(x_j, \Theta_{j,n}) + \frac{\partial^4 u}{\partial t^4}(x_j, \Theta_{j,n+1}) \right) + \bar{c}_3 - \bar{c}_1 \right) \tau^2. \end{aligned}$$

结合初值条件(3)和边值条件(4), 并用  $\varphi_j^n, u_j^n$  分别代替  $\Phi_j^n, U_j^n$ , 得到 Crank-Nicolson 差分格式为

$$i\delta_i^+ \varphi_j^n + \frac{1}{2} \delta_x^2 \varphi_j^{n+1/2} + u_j^{n+1/2} \varphi_j^{n+1/2} = 0, \quad 1 \leq j \leq J-1, \quad 0 \leq n \leq N-1, \tag{29}$$

$$\delta_i^2 u_j^{n+1/2} - \delta_x^2 u_j^{n+1/2} + u_j^{n+1/2} - \frac{1}{2} (|\varphi_j^n|^2 + |\varphi_j^{n+1}|^2) = 0, \quad 1 \leq j \leq J-1, \quad 1 \leq n \leq N-1, \tag{30}$$

$$\varphi_j^0 = \varphi_0(x_j), \quad u_j^0 = u_0(x_j), \quad u_j^1 = u_0(x_j) + \tau u_1(x_j), \quad 0 \leq j \leq J, \tag{31}$$

$$\varphi_j^n = \varphi_j^n = 0, \quad u_j^n = u_j^n = 0, \quad 1 \leq n \leq N. \tag{32}$$

式(29)~(32)即为 KGS 方程的 Crank-Nicolson 格式。称  $R_{j,n}^{(3)}$  和  $R_{j,n}^{(4)}$  为差分格式(23)和差分格式(28)的局部截断误差。记

$$\begin{aligned} c_3 &= \max \left\{ \frac{i}{24} \max_{0 \leq t \leq T} \left| \frac{\partial^3 \varphi}{\partial t^3}(x, t) \right|, \frac{1}{16} \max_{0 \leq t \leq T} \left| \frac{\partial^4 u}{\partial x^2 \partial t^2}(x, t) \right|, \frac{1}{48} \max_{0 \leq t \leq T} \left| \frac{\partial^4 \varphi}{\partial t^4}(x, t) \right|, |\bar{c}_1|, |\bar{c}_3| \right\}, \\ c_4 &= \max_{0 \leq t \leq T} \left\{ \frac{-1}{24} \max_{a \leq x \leq b} \left| \frac{\partial^2 u}{\partial x^2}(x, t) \right|, \frac{1}{8} \left| \frac{\partial^4 u}{\partial t^4}(x, t) \right|, \frac{-1}{8} \left| \frac{\partial^4 u}{\partial x^2 \partial t^2}(x, t) \right|, \bar{c}_3, -\bar{c}_1 \right\}, \end{aligned}$$

则可知截断误差  $R_{j,n}^{(3)}, R_{j,n}^{(4)}$  满足

$$\begin{aligned} |R_{j,n}^{(3)}| &\leq c_3(\tau^2 + h^2), & 0 \leq n \leq N-1, & \quad 1 \leq j \leq J-1, \\ |R_{j,n}^{(4)}| &\leq c_4(\tau^2 + h^2), & 1 \leq n \leq N-1, & \quad 1 \leq j \leq J-1. \end{aligned}$$

其中:  $c_3, c_4$  是与  $h$  和  $\tau$  无关的常数。

**注 2** 与向前 Euler 格式不同, Crank-Nicolson 格式(29)~(32)是一个非线性隐性格式, 并且该格式下  $\varphi$  和  $u$  的数值解在时间方向和空间方向上都具有 2 阶精度。

### 2.3 紧差分格式

在点  $(x_j, t_{n+1/2})$  处考虑方程(1), 有

$$i \frac{\partial \varphi}{\partial t}(x_j, t_{n+1/2}) + \frac{1}{2} \frac{\partial^2 \varphi}{\partial x^2}(x_j, t_{n+1/2}) + u(x_j, t_{n+1/2}) \varphi(x_j, t_{n+1/2}) = 0.$$

其中:  $0 \leq n \leq N-1; 1 \leq j \leq J-1$ 。

结合式(19)~(22), 有

$$i \delta_i^+ \Phi_j^n + \frac{1}{2} \frac{\partial^2 \varphi}{\partial x^2}(x_j, t_{n+1/2}) + U_j^{n+1/2} \Phi_j^{n+1/2} = \left( \frac{i}{24} \frac{\partial^3 \varphi}{\partial x^3}(x_j, \tilde{\eta}_{j,n}) + \frac{1}{16} \frac{\partial^4 u}{\partial x^2 \partial t^2}(x_j, \xi_{j,n}) - \bar{c}_1 \bar{c}_2 \right) \tau^2. \quad (33)$$

式(33)中:  $0 \leq n \leq N-1; 1 \leq j \leq J-1$ 。

式(33)两边同时左乘紧差分算子  $A_h$ , 可以得到

$$\begin{aligned} i A_h \delta_i^+ \Phi_j^n + \frac{1}{2} A_h \frac{\partial^2 \varphi}{\partial x^2}(x_j, t_{n+1/2}) + A_h (U_j^{n+1/2} \Phi_j^{n+1/2}) = \\ A_h \left( \frac{i}{24} \frac{\partial^3 \varphi}{\partial x^3}(x_j, \tilde{\eta}_{j,n}) + \frac{1}{16} \frac{\partial^4 u}{\partial x^2 \partial t^2}(x_j, \xi_{j,n}) - \bar{c}_1 \bar{c}_2 \right) \tau^2. \end{aligned} \quad (34)$$

由于有

$$A_h \frac{\partial^2 \varphi}{\partial x^2}(x_j, t_n) = \delta_x^2 \Phi_j^n + \frac{h^4}{240} \frac{\partial^6 \varphi}{\partial x^6}(\zeta_{j,n}, t_n), \quad \zeta_{j,n} \in (x_{j-1}, x_{j+1}),$$

