

半经典 Schrödinger 方程的几个分裂数值格式

许秋滨

(南京审计大学数学学院, 江苏 南京 211815)

摘要: 本文研究了半经典的 Schrödinger 方程的两个分裂龙格-库塔格式和分裂谱格式. 给出了格式的稳定性, 并研究了当 $\beta = 0$ 时的平面波解. 通过线性化的分析方法可知两个龙格-库塔格式是条件稳定的, 谱格式是绝对稳定的. 最后给出了格式的截断误差并与文 [1] 中的格式进行了数值比较, 结果表明本文的格式是有效的和可靠的.

关键词: 非线性 Schrödinger 方程; 分裂龙格-库塔格式; 分裂谱格式; 差分格式

MR(2010) 主题分类号: 65M06; 65M30

中图分类号: O241.82

文献标识码: A

文章编号: 0255-7797(2025)02-0161-12

1 引言

本文考虑如下的 Schrödinger 方程初值问题 [1],

$$i\varepsilon u_t^\varepsilon + \frac{\varepsilon^2}{2} u_{xx}^\varepsilon - V u^\varepsilon - f(|u^\varepsilon|^2) u^\varepsilon - \varepsilon \beta \arg(u^\varepsilon) u^\varepsilon = 0, t > 0, x \in R. \quad (1.1)$$

$$u^\varepsilon(x, t = 0) = u_0^\varepsilon(x), x \in R. \quad (1.2)$$

其中 $V = V(x) > 0$ 为已知的实函数, ε 为普朗克常数, f 为足够光滑的实函数, $\beta \geq 0$ 为常数, $u^\varepsilon = u^\varepsilon(x, t)$ 为复波函数, 并有

$$\varepsilon \arg(u^\varepsilon(x, t)) = S^\varepsilon(x, t). \quad (1.3)$$

方程 (1.1) 包含很多的 Schrödinger 方程 [1]. 例如, 当 $f \equiv 0$ 且 $\beta = 0$ 时, (1.1) 变为线性 Schrödinger 方程; 当 $V \equiv 0, f(\rho) \equiv \gamma_\varepsilon \rho$ 且 $\beta = 0$ 时, 变为广义 Schrödinger 方程; 当 $f(\rho) = \alpha(\rho - 1)$ 且 $\beta = 0$ 时, 变为潜水波方程. 方程 (1.1) ~ (1.2) 遵守以下守恒律,

$$\int_{-\infty}^{+\infty} |u^\varepsilon(x, t)|^2 dx = const, \quad (1.4)$$

如果 $\beta = 0$ 还遵守下面的守恒律,

$$\int_{-\infty}^{+\infty} E^\varepsilon(x, t) dx = const, \quad (1.5)$$

*收稿日期: 2024-10-08

接收日期: 2024-12-25

基金项目: 国家社会科学基金资助 (21BTJ030).

作者简介: 许秋滨 (1980-), 男, 副教授, 主要研究方向: 偏微分方程数值解, E-mail: xqb0209@nau.edu.cn

其中

$$E^\varepsilon(x, t) = \frac{\varepsilon^2}{2} |u_x^\varepsilon(x, t)|^2 + F(|u^\varepsilon(x, t)|^2) + V(x) |u^\varepsilon(x, t)|^2, \quad (1.6)$$

并且

$$F(s) = \int_0^s f(z) dz.$$

在文 [1] 中作者对方程 (1.1)–(1.2) 的周期初边值问题研究了两个分裂的谱格式, 文 [2] 对一类半经典长短波方程构造了分裂龙格 - 库塔格式, 文 [3] 将分裂的龙格 - 库塔格式用于耦合 Schrödinger 方程, 都取得了很好的数值结果. 本文将分裂的三点、四点龙格 - 库塔格式和一个分裂谱格式应用于半经典 Schrödinger 方程, 数值结果表明本文的算法是有效的和可靠的. 周期边值问题如下:

$$u^\varepsilon(x_L + x, t) = u^\varepsilon(x_R + x, t), \quad u_x^\varepsilon(x_L + x, t) = u_x^\varepsilon(x_R + x, t),$$

方程 (1.1)–(1.2) 变为

$$i\varepsilon u_t^\varepsilon + \frac{\varepsilon^2}{2} u_{xx}^\varepsilon - V(x) u^\varepsilon - f(|u^\varepsilon|^2) u^\varepsilon - \varepsilon \beta \arg(u^\varepsilon) u^\varepsilon = 0, \quad x_L < x < x_R, \quad t > 0. \quad (1.7)$$

$$u^\varepsilon(x, t = 0) = u_0^\varepsilon(x), \quad x_L < x < x_R, \quad t > 0. \quad (1.8)$$

$$u^\varepsilon(x_L + x, t) = u^\varepsilon(x_R + x, t), \quad u_x^\varepsilon(x_L + x, t) = u_x^\varepsilon(x_R + x, t), \quad t > 0. \quad (1.9)$$

本文作如下的安排: 第 2 节提出了三个新的格式, 第 3 节研究了格式的守恒律, 第 4 节研究了 $\beta = 0$ 时的平面波解, 第 5 节给出了稳定性条件, 第 6 节给出了模型问题, 第 7 节给出了数值实验.

2 差分格式

下面对方程 (1.7)–(1.9) 构造几个差分格式, 首先引入如下的符号:

$$x_j = x_L + jh, \quad t^n = n\tau, \quad 0 \leq j \leq J = \left[\frac{x_R - x_L}{h} \right], \quad n = 0, 1, 2, \dots, \left[\frac{T}{\tau} \right],$$

$$u^\varepsilon(j, n) \equiv u^\varepsilon(x_j, t^n), \quad u_j^{\varepsilon, n} \sim u^\varepsilon(j, n), \quad V_j = V(x_j),$$

$$(w_j^n)_x = \frac{w_{j+1}^n - w_j^n}{h}, \quad (w_j^n)_{\bar{x}} = \frac{w_j^n - w_{j-1}^n}{h},$$

$$(w_j^n)_t = \frac{w_j^{n+1} - w_j^n}{\tau}, \quad r \equiv \frac{\tau}{h^2},$$

$$\|w^n\|_2^2 = h \sum_{j=1}^J |w_j^n|^2, \quad \|w^n\|_\infty = \sup_{1 \leq j \leq J} |w_j^n|.$$

其中 C 表示一个常数. 从 t^n 到 t^{n+1} , 方程 (1.7) 可分为两步求解 [1], 首先求解

$$i\varepsilon u_t^\varepsilon - Vu^\varepsilon - f(|u^\varepsilon|^2)u^\varepsilon - \varepsilon\beta \arg(u^\varepsilon)u^\varepsilon = 0, \quad (2.1)$$

接下来求解

$$i\varepsilon u_t^\varepsilon + \frac{\varepsilon^2}{2}u_{xx}^\varepsilon = 0. \quad (2.2)$$

2.1 三点分裂龙格 - 库塔格式 (二阶精度)(R-K(2))

龙格 - 库塔方法是一种具有很高精度的算法, 我们用三点格式离散 (2.2) 中的导数项 u_{xx}^ε , 然后将离散后的方程用龙格 - 库塔方法求解, 格式如下

$$u_j^{\varepsilon,*} = \begin{cases} e^{-\frac{i\tau}{\varepsilon}(V_j + f(|u_j^{\varepsilon,n}|^2))}u_j^{\varepsilon,n}, \beta = 0 \\ e^{-\frac{i}{\varepsilon\beta}(V_j + f(|u_j^{\varepsilon,n}|^2))(1 - e^{-\tau\beta}) + iS_j^\varepsilon(u_j^{\varepsilon,n}, \tau)}|u_j^{\varepsilon,n}|, \beta \neq 0 \end{cases} \quad (2.3)$$

$$u_j^{\varepsilon,n+1} = u_j^{\varepsilon,*} + (K1_j + 2K2_j + 2K3_j + K4_j)/6, \quad (2.4)$$

$$K1_j = G(u_j^{\varepsilon,*}), K2_j = G(u_j^{\varepsilon,*} + 0.5K1_j), K3_j = G(u_j^{\varepsilon,*} + 0.5K2_j), K4_j = G(u_j^{\varepsilon,*} + K3_j),$$

$$G(\eta_j^n) = \frac{i\varepsilon\tau}{2h^2}(\eta_{j+1}^n - 2\eta_j^n + \eta_{j-1}^n). \quad (2.5)$$

$S^\varepsilon(u^\varepsilon, t)$ 如下

$$S^\varepsilon(u^\varepsilon, t) = e^{-\beta(t-t_n)} \operatorname{Im} \left(\int_a^x \frac{u_v^\varepsilon(v, t_n)}{u^\varepsilon(v, t_n)} dv \right), \quad (2.6)$$

离散后为

$$S_j^\varepsilon(u^\varepsilon, t) = e^{-\beta t} \sum_{l=1}^j \frac{h}{2} \operatorname{Im} \left(\frac{D_x^s u|_{x=x_l-1}}{u_l-1} + \frac{D_x^s u|_{x=x_l}}{u_l} \right), \quad (2.7)$$

$$j = 1, 2, \dots, J, \quad s_0(u, \tau) = 0. \quad (2.8)$$

D_x^s 为导数项 ∂_x 的谱格式:

$$D_x^s u|_{x=x_j} = \frac{1}{J} \sum_{l=-J/2}^{J/2-1} i\mu_l \hat{u}_l e^{i\mu_l(x_j-a)}, \quad (2.9)$$

其中

$$\hat{u}_l = \sum_{j=0}^{J-1} u_j e^{-i\mu_l(x_j-a)}, \quad l = -\frac{J}{2}, \dots, \frac{J}{2} - 1, \quad (2.10)$$

格式 (2.3)–(2.5) 的截断误差为 $O(\tau^2 + h^2)$.