所以有

$$\frac{1}{2} A_h \frac{\partial^2 \varphi}{\partial x^2}(x_j, t_{n+1/2}) = \frac{1}{2} \delta_x^2 \Phi_j^{n+1/2} + \frac{h^4}{240} \frac{\partial^6 \varphi}{\partial x^6}(\tilde{\zeta}_{j,n}, \tilde{t}_{j,n}). \quad (35)$$

式(35)中:  $x_{j-1} < \tilde{\zeta}_{j,n} < x_{j+1}; t_{n-1} < \tilde{t}_{j,n} < t_{n+1}$ 。

将式(35)代入式(34), 有

$$\begin{aligned} i A_h \delta_t^+ \Phi_j^n + \frac{1}{2} \delta_x^2 \Phi_j^{n+1/2} + A_h (U_j^{n+1/2} \Phi_j^{n+1/2}) = \\ - \frac{1}{480} \left( \frac{\partial^6 \varphi}{\partial x^6}(\tilde{\zeta}_{j,n}, \tilde{t}_{j,n}) \right) h^4 + A_h \left( \frac{i}{24} \frac{\partial^3 \varphi}{\partial x^3}(x_j, \tilde{\eta}_{j,n}) + \frac{1}{16} \frac{\partial^4 u}{\partial x^2 \partial t^2}(x_j, \xi_{j,n}) - \bar{c}_1 \bar{c}_2 \right) \tau^2. \end{aligned} \quad (36)$$

在点  $(x_j, t_{n+1/2})$  处考虑方程(2), 有

$$\frac{\partial^2 u}{\partial t^2}(x_j, t_{n+1/2}) - \frac{\partial^2 u}{\partial x^2}(x_j, t_{n+1/2}) + u(x_j, t_{n+1/2}) - |\varphi(x_j, t_{n+1/2})|^2 = 0. \quad (37)$$

式(37)中:  $1 \leq n \leq N-1; 1 \leq j \leq J-1$ 。

将式(25)~(27)代入式(37), 可以得到

$$\begin{aligned} \frac{1}{2} \left( \frac{\partial^2 u}{\partial t^2}(x_j, t_{n+1}) + \frac{\partial^2 u}{\partial t^2}(x_j, t_n) \right) + \frac{1}{2} \left( \frac{\partial^2 u}{\partial x^2}(x_j, t_{n+1}) + \frac{\partial^2 u}{\partial x^2}(x_j, t_n) \right) + U_j^{n+1/2} - \\ \frac{1}{2} (|\Phi_j^n|^2 + |\Phi_j^{n+1}|^2) = \left( \frac{1}{8} \frac{\partial^4 u}{\partial x^2 \partial t^2}(x_j, \tilde{\theta}_{j,n}) + \frac{1}{8} \frac{\partial^4 u}{\partial t^4}(x_j, \tilde{\Theta}_{j,n}) + \bar{c}_3 - \bar{c}_1 \right) \tau^2. \end{aligned} \quad (38)$$

将式(38)两边同时左乘紧差分算子  $A_h$ , 并利用式(11)及

$$A_h \frac{\partial^2 u}{\partial x^2}(x_j, t_n) = \delta_x^2 U_j^n + \frac{h^4}{240} \frac{\partial^6 u}{\partial x^6}(\gamma_{j,n}, t_n), \quad \gamma_{j,n} \in (x_{j-1}, x_{j+1}),$$

可得

$$A_h \delta_t^2 U_j^{n+1/2} - \delta_x^2 U_j^{n+1/2} + A_h U_j^{n+1/2} - \frac{1}{2} A_h (|\Phi_j^n|^2 + |\Phi_j^{n+1}|^2) =$$

$$\begin{aligned} & \frac{1}{480} \left( \frac{\partial^6 u}{\partial x^6}(\gamma_{j,n}, t_n) + \frac{\partial^6 u}{\partial x^6}(\gamma_{j,n+1}, t_{n+1}) \right) h^4 + \\ & A_h \left( \frac{1}{8} \frac{\partial^4 u}{\partial x^2 \partial t^2}(x_j, \tilde{\theta}_{j,n}) + \frac{1}{8} \frac{\partial^4 u}{\partial t^4}(x_j, \tilde{\Theta}_{j,n}) + \bar{c}_3 - \bar{c}_1 + \right. \\ & \left. \frac{1}{24} \frac{\partial^4 u}{\partial t^4}(x_j, \Theta_{j,n}) + \frac{1}{24} \frac{\partial^4 u}{\partial t^4}(x_j, \Theta_{j,n}) \right) \tau^2. \end{aligned} \tag{39}$$

略去式(36)和式(39)中的小量项,则有

$$R_{j,n}^{(5)} = A_h \left( \frac{1}{24} \frac{\partial^3 \varphi}{\partial x^3}(x_j, \tilde{\eta}_{j,n}) + \frac{1}{16} \frac{\partial^4 u}{\partial x^2 \partial t^2}(x_j, \xi_{j,n}) - \bar{c}_1 \bar{c}_2 \right) \tau^2 - \frac{1}{480} \left( \frac{\partial^6 \varphi}{\partial x^6}(\tilde{\zeta}_{j,n}, \tilde{t}_{j,n}) \right) h^4,$$

$$\begin{aligned} R_{j,n}^{(6)} &= \frac{1}{480} \left( \frac{\partial^6 u}{\partial x^6}(\gamma_{j,n}, t_n) + \frac{\partial^6 u}{\partial x^6}(\gamma_{j,n+1}, t_{n+1}) \right) h^4 + \\ & A_h \left( \frac{1}{8} \frac{\partial^4 u}{\partial x^2 \partial t^2}(x_j, \tilde{\theta}_{j,n}) + \frac{1}{8} \frac{\partial^4 u}{\partial t^4}(x_j, \tilde{\Theta}_{j,n}) + \bar{c}_3 - \bar{c}_1 + \frac{1}{24} \frac{\partial^4 u}{\partial t^4}(x_j, \Theta_{j,n}) + \frac{1}{24} \frac{\partial^4 u}{\partial t^4}(x_j, \Theta_{j,n}) \right) \tau^2, \end{aligned}$$

结合初值条件(3)和边值条件(4),并且用  $\varphi_j^n, u_j^n$  分别代替  $\Phi_j^n, U_j^n$ ,得到 KGS 方程的紧差分格式为

$$iA_h \delta_t^+ \varphi_j^n + \frac{1}{2} \delta_x^2 \varphi_j^{n+1/2} + A_h (u_j^{n+1/2} \varphi_j^{n+1/2}) = 0, \quad 0 \leq n \leq N-1, \quad 1 \leq j \leq J-1, \tag{40}$$

$$\begin{aligned} & A_h \delta_t^2 u_j^{n+1/2} - \delta_x^2 u_j^{n+1/2} + A_h u_j^{n+1/2} - \frac{1}{2} A_h (|\varphi_j^n|^2 + |\varphi_j^{n+1}|^2) = 0, \\ & 1 \leq n \leq N-1, \quad 1 \leq j \leq J-1, \end{aligned} \tag{41}$$

$$\varphi_j^0 = \varphi_0(x_j), \quad u_j^0 = u_0(x_j), \quad u_j^1 = u_0(x_j) + \tau u_1(x_j), \quad 0 \leq j \leq J, \tag{42}$$

$$\varphi_0^n = \varphi_j^n = 0, \quad u_0^n = u_j^n = 0, \quad 1 \leq n \leq N. \tag{43}$$

式(40)~(43)即为 KGS 方程的紧差分格式。称  $R_{j,n}^{(5)}$  和  $R_{j,n}^{(6)}$  为差分格式(36)和差分格式(39)的局部截断误差。记

$$\begin{aligned} c_5 &= \max \left\{ \frac{1}{8} \max_{\substack{a \leq x \leq b \\ 0 \leq t \leq T}} \left| \frac{\partial^4 u}{\partial t^4}(x, t) \right|, \frac{1}{8} \max_{\substack{a \leq x \leq b \\ 0 \leq t \leq T}} \left| A_h \frac{\partial^4 u}{\partial x^2 \partial t^2}(x, t) \right|, \frac{1}{480} \max_{\substack{a \leq x \leq b \\ 0 \leq t \leq T}} \left| \frac{\partial^6 u}{\partial x^6}(x, t) \right|, -\bar{c}_1, \bar{c}_3 \right\}, \\ c_6 &= \max_{\substack{a \leq x \leq b \\ 0 \leq t \leq T}} \left\{ \frac{1}{480} \max_{\substack{a \leq x \leq b \\ 0 \leq t \leq T}} \left| \frac{\partial^6 u}{\partial t^6}(x, t) \right|, \frac{1}{8} \max_{\substack{a \leq x \leq b \\ 0 \leq t \leq T}} \left| A_h \frac{\partial^4 u}{\partial x^2 \partial t^2}(x, t) \right|, \frac{1}{8} \max_{\substack{a \leq x \leq b \\ 0 \leq t \leq T}} \left| A_h \frac{\partial^4 u}{\partial x^4}(x, t) \right|, -\bar{c}_1, \bar{c}_3 \right\}, \end{aligned}$$

则可知截断误差  $R_{j,n}^{(5)}, R_{j,n}^{(6)}$  分别满足

$$\begin{aligned} |R_{j,n}^{(5)}| &\leq c_5 (\tau^2 + h^4), \quad 0 \leq n \leq N-1, \quad 1 \leq j \leq J-1, \\ |R_{j,n}^{(6)}| &\leq c_6 (\tau^2 + h^4), \quad 1 \leq n \leq N-1, \quad 1 \leq j \leq J-1. \end{aligned}$$

其中:  $c_5, c_6$  是与  $h$  和  $\tau$  无关的常数。

**注 3** 紧差分格式(40)~(43)也是一个非线性隐性格式,并且该格式下的  $\varphi$  和  $u$  的数值解在时间方向和空间方向上分别具有 2 阶和 4 阶精度。

3 守恒性

**引理 1**<sup>[18]</sup> 对于任意的  $u, v \in V_h^0$ , 有  $\langle \delta_x^2 u, v \rangle = -\langle \delta_x^+ u, \delta_x^+ v \rangle$ 。

**引理 2**<sup>[18]</sup> 对于任意的  $u \in V_h, n=0, 1, \dots, N-1$ , 则有

$$\begin{aligned} \operatorname{Re} \langle -B^{-1} A(u^{n+1} + u^n), (u^{n+1} - u^n) \rangle &= \| \delta_x u^{n+1} \|^2 - \| \delta_x u^n \|^2, \\ \operatorname{Im} \langle B^{-1} A(u^{n+1} + u^n), (u^{n+1} - u^n) \rangle &= 0. \end{aligned}$$

其中:  $\operatorname{Re}$  和  $\operatorname{Im}$  分别表示取函数的实部和虚部。

**定理 1** Crank-Nicolson 格式(29)~(32)能够精确地保持离散的电荷和能量守恒,即

$$Q^n = \| \varphi^n \|^2 \equiv Q^0, \quad n=1, 2, \dots, N, \tag{44}$$

$$E^n = \| u^n \|^2 + \| \delta_t^+ u^n \|^2 + \| \delta_x^+ u^n \|^2 + \| \delta_x^+ \varphi^n \|^2 - 2 \langle u^n, |\varphi^n|^2 \rangle = E^0, \quad n=1, 2, \dots, N-1. \tag{45}$$

证明: 式(29), (30)可以表示为

$$i \delta_t^+ \varphi^n + \frac{1}{2} \delta_x^2 \varphi^{n+1/2} + u^{n+1/2} \varphi^{n+1/2} = 0, \tag{46}$$

$$\delta_t^2 u^{n+1/2} - \delta_x^2 u^{n+1/2} + u^{n+1/2} - \frac{1}{2}(|\varphi^n|^2 + |\varphi^{n+1}|^2) = 0. \quad (47)$$

将式(46)与  $\varphi^{n+1/2}$  作内积, 并取虚部, 有

$$\operatorname{Im}\left(\langle \mathrm{id}_t^+ \varphi^n, \varphi^{n+1/2} \rangle + \frac{1}{2} \langle \delta_x^2 \varphi^{n+1/2}, \varphi^{n+1/2} \rangle + \langle u^{n+1/2} \varphi^{n+1/2}, \varphi^{n+1/2} \rangle\right) = 0.$$