2.2 五点分裂龙格 - 库塔格式 (四阶精度)(R-K(4))

类似 (2.3)–(2.5) 我们考虑如下的五点龙格 - 库塔格式,

$$u_j^{\varepsilon,*} = \begin{cases} e^{-\frac{i\tau}{\varepsilon}(V_j + f(|u_j^{\varepsilon,n}|^2))} u_j^{\varepsilon,n}, \beta = 0 \\ e^{-\frac{i}{\varepsilon\beta}(V_j + f(|u_j^{\varepsilon,n}|^2))(1 - e^{-\tau\beta}) + iS_j^\varepsilon(u_j^{\varepsilon,n}, \tau)} |u_j^{\varepsilon,n}|, \beta \neq 0 \end{cases} \quad (2.11)$$

$$u_j^{\varepsilon,n+1} = u_j^{\varepsilon,*} + (K1_j + 2K2_j + 2K3_j + K4_j)/6, \quad (2.12)$$

$$K1_j = G(u_j^{\varepsilon,*}), K2_j = G(u_j^{\varepsilon,*} + 0.5K1_j), K3_j = G(u_j^{\varepsilon,*} + 0.5K2_j), K4_j = G(u_j^{\varepsilon,*} + K3_j),$$

$$G(\eta_j^n) = \frac{i\varepsilon\tau}{2h^2}(-\eta_{j+2}^n/12 + 4\eta_{j+1}^n/3 - 5\eta_j^n/2 + 4\eta_{j-1}^n/3 - \eta_{j-2}^n/12), \quad (2.13)$$

格式 (2.11)–(2.13) 的精度为 $O(\tau^2 + h^4)$.

2.3 分裂谱格式 (SP0)

方程 (2.2) 是一个线性方程可以用傅里叶方法精确求解, 我们构造下面的格式,

$$u_j^{\varepsilon,*} = \begin{cases} e^{-\frac{i\tau}{\varepsilon}(V_j + f(|u_j^{\varepsilon,n}|^2))} u_j^{\varepsilon,n}, \beta = 0 \\ e^{-\frac{i}{\varepsilon\beta}(V_j + f(|u_j^{\varepsilon,n}|^2))(1 - e^{-\tau\beta}) + iS_j^\varepsilon(u_j^{\varepsilon,n}, \tau)} |u_j^{\varepsilon,n}|, \beta \neq 0 \end{cases} \quad (2.14)$$

$$u_j^{\varepsilon,n+1} = \frac{1}{J} \sum_{l=-J/2}^{J/2-1} e^{-i\varepsilon\mu_l^2\tau/2} \hat{u}_l^{\varepsilon,*} e^{i\mu_l(x_j - x_L)}, \quad j = 0, 1, 2, \dots, J-1, \quad (2.15)$$

$$\mu_l = \frac{2\pi l}{x_R - x_L}, \hat{u}_l^{\varepsilon,*} = \sum_{j=0}^{J-1} u_j^{\varepsilon,*} e^{-i\mu_l(x_j - x_L)}, l = -\frac{J}{2}, \dots, \frac{J}{2} - 1, \quad (2.16)$$

格式 (2.14)–(2.16) 的精度为 $O(\tau^2 + h^m)$, m 为方程 (1.7)–(1.9) 的光滑度.

2.4 分裂谱格式 (BSP1 和 BSP2)

作为比较我们给出文 [1] 中的两个格式.

(1)BSP1

$$u_j^{\varepsilon,*} = \frac{1}{J} \sum_{l=-J/2}^{J/2-1} e^{-i\varepsilon\mu_l^2\tau/2} \hat{u}_l^{\varepsilon,n} e^{i\mu_l(x_j - x_L)}, \quad j = 0, 1, 2, \dots, J-1, \quad (2.17)$$

$$u_j^{\varepsilon, n+1} = \begin{cases} e^{-\frac{i\tau}{\varepsilon}(V_j + f(|u_j^{\varepsilon, *}|^2))} u_j^{\varepsilon, *}, & \beta = 0 \\ e^{-\frac{i}{2\varepsilon\beta}(V_j + f(|u_j^{\varepsilon, *}|^2))(1 - e^{-\tau\beta}) + iS_j^\varepsilon(u_j^{\varepsilon, *}, \tau)} |u_j^{\varepsilon, *}|, & \beta \neq 0 \end{cases} \quad (2.18)$$

$$\mu_l = \frac{2\pi l}{x_R - x_L}, \hat{u}_l^{\varepsilon, n} = \sum_{j=0}^{J-1} u_j^{\varepsilon, n} e^{-i\mu_l(x_j - x_L)}, l = -\frac{J}{2}, \dots, \frac{J}{2} - 1. \quad (2.19)$$