由引理 1 可知

$$\langle \delta_x^2 \varphi^{n+1/2}, \varphi^{n+1/2} \rangle = -\langle \delta_x^+ \varphi^{n+1/2}, \delta_x^+ \varphi^{n+1/2} \rangle = -\|\delta_x^+ \varphi^{n+1/2}\|^2 \in \mathbf{R}.$$

又

$$\langle u^{n+1/2} \varphi^{n+1/2}, \varphi^{n+1/2} \rangle = \sum_{n=0}^{N-1} u_j^{n+1/2} |\varphi_j^{n+1/2}|^2 \in \mathbf{R},$$

因此, 有

$$\operatorname{Im}\langle \mathrm{id}_t^+ \varphi^n, \varphi^{n+1/2} \rangle = \frac{1}{2\tau} (\|\varphi^{n+1}\|^2 - \|\varphi^n\|^2) = 0.$$

故有

$$\|\varphi^{n+1}\|^2 = \|\varphi^n\|^2. \quad (48)$$

因此, 式(44)成立。

将式(46)与  $\varphi^{n+1} - \varphi^n$  做内积, 并取实部, 有

$$\operatorname{Re}\left(\langle \mathrm{id}_t^+ \varphi^n, \varphi^{n+1} - \varphi^n \rangle + \frac{1}{2} \langle \delta_x^2 \varphi^{n+1/2}, \varphi^{n+1} - \varphi^n \rangle + \langle u^{n+1/2} \varphi^{n+1/2}, \varphi^{n+1} - \varphi^n \rangle\right) = 0.$$

对上式进行逐项分析, 即

$$\begin{aligned} \operatorname{Re}\langle \mathrm{id}_t^+ \varphi^n, \varphi^{n+1} - \varphi^n \rangle &= 0, \\ \operatorname{Re}\left(\frac{1}{2} \langle \delta_x^2 \varphi^{n+1/2}, \varphi^{n+1} - \varphi^n \rangle\right) &= \operatorname{Re}\left(\frac{1}{4} \langle \delta_x^2 \varphi^{n+1}, \varphi^{n+1} - \varphi^n \rangle + \frac{1}{4} \langle \delta_x^2 \varphi^n, \varphi^{n+1} - \varphi^n \rangle\right) = \\ &= \operatorname{Re}\left(-\frac{1}{4} \langle \delta_x^+ \varphi^{n+1}, \delta_x^+ \varphi^{n+1} \rangle + \frac{1}{4} \langle \delta_x^+ \varphi^n, \delta_x^+ \varphi^n \rangle\right) = \\ &= -\frac{1}{4} \|\delta_x^+ \varphi^{n+1}\|^2 + \frac{1}{4} \|\delta_x^+ \varphi^n\|^2, \\ \operatorname{Re}\langle u^{n+1/2} \varphi^{n+1/2}, \varphi^{n+1} - \varphi^n \rangle &= \frac{1}{4} \langle u^{n+1} + u^n, |\varphi^{n+1}|^2 \rangle - \frac{1}{4} \langle u^{n+1} + u^n, |\varphi^n|^2 \rangle. \end{aligned}$$

整理可以得到

$$-\|\delta_x^+ \varphi^{n+1}\|^2 + \|\delta_x^+ \varphi^n\|^2 + \langle u^{n+1} + u^n, |\varphi^{n+1}|^2 \rangle - \langle u^{n+1} + u^n, |\varphi^n|^2 \rangle = 0. \quad (49)$$

将式(47)与  $u^{n+1} - u^n$  做内积, 有

$$\langle \delta_t^2 u^{n+1/2}, u^{n+1} - u^n \rangle - \langle \delta_x^2 u^{n+1/2}, u^{n+1} - u^n \rangle + \langle u^{n+1/2}, u^{n+1} - u^n \rangle - \frac{1}{2} \langle |\varphi^n|^2 + |\varphi^{n+1}|^2, u^{n+1} - u^n \rangle = 0.$$

对上式进行逐项分析, 可得到

$$\begin{aligned} \langle \delta_t^2 u^{n+1/2}, u^{n+1} - u^n \rangle &= \frac{1}{2} \|\delta_t^+ u^{n+1}\|^2 - \frac{1}{2} \|\delta_t^+ u^n\|^2, \\ -\langle \delta_x^2 u^{n+1/2}, u^{n+1} - u^n \rangle &= \frac{1}{2} \|\delta_x^+ u^{n+1}\|^2 - \frac{1}{2} \|\delta_x^+ u^n\|^2, \\ \frac{1}{2} \langle u^{n+1} + u^n, u^{n+1} - u^n \rangle &= \frac{1}{2} \|u^{n+1}\|^2 - \frac{1}{2} \|u^n\|^2. \end{aligned}$$

整理得到

$$\begin{aligned} \|\delta_t^+ u^{n+1}\|^2 - \|\delta_t^+ u^n\|^2 + \|\delta_x^+ u^{n+1}\|^2 - \|\delta_x^+ u^n\|^2 + \|u^{n+1}\|^2 - \\ \|u^n\|^2 - \langle |\varphi^n|^2 + |\varphi^{n+1}|^2, u^{n+1} - u^n \rangle = 0. \end{aligned} \quad (50)$$

用式(50)减去式(49)得到

$$\begin{aligned} \|u^{n+1}\|^2 + \|\delta_t^+ u^{n+1}\|^2 + \|\delta_x^+ u^{n+1}\|^2 + \|\delta_x^+ \varphi^{n+1}\|^2 - 2\langle u^{n+1}, |\varphi^{n+1}|^2 \rangle = \\ \|u^n\|^2 + \|\delta_t^+ u^n\|^2 + \|\delta_x^+ u^n\|^2 + \|\delta_x^+ \varphi^n\|^2 - 2\langle u^n, |\varphi^n|^2 \rangle, \end{aligned}$$

因此, 式(45)成立。



**定理 2** 紧差分格式(40)~(43)能够精确保持离散电荷和能量守恒,即

$$Q^n = \|\boldsymbol{\varphi}^n\|^2 \equiv Q^n, \quad n=0,1,\cdots,N, \quad (51)$$

$$E^n = \|\boldsymbol{u}^n\|^2 + \|\delta_t^+ \boldsymbol{u}^n\|^2 + \|\delta_x \boldsymbol{u}^n\|^2 + \|\delta_x \boldsymbol{\varphi}^n\|^2 - 2\langle \boldsymbol{u}^n, |\boldsymbol{\varphi}^n|^2 \rangle \equiv E^n, \quad n=0,1,\cdots,N-1. \quad (52)$$

证明:利用前面定义的矩阵  $\mathbf{A}$  和  $\mathbf{B}$ , 式(40), (41)可以表示为

$$i\delta_t^+ \boldsymbol{\varphi}^n + \frac{1}{2} \mathbf{B}^{-1} \mathbf{A} \boldsymbol{\varphi}^{n+1/2} + \boldsymbol{u}^{n+1/2} \boldsymbol{\varphi}^{n+1/2} = 0, \quad (53)$$

$$\delta_t^2 \boldsymbol{u}^{n+1/2} - \mathbf{B}^{-1} \mathbf{A} \boldsymbol{u}^{n+1/2} + \boldsymbol{u}^{n+1/2} - \frac{1}{2} (|\boldsymbol{\varphi}^n|^2 + |\boldsymbol{\varphi}^{n+1}|^2) = 0. \quad (54)$$

将式(53)与  $\boldsymbol{\varphi}^{n+1/2}$  作内积, 并取虚部, 则有

$$\text{Im}\langle i\delta_t^+ \boldsymbol{\varphi}^n, \boldsymbol{\varphi}^{n+1/2} \rangle + \frac{1}{2} \text{Im}\langle \mathbf{B}^{-1} \mathbf{A} \boldsymbol{\varphi}^{n+1/2}, \boldsymbol{\varphi}^{n+1/2} \rangle + \text{Im}\langle \boldsymbol{u}^{n+1/2} \boldsymbol{\varphi}^{n+1/2}, \boldsymbol{\varphi}^{n+1/2} \rangle = 0. \quad (55)$$

对上式进行逐项分析, 有

$$\text{Im}\langle i\delta_t^+ \boldsymbol{\varphi}^n, \boldsymbol{\varphi}^{n+1/2} \rangle = \frac{1}{2\tau} (\|\boldsymbol{\varphi}^{n+1}\|^2 - \|\boldsymbol{\varphi}^n\|^2),$$

$$\frac{1}{2} \text{Im}\langle \mathbf{B}^{-1} \mathbf{A} \boldsymbol{\varphi}^{n+1/2}, \boldsymbol{\varphi}^{n+1/2} \rangle = 0.$$

又  $\langle \boldsymbol{u}^{n+1/2} \boldsymbol{\varphi}^{n+1/2}, \boldsymbol{\varphi}^{n+1/2} \rangle \in \mathbf{R}$ , 所以有

$$\frac{1}{2\tau} (\|\boldsymbol{\varphi}^{n+1}\|^2 - \|\boldsymbol{\varphi}^n\|^2) = 0.$$

由此可知, 式(51)成立。

将式(53)与  $\delta_t^+ \boldsymbol{\varphi}^n$  作内积, 并取实部, 有

$$\text{Re}\langle i\delta_t^+ \boldsymbol{\varphi}^n, \delta_t^+ \boldsymbol{\varphi}^n \rangle + \frac{1}{2} \text{Re}\langle \mathbf{B}^{-1} \mathbf{A} \boldsymbol{\varphi}^{n+1/2}, \delta_t^+ \boldsymbol{\varphi}^n \rangle + \text{Re}\langle \boldsymbol{u}^{n+1/2} \boldsymbol{\varphi}^{n+1/2}, \delta_t^+ \boldsymbol{\varphi}^n \rangle = 0. \quad (56)$$

逐项分析, 有

$$\text{Re}\langle i\delta_t^+ \boldsymbol{\varphi}^n, \delta_t^+ \boldsymbol{\varphi}^n \rangle = 0,$$

$$\frac{1}{2\tau} \text{Re}\langle \mathbf{B}^{-1} \mathbf{A} \boldsymbol{\varphi}^{n+1/2}, \boldsymbol{\varphi}^{n+1} - \boldsymbol{\varphi}^n \rangle = -\frac{1}{4\tau} (\|\delta_x \boldsymbol{\varphi}^{n+1}\|^2 - \|\delta_x \boldsymbol{\varphi}^n\|^2),$$

$$\begin{aligned} \text{Re}\langle \boldsymbol{u}^{n+1/2} \boldsymbol{\varphi}^{n+1/2}, \delta_t^+ \boldsymbol{\varphi}^n \rangle &= \frac{1}{4\tau} \langle (\boldsymbol{u}^{n+1} + \boldsymbol{u}^n) \boldsymbol{\varphi}^{n+1}, \boldsymbol{\varphi}^{n+1} \rangle - \frac{1}{4\tau} \langle (\boldsymbol{u}^{n+1} + \boldsymbol{u}^n) \boldsymbol{\varphi}^n, \boldsymbol{\varphi}^n \rangle = \\ &= \frac{1}{4\tau} \langle \boldsymbol{u}^{n+1} + \boldsymbol{u}^n, |\boldsymbol{\varphi}^{n+1}|^2 \rangle - \frac{1}{4\tau} \langle \boldsymbol{u}^{n+1} + \boldsymbol{u}^n, |\boldsymbol{\varphi}^n|^2 \rangle. \end{aligned}$$

则式(56)可表示为

$$\|\delta_x \boldsymbol{\varphi}^{n+1}\|^2 - \|\delta_x \boldsymbol{\varphi}^n\|^2 - \langle \boldsymbol{u}^{n+1} + \boldsymbol{u}^n, |\boldsymbol{\varphi}^{n+1}|^2 \rangle + \langle \boldsymbol{u}^{n+1} + \boldsymbol{u}^n, |\boldsymbol{\varphi}^n|^2 \rangle = 0. \quad (57)$$