(2)BSP2

$$u_j^{\varepsilon, *} = \begin{cases} e^{-\frac{i\tau}{2\varepsilon}(V_j + f(|u_j^{\varepsilon, n}|^2))} u_j^{\varepsilon, n}, & \beta = 0 \\ e^{-\frac{i}{2\varepsilon\beta}(V_j + f(|u_j^{\varepsilon, n}|^2))(1 - e^{-\tau\beta}) + iS_j^\varepsilon(u_j^{\varepsilon, n}, \tau/2)} |u_j^{\varepsilon, n}|, & \beta \neq 0 \end{cases} \quad (2.20)$$

$$u_j^{\varepsilon, **} = \frac{1}{J} \sum_{l=-J/2}^{J/2-1} e^{-i\varepsilon\mu_l^2\tau/2} \hat{u}_l^{\varepsilon, *} e^{i\mu_l(x_j - x_L)}, \quad j = 0, 1, 2, \dots, J-1, \quad (2.21)$$

$$u_j^{\varepsilon, n+1} = \begin{cases} e^{-\frac{i\tau}{2\varepsilon}(V_j + f(|u_j^{\varepsilon, **}|^2))} u_j^{\varepsilon, **}, & \beta = 0 \\ e^{-\frac{i}{2\varepsilon\beta}(V_j + f(|u_j^{\varepsilon, **}|^2))(1 - e^{-\tau\beta}) + iS_j^\varepsilon(u_j^{\varepsilon, **}, \tau/2)} |u_j^{\varepsilon, **}|, & \beta \neq 0 \end{cases} \quad (2.22)$$

格式 (2.17)–(2.19) 和 (2.20)–(2.22) 的精度为 $O(\tau^2 + h^m)$, m 为方程 (1.7)–(1.9) 的光滑度.

3 格式的守恒律

考虑如下的两个守恒律:

$$H_1^n = \|u^{\varepsilon, n}\|^2, \quad (3.1)$$

$$H_2^n = \frac{\varepsilon^2}{2} h \sum_{j=0}^{j=J-1} \left| \frac{u_{j+1}^{\varepsilon, n} - u_j^{\varepsilon, n}}{h} \right|^2 + F(\|u^{\varepsilon, n}\|^2) + h \sum_{j=0}^{J-1} V_j |u_j^{\varepsilon, n}|^2. \quad (3.2)$$

定理 3.1 格式 SP0, BSP1 和 BSP2 满足守恒律 $\|u^{\varepsilon, n}\|^2 = const.$

证 由 (2.3) 得 $|u_j^{\varepsilon, *}| = |u_j^{\varepsilon, n}|$, 对 SP0 由巴什瓦定理得

$$\|u^{\varepsilon, n+1}\|^2 = (x_R - x_L) \sum_{l=-J/2}^{J/2-1} (\hat{u}_l^{\varepsilon, *})^2 = h \sum_{j=1}^J |u_j^{\varepsilon, *}|^2 = h \sum_{j=1}^J |u_j^{\varepsilon, n}|^2 = \|u^{\varepsilon, n}\|^2,$$

于是有

$$\|u^{\varepsilon, n+1}\|^2 = \dots = \|u^{\varepsilon, 0}\|^2 = \|u_0^\varepsilon\|^2 = const,$$

对于格式 BSP1 有

$$\|u^{\varepsilon, n+1}\|^2 = \|u^{\varepsilon, *}\|^2 = (x_R - x_L) \sum_{l=-J/2}^{J/2-1} (\hat{u}_l^{\varepsilon, n})^2 = h \sum_{j=1}^J |u_j^{\varepsilon, n}|^2 = \|u^{\varepsilon, n}\|^2,$$

所以

$$\|u^{\varepsilon, n+1}\|^2 = \dots = \|u^{\varepsilon, 0}\|^2 = \|u_0^\varepsilon\|^2 = \text{const},$$

与格式 SP0 和 BSP1 类似, 可以证明格式 BSP2 有

$$\|u^{\varepsilon, n+1}\|^2 = \|u^{\varepsilon, **}\|^2 = (x_R - x_L) \sum_{l=-J/2}^{J/2-1} (\hat{u}_l^{\varepsilon, **})^2 = h \sum_{j=1}^J |u_j^{\varepsilon, **}|^2 = h \sum_{j=1}^J |u_j^{\varepsilon, n}|^2 = \|u^{\varepsilon, n}\|^2,$$

所以

$$\|u^{\varepsilon, n+1}\|^2 = \dots = \|u^{\varepsilon, 0}\|^2 = \|u_0^\varepsilon\|^2 = \text{const}.$$

尽管三点龙格 - 库塔格式 (2.3)–(2.5) 和五点龙格 - 库塔格式 (2.11)–(2.15) 不能够满足守恒律 (3.1) 和 (3.2), 在数值实验中我们可以看到, 它们也可以很好地满足两个守恒律.