将式(54)与  $\delta_t^+ \boldsymbol{u}^n$  作内积, 并取实部, 有

$$\langle \delta_t^2 \boldsymbol{u}^{n+1/2}, \delta_t^+ \boldsymbol{u}^n \rangle - \langle \mathbf{B}^{-1} \mathbf{A} \boldsymbol{u}^{n+1/2}, \delta_t^+ \boldsymbol{u}^n \rangle + \langle \boldsymbol{u}^{n+1/2}, \delta_t^+ \boldsymbol{u}^n \rangle - \frac{1}{2} \langle |\boldsymbol{\varphi}^n|^2 + |\boldsymbol{\varphi}^{n+1}|^2, \delta_t^+ \boldsymbol{u}^n \rangle = 0. \quad (58)$$

分析式(58)的每一项, 可得

$$\begin{aligned} \langle \delta_t^2 \boldsymbol{u}^{n+1/2}, \delta_t^+ \boldsymbol{u}^n \rangle &= \frac{1}{2\tau} \|\delta_t^+ \boldsymbol{u}^{n+1}\|^2 - \frac{1}{2\tau} \|\delta_t^+ \boldsymbol{u}^n\|^2, \\ -\langle \mathbf{B}^{-1} \mathbf{A} \boldsymbol{u}^{n+1/2}, \delta_t^+ \boldsymbol{u}^n \rangle &= \frac{1}{2\tau} (\|\delta_x \boldsymbol{u}^{n+1}\|^2 - \|\delta_x \boldsymbol{u}^n\|^2), \\ \langle \boldsymbol{u}^{n+1/2}, \delta_t^+ \boldsymbol{u}^n \rangle &= \frac{1}{2\tau} \|\boldsymbol{u}^{n+1}\|^2 - \frac{1}{2\tau} \|\boldsymbol{u}^n\|^2. \end{aligned}$$

则式(58)可以写成

$$\begin{aligned} \|\delta_t^+ \boldsymbol{u}^{n+1}\|^2 - \|\delta_t^+ \boldsymbol{u}^n\|^2 + \|\delta_x \boldsymbol{u}^{n+1}\|^2 - \|\delta_x \boldsymbol{u}^n\|^2 + \|\boldsymbol{u}^{n+1}\|^2 - \|\boldsymbol{u}^n\|^2 - \\ \langle |\boldsymbol{\varphi}^n|^2 + |\boldsymbol{\varphi}^{n+1}|^2, \boldsymbol{u}^{n+1} - \boldsymbol{u}^n \rangle = 0. \end{aligned} \quad (59)$$

结合式(57)与式(59), 有

$$\|\boldsymbol{u}^{n+1}\|^2 + \|\delta_t^+ \boldsymbol{u}^{n+1}\|^2 + \|\delta_x \boldsymbol{u}^{n+1}\|^2 + \|\delta_x \boldsymbol{\varphi}^{n+1}\|^2 - 2\langle \boldsymbol{u}^{n+1}, |\boldsymbol{\varphi}^{n+1}|^2 \rangle =$$

$$\|u^n\|^2 + \|\delta_t^+ u^n\|^2 + \|\delta_x u^n\|^2 + \|\delta_x \phi^n\|^2 - 2\langle u^n, |\phi^n|^2 \rangle.$$

由此可知,式(52)成立。

4 数值实验

通过数值实验验证前面的理论结果。根据文献[19]可以得到 KGS 方程的解析解,即

$$\varphi(x,t,v,x_0)=\frac{3\sqrt{2}}{4\sqrt{1-v^2}}\operatorname{sech}^2\left(\frac{1}{2\sqrt{1-v^2}}(x-vt-x_0)\right)\exp\left(i\left(vx+\frac{1-v^2+v^4}{2(1-v^2)}t\right)\right), \tag{60}$$

$$u(x,t,v,x_0)=\frac{3}{4(1-v^2)}\operatorname{sech}^2\left(\frac{1}{2\sqrt{1-v^2}}(x-vt-x_0)\right). \tag{61}$$

式(60),(61)中: $v$  为孤立波的传播速度; $x_0$  为初始相位。

对于固定的  $t$ ,当  $\|x\|\rightarrow\infty$  时, $\varphi(x,t)$  和  $u(x,t)$  迅速衰减到 0。因此,在数值上可以在有限区域  $(a,b)$  中求解 KGS 方程。其中, $-a,b\gg 1$ ,边界条件为零边界。

4.1 数值解

考虑初值条件

$$\varphi_0(x)=\varphi(x,0,v,0), \quad u_0(x)=u(x,0,v,0), \quad u_1(x)=u_t(x,0,v,0)。$$

计算主要在区间  $[-20,20]$  中进行,选取空间步长  $h$  为 0.2,时间步长  $\tau$  为 0.001 s,传播速度  $v$  为 0.1。向前 Euler 格式、Crank-Nicolson 格式和紧差分格式在数值运算时间  $(T)$  分别为 1,16 s 时得到的数值解,如图 1~3 所示。