4 平面波解

考虑当 $\beta = 0$ 时方程 (1.7)–(1.9) 的平面波解, 令

$$V = d, u^\varepsilon = Ae^{i(k\pi x/p - \omega t)}, \quad (4.1)$$

其中 d, A, k 和 ω 为常数. 将 (4.1) 代入到 (1.7) 中, 得如下等式

$$i\varepsilon(-i\omega)u^\varepsilon + \frac{\varepsilon^2}{2}(i \cdot \frac{k\pi}{p})^2 u^\varepsilon - (f(A^2) + d)u^\varepsilon = 0, \quad (4.2)$$

得

$$\omega = \frac{\frac{\pi^2 \varepsilon^2 k^2}{2p^2} + f(A^2) + d}{\varepsilon}.$$

在下面的论述中我们考虑如下离散形式的平面波解

$$V = d, u^\varepsilon = Ae^{i(k\pi jh/p - \omega n\tau)}. \quad (4.3)$$

4.1 三点龙格 - 库塔格式

将 (4.3) 代入到 (2.3)–(2.5), 得

$$u_j^{\varepsilon, *} = Ae^{-\frac{i\tau}{\varepsilon}(d+f(A^2))} \cdot e^{i(k\pi jh/p - \omega n\tau)}, u_j^{\varepsilon, n+1} = u_j^{\varepsilon, *} + \frac{1}{6}(K1_j + 2K2_j + 2K3_j + K4_j),$$

整理得,

$$u_j^{\varepsilon, n+1} = (1 + q + \frac{q^2}{2} + \frac{q^3}{6} + \frac{q^4}{24})u_j^{\varepsilon, *},$$

其中

$$q = \frac{i\varepsilon\tau}{h^2} \left(\cos \frac{k\pi h}{p} - 1 \right) = \frac{i\varepsilon\tau}{h^2} \left(-\frac{k^2\pi^2 h^2}{2p^2} + O(h^4) \right) = -\frac{i\varepsilon k^2 \pi^2 \tau}{2p^2} + O(h^2),$$

于是有

$$u_j^{\varepsilon, n+1} = u_j^{\varepsilon, *} \left(1 - \frac{i\varepsilon k^2 \pi^2 \tau}{2p^2} + O(\tau^2 + h^2) \right),$$

因为 $u_j^{\varepsilon, n+1} = A e^{k\pi j h/p - \omega(n+1)\tau}$, 所以有

$$\omega = \frac{\frac{\pi^2 \varepsilon^2 k^2}{2p^2} + f(A^2) + d}{\varepsilon} + O(\tau^2 + h^2),$$

所以三点龙格 - 库塔方法的精度为 $O(\tau^2 + h^2)$, 同理可得五点龙格 - 库塔格式 (2.11)–(2.13) 的精度为 $O(\tau^2 + h^4)$.

4.2 分裂谱格式

将 (4.3) 代入到格式 SP0 中, 由离散的傅里叶变换,

$$u_j^{\varepsilon, *} = e^{-\frac{i\tau}{\varepsilon}(d+f(A^2))} \cdot A e^{i\left(\frac{k\pi j h}{p} - \omega n \tau\right)} = A e^{-\frac{i\tau}{\varepsilon}(d+f(A^2)) + i\frac{k\pi j h}{p} - i\omega n \tau},$$

$$\begin{aligned} \hat{u}_j^{\varepsilon, *} &= \sum_{j=0}^{J-1} u_j^{\varepsilon, *} e^{-i\frac{l\pi j h}{p}} = A e^{[-\frac{i\tau}{\varepsilon}(d+f(A^2)) - i\omega n \tau]} \cdot \sum_{j=0}^{J-1} e^{i\left(\frac{k\pi j h}{p} - \frac{l\pi j h}{p}\right)} \\ &= \begin{cases} 0, l \neq k \\ J \cdot A e^{[-\frac{i\tau}{\varepsilon}(d+f(A^2)) - i\omega n \tau]}, l = k \end{cases} \end{aligned}$$

并且

$$u_j^{\varepsilon, n+1} = \frac{1}{J} \sum_{l=-\frac{J}{2}}^{\frac{J}{2}-1} e^{-\frac{i\varepsilon n^2 l^2 \tau}{2p^2}} \cdot \hat{u}_j^{\varepsilon, *} \cdot e^{i\frac{\pi l j h}{p}} = A e^{-\frac{i\tau}{\varepsilon}(d+f(A^2)) - i\omega n \tau} \cdot e^{-\frac{i\varepsilon n^2 k^2 \tau}{2p^2}} \cdot e^{i\frac{\pi k j h}{p}},$$

又因为

$$u_j^{\varepsilon, n+1} = A e^{i\left(\frac{k\pi j h}{p} - \omega(n+1)\tau\right)},$$

整理得

$$\omega = \frac{\frac{\pi^2 \varepsilon^2 k^2}{2p^2} + f(A^2) + d}{\varepsilon},$$

所以分裂谱格式可以精确满足平面波解, 同理 BSP1 和 BSP2 也精确满足平面波解.

5 格式的稳定性

关于格式的稳定性有如下的定理:

定理 5.1 三点龙格 - 库塔格式 (2.3)–(2.5)、五点龙格 - 库塔格式 (2.11)–(2.13) 的稳定性条件分别为 $r \leq \frac{\sqrt{2}}{\varepsilon}$, $r \leq \frac{12\sqrt{2}}{7\varepsilon}$, 其中 $r = \tau/h^2$.

证明 假设 $V(x) = d$, 其中 d 是个常数. 下面用线性化的方法证明三点龙格 - 库塔格式和五点龙格 - 库塔格式的稳定性. 考虑如下的解的形式

$$u_j^{\varepsilon, n} = \xi^{\varepsilon, n} e^{ikjh}, \quad (5.1)$$

将 (5.1) 式代入到 (2.3)–(2.5), 我们得

$$\begin{aligned} u_j^{\varepsilon, *} &= e^{-\frac{i\tau}{\varepsilon}(d+f(|\xi^n|^2))} \xi^n e^{ikjh}, \\ u_j^{\varepsilon, n+1} &= u_j^{\varepsilon, *} + \frac{1}{6}(K1_j + 2K2_j + 2K3_j + K4_j), \\ K1_j &= G(u_j^{\varepsilon, *}) = \frac{i\varepsilon\tau}{2h^2} \cdot (e^{ikh} - 2 + e^{-ikh})u_j^{\varepsilon, *} \\ &= i\varepsilon r(\cos kh - 1)u_j^{\varepsilon, *} \equiv qu_j^{\varepsilon, *}, \end{aligned}$$

其中

$$\begin{aligned} q &= i\varepsilon r(\cos kh - 1), \\ K2_j &= G\left(\left(1 + \frac{q}{2}\right)u_j^{\varepsilon, *}\right) = q\left(1 + \frac{q}{2}\right)u_j^{\varepsilon, *}, \\ K3_j &= q\left(1 + \frac{q}{2}\left(1 + \frac{q}{2}\right)\right)u_j^{\varepsilon, *}, \\ K4_j &= q\left(1 + q\left(1 + \frac{q}{2}\left(1 + \frac{q}{2}\right)\right)\right)u_j^{\varepsilon, *}, \end{aligned}$$

因为

$$u_j^{\varepsilon, n+1} = \left(1 + q + \frac{q^2}{2} + \frac{q^3}{6} + \frac{q^4}{24}\right)u_j^{\varepsilon, *},$$

又因为

$$u_j^{\varepsilon, n+1} = \xi^{\varepsilon, n+1} e^{ikjh},$$

所以有

$$\xi^{\varepsilon, n+1} = \left(1 + q + \frac{q^2}{2} + \frac{q^3}{6} + \frac{q^4}{24}\right)e^{-\frac{i\tau}{\varepsilon}(d+f(|\xi^n|^2))} \xi^{\varepsilon, n}.$$

令

$$G(\tau, k) = \left(1 + q + \frac{q^2}{2} + \frac{q^3}{6} + \frac{q^4}{24}\right)e^{-\frac{i\tau}{\varepsilon}(d+f(|\xi^n|^2))}, p = \varepsilon r(\cos kh - 1), \quad (5.2)$$

则

$$G(\tau, k) = \left(1 + ip - \frac{p^2}{2} - i\frac{p^3}{6} + \frac{p^4}{24}\right)e^{-\frac{i\tau}{\varepsilon}(d+f(|\xi^n|^2))}, \quad (5.3)$$

格式 (2.3)–(2.5) 是稳定的, 则 $G(\tau, k)$ 满足

$$|G(\tau, k)|^2 = \left(1 - \frac{p^2}{2} + \frac{p^4}{24}\right)^2 + \left(p - \frac{p^3}{6}\right)^2 \leq 1,$$

于是有

$$\varepsilon^2 r^2 \sin^4 \frac{kh}{2} - 2 \leq 0,$$

三点龙格 - 库塔格式 (2.3)–(2.5) 的稳定性条件为 $r \leq \frac{\sqrt{2}}{\varepsilon}$. 同理可证, 五点龙格 - 库塔格式的稳定性条件为 $r \leq \frac{12\sqrt{2}}{7\varepsilon}$. 另外, 由定理 3.1 可知谱格式 SP0, BSP1 和 BSP2 是无条件稳定的 [1].

6 模型问题

令

$$u_0^\varepsilon(x) \equiv A_0(x)e^{\frac{i}{\varepsilon}s_0(x)}.$$

模型 I 平面波解的初值问题: 当 $\beta = 0$ 时, 我们给出了 (1.7)–(1.9) 的平面波解, 令初值 $A_0(x) = A, S_0(x) = \frac{\varepsilon k \pi x}{p}, V_0^\varepsilon(x) = d$. 精确解为

$$u^\varepsilon(x, t) = Ae^{i(\frac{k\pi x}{p} - \omega t)}, V_0^\varepsilon(x) = d,$$

并且

$$\omega = \frac{\frac{\pi^2 \varepsilon^2 k^2}{2p^2} + f(A^2) + d}{\varepsilon},$$

在计算中取如下参数: $A = 5, k = 1, p = 10, d = 1$.