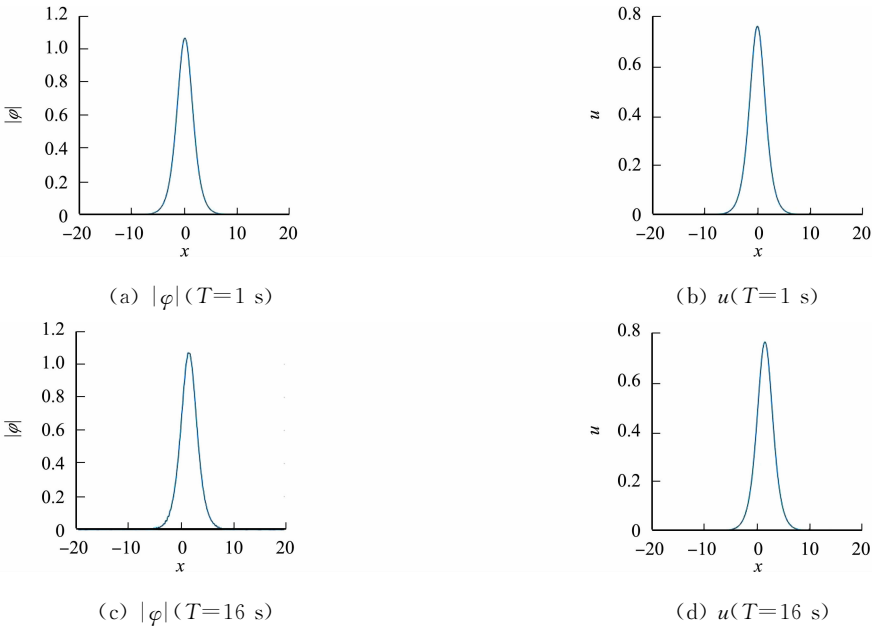
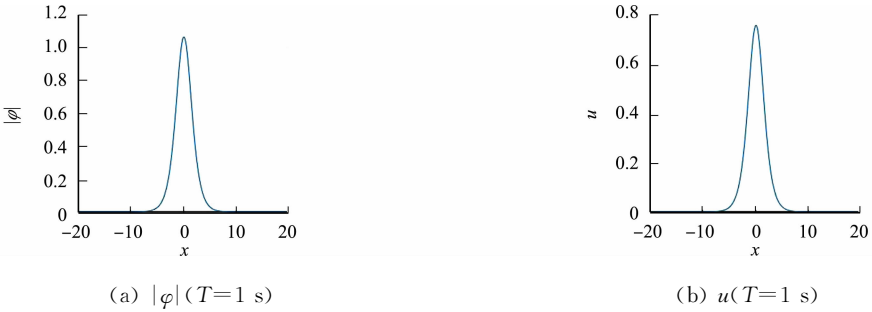


图 1 向前 Euler 格式在不同数值运算时间得到的数值解

Fig. 1 Numerical solutions of forward Euler scheme at different numerical operation times



由图 1~3 可知:当  $T=16$  时,向前 Euler 格式的数值解出现了一些轻微的振荡,Crank-Nicolson 格式和紧差分格式的数值解较为光滑。这表明相较于其他两种稳定的隐式格式,作为显式格式的向前 Euler 格

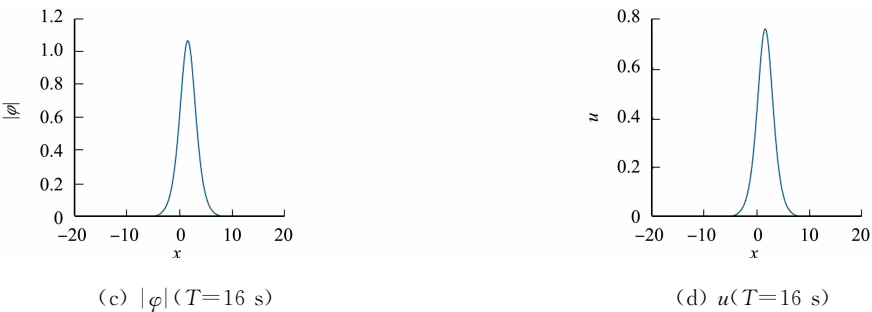


图 2 Crank-Nicolson 格式在不同数值运算时间得到的数值解

Fig. 2 Numerical solutions of Crank-Nicolson scheme at different numerical operation times

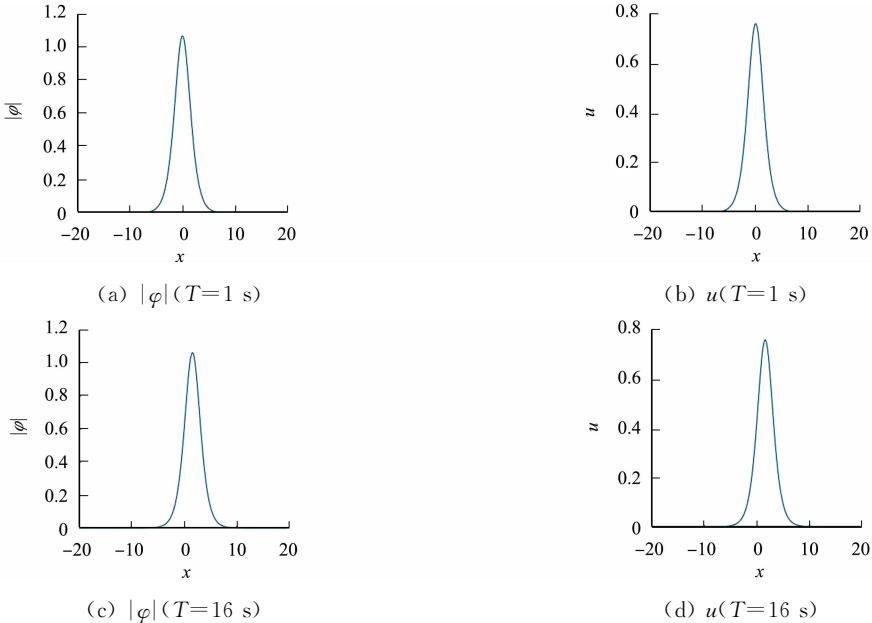


图 3 紧差分格式在不同数值运算时间得到的数值解

Fig. 3 Numerical solutions of compact difference scheme at different numerical operation times

式相对不稳定。

当  $T$  分别为 1, 16 s 时, 分别运用向前 Euler 格式、Crank-Nicolson 格式和紧差分格式求解 KGS 方程时的 CPU 运行时间( $t_{\text{CPU}}$ ), 结果如表 1 所示。由表 1 可知: 显式的向前 Euler 格式的计算速度明显优于隐式的 Crank-Nicolson 格式和紧差分格式, 这是因为向前 Euler 格式在计算过程中没有迭代。

表 1 不同数值运算时间时 3 种格式的 CPU 运行时间

Tab. 1 CPU runtimes of three schemes under different numerical operation times

$T/\text{s}$	$t_{\text{CPU}}/\text{s}$		
	向前 Euler 格式	Crank-Nicolson 格式	紧差分格式
1	0.443 491	24.160 042	36.455 731
16	4.235 344	428.940 976	650.413 849

4.2 电荷守恒与能量守恒

分别定义离散电荷误差 error  $Q$  和能量误差 error  $E$  为

$$\text{error } Q = \frac{Q^n - Q^0}{Q^0},$$

(62)

$$\text{error } E = \frac{E^n - E^0}{E^0}.$$

(63)