模型 II 当 $\beta \neq 0$ 时, 我们用第 2 节中的格式来计算密度函数 $\rho^\varepsilon(x, t) = |u^\varepsilon(x, t)|^2$. 初值条件为 $A_0(x) = e^{-x^2}, S_0(x) = \frac{1}{e^{3x} + e^{-3x}}, \beta = 1.0, V(x) = 0, f(\rho) = -\rho$.

7 数值实验

本节用第 2 节的数值格式来计算模型 I 和模型 II. 在计算模型 I 时, 固定精度 (L_∞), 让步长 h 和 τ 自由. 对每个格式, 令步长 h 和 τ 尽量大, 既要达到给定的精度, 又能使格式保持稳定, 比较格式的计算时间. 计算的量如下:

守恒律

$$H_1^n = \|u^{\varepsilon, n}\|^2,$$

和

$$H_2^n = \frac{\varepsilon^2}{2} h \sum_{j=0}^{j=J-1} \left| \frac{u_{j+1}^{\varepsilon, n} - u_j^{\varepsilon, n}}{h} \right|^2 + F(\|u^{\varepsilon, n}\|^2) + h \sum_{j=0}^{j=J-1} V_j |u_j^{\varepsilon, n}|^2,$$

误差为

$$E_1 = \frac{H_1^n - H_1^0}{H_1^0}, E_2 = \frac{H_2^n - H_2^0}{H_2^0},$$

精确解的误差

$$L_\infty = \max_j |u_j^{\varepsilon, n} - u^\varepsilon(x_j, t^n)|,$$

其中 $u^\varepsilon(x_j, t^n)$ 为在点 (x_j, t_n) 处的精确解. 模型 I 的计算结果见表 1.

文 [4][5] 中对小 ε 的线性 schrödinger 方程的有限差分进行了研究, 结果表明为了保证良好的近似, 时间步长 τ 和空间步长 h 满足如下关系:

$$h = o(\varepsilon), \tau = o(\varepsilon).$$

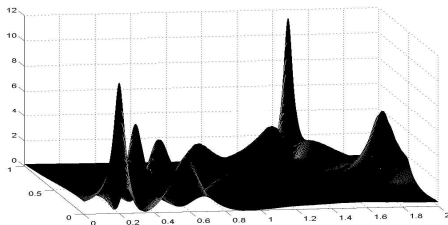
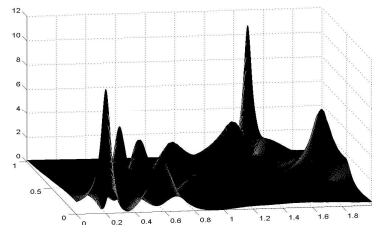
对于模型 II, 我们取 $\varepsilon = 0.1$, 为了画出密度函数的较精确图像, 令空间步长 $h = 0.015625$ 和一个较小的时间步长 $\tau = 0.002$. 图 1 和图 2 给出了用五点龙格 - 库塔格式和 Bsp2 计算的结果, 表 2 给出了所有格式的计算时间.

表 1 表 1: $\beta = 0$, $f(\rho) = -\rho$, $T=1.0$, $A=5.0$, $k=1.0$, 精度 $L_\infty < 0.05$, $t=1.0$ 平面波解计算结果比较