式(62)中:  $Q^n$  和  $E^n$  分别表示第  $n$  步的电荷值和能量值。

计算在区间  $[-20, 20]$  中进行, 选取空间步长  $h$  为 0.2, 时间步长  $\tau$  为 0.001 s, 传播速度  $v$  为 0.1。分别绘制  $T=10\text{ s}$  时 Crank-Nicolson 格式和紧差分格式的电荷、能量值及其离散误差, 如图 4, 5 所示。

由图 4 可知: 电荷误差和能量误差分别在  $10^{-13}$  和  $10^{-12}$  左右, 表明 Crank-Nicolson 格式的电荷和能量

是守恒的。由图 5 可知:紧差分格式的守恒量误差分别在  $10^{-11}$  和  $10^{-12}$  左右,表明紧差分格式能够很好地保持离散电荷和能量守恒。

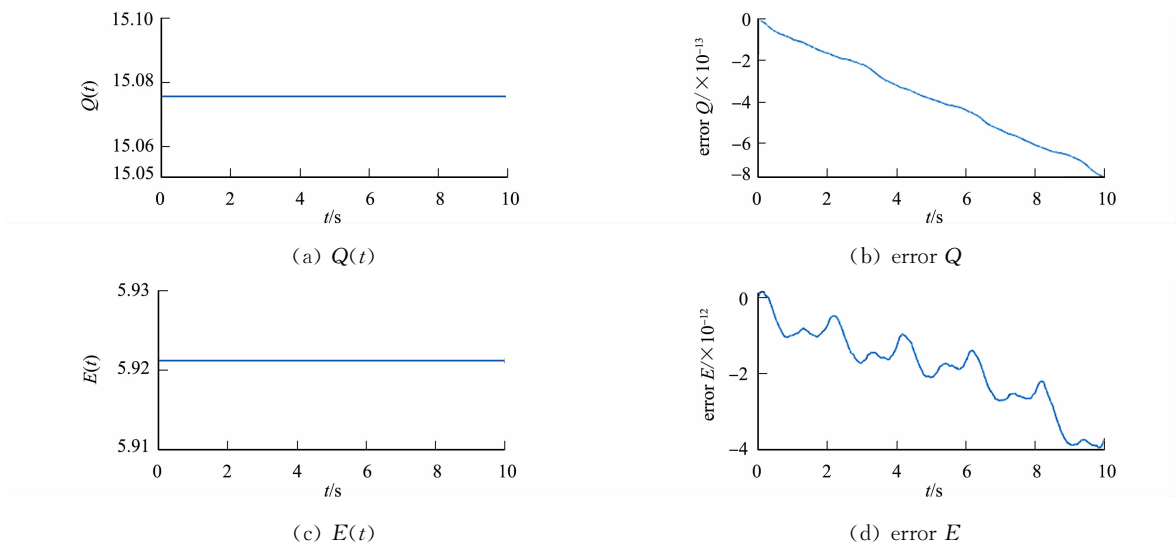


图 4 Crank-Nicolson 格式对守恒量的保持情况  
Fig. 4 Conservation of conserved quantities in Crank-Nicolson scheme

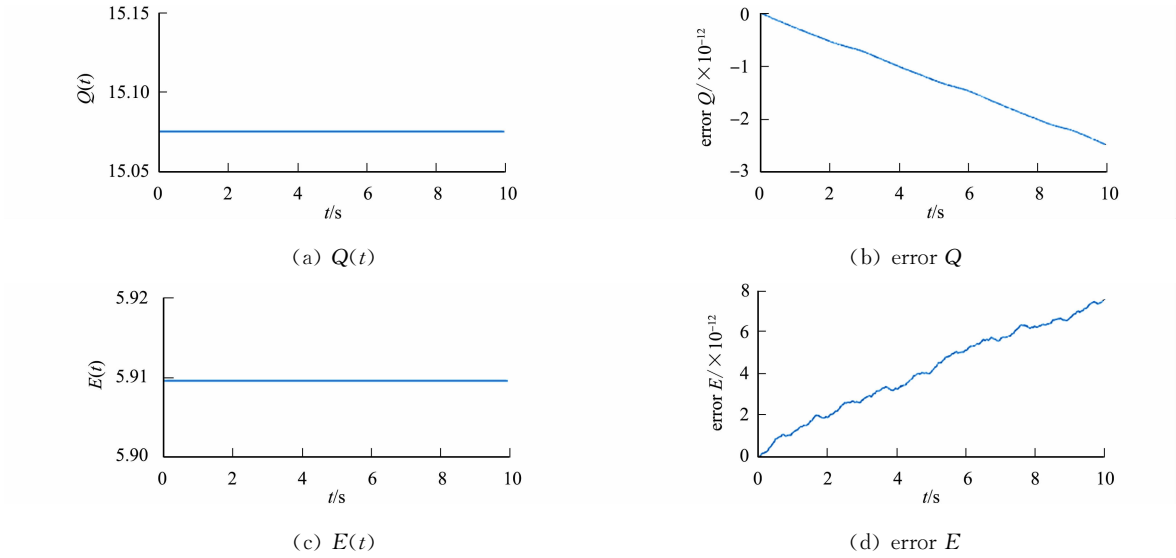


图 5 紧差分格式对守恒量的保持情况  
Fig. 5 Conservation of conserved quantities in compact difference scheme

## 5 结束语

利用经典的差分算子为一维 KGS 方程分别构造向前 Euler 格式、Crank-Nicolson 格式和紧差分格式。利用相关理论知识讨论了 3 种格式的精度,详细证明了 Crank-Nicolson 格式和紧差分格式能够精确保持离散电荷守恒及能量守恒。数值实验结果表明,与 Crank-Nicolson 格式和紧差分格式相比,向前 Euler 格式长时间计算的稳定性稍差,但是其计算效率更高。另外,在数值上,Crank-Nicolson 格式和紧差分格式能够精确地保持离散的电荷和能量守恒,验证了理论结果的正确性。通过对 3 种格式的比较,可以看出它们在求解 KGS 方程时的优缺点,为不同工程应用提供合适的选择。

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