	格式	步长	时间	L_∞	E_1	E_2
$\varepsilon = 1$	BSP1	$h=2.5, \tau=0.5$	1.90(-5)	1.00(-5)	1.82(-7)	3.64(-7)
	BSP2	$h=2.5, \tau=0.5$	2.32(-5)	3.64(-6)	1.22(-7)	1.18(-5)
	SP0	$h=2.5, \tau=0.5$	1.90(-5)	2.31(-5)	7.22(-8)	1.44(-7)
	R-K(4)	$h=2.5, \tau=0.5$	1.10(-5)	9.90(-4)	1.15(-7)	2.29(-7)
	R-K(2)	$h=2.5, \tau=0.5$	1.00(-5)	1.24(-2)	3.99(-8)	3.98(-8)
$\varepsilon = 0.1$	BSP1	$h=2.5, \tau=0.5$	1.92(-5)	1.53(-4)	1.94(-7)	3.87(-7)
	BSP2	$h=2.5, \tau=0.5$	2.30(-5)	1.51(-4)	2.93(-8)	5.86(-8)
	SP0	$h=2.5, \tau=0.5$	1.90(-5)	2.64(-4)	2.10(-7)	4.20(-7)
	R-K(4)	$h=2.5, \tau=0.5$	1.09(-5)	1.40(-4)	9.59(-9)	1.91(-8)
	R-K(2)	$h=2.5, \tau=0.5$	1.00(-5)	1.29(-3)	2.33(-8)	4.64(-8)
$\varepsilon = 0.01$	BSP1	$h=2.5, \tau=0.5$	1.89(-5)	1.17(-3)	1.17(-7)	2.34(-7)
	BSP2	$h=2.5, \tau=0.5$	2.32(-5)	2.12(-3)	1.68(-7)	3.36(-7)
	SP0	$h=2.5, \tau=0.5$	1.92(-5)	4.91(-3)	2.11(-7)	4.21(-7)
	R-K(4)	$h=2.5, \tau=0.5$	1.10(-5)	3.75(-4)	9.59(-9)	1.91(-8)
	R-K(2)	$h=2.5, \tau=0.5$	1.00(-5)	6.61(-4)	1.29(-7)	2.57(-7)
$\varepsilon = 0.001$	BSP1	$h=2.5, \tau=0.5$	1.92(-5)	6.58(-3)	2.38(-8)	4.76(-8)
	BSP2	$h=2.5, \tau=0.5$	2.32(-5)	3.09(-2)	2.33(-7)	4.66(-7)
	SP0	$h=2.5, \tau=0.5$	1.91(-5)	1.10(-2)	1.14(-7)	2.28(-7)
	R-K(4)	$h=2.5, \tau=0.5$	1.10(-5)	3.81(-3)	7.98(-8)	1.59(-7)
	R-K(2)	$h=2.5, \tau=0.5$	1.00(-5)	1.68(-3)	2.50(-8)	5.00(-8)
$\varepsilon = 0.0001$	BSP1	$h=2.5, \tau=0.6$	1.95(-5)	1.58(-2)	6.68(-8)	1.33(-7)
	BSP2	$h=2.5, \tau=0.6$	2.40(-5)	4.75(-2)	3.20(-7)	6.40(-7)
	SP0	$h=2.5, \tau=0.6$	1.95(-5)	4.27(-2)	5.74(-8)	1.14(-7)
	R-K(4)	$h=2.5, \tau=0.6$	1.16(-5)	3.81(-2)	2.82(-8)	5.64(-8)
	R-K(2)	$h=2.5, \tau=0.6$	1.05(-5)	3.52(-2)	3.63(-8)	7.25(-8)

表 2 $\beta = 1.0, \varepsilon = 0.1, h = 0.015625, \tau = 0.002$, 模型 II 计算结果比较

	scheme	cpu-time	E_1
$\varepsilon = 0.1$	BSP1	0.42	4.05(-3)
	BSP2	0.48	3.97(-3)
	SP0	0.42	3.88(-3)
	R-K(4)	0.38	1.99(-3)
	R-K(2)	0.35	1.56(-3)

图 1: 五点龙格 - 库塔格式计算的密度 $\rho^\varepsilon(x, t) = |u^\varepsilon(x, t)|^2$ 图 2: Bsp2 格式计算的密度 $\rho^\varepsilon(x, t) = |u^\varepsilon(x, t)|^2$

由表 1 可知, 当 $\varepsilon=1, 0.1, 0.01, 0.001, 0.0001$ 时, 所有的格式都能够很好的计算平面波解. 其中, 分裂的五点龙格 - 库塔格式和三点龙格 - 库塔格式用的时间较少. 表 2 中数据也表明五点龙格 - 库塔格式和三点龙格 - 库塔格式用的时间较少, 具有较高的计算效率. 由计算结果可知, 所有的格式都可以很好的计算, 其中分裂的五点龙格 - 库塔格式精度高, 计算时间少, 是最有效的和可靠的.

参 考 文 献

- [1] W.Bao,S.Jin,P.A.Markowich. Numerical study of time-splitting spectral discretizations of nonlinear schrödinger equation in the semiclassical regimes[J]. SIAM J.sci.Compt, 2003, 25(1): 27-64.
- [2] Qianshun Chang,Yau-shu Wang,Chi-kun Lin. Numerical computations for long-wave short-wave interaction equations in semi-classical limit[J]. J.Comput.Phys, 2008, 227(19): 8489-8507.
- [3] Qiubin Xu, Qianshun Chang. New numerical methods for the coupled Nonlinear Schrodinger equations[J]. Acta. Mathematicae. Applicatae Sinica., 2010, 26(2): 205-218.
- [4] Peter Markowich, Paola Pietra, Carsten Pohl. Numerical approximation of quadratic observables of schrödinger type equations in the semiclassical limit[J]. Numer. Math, 1999, 81(4): 595-630.
- [5] Peter Markowich, Paola Pietra, Carsten Pohl, Hans Stimming. A Wigner measure analysis of the Dufort-Frankel scheme for the schrödinger equation[J]. SIAM J. Numer.Anal, 2002, 40(4): 1281-1310.
- [6] Q.Chang,B.Guo,H.Jiang. Finite difference method for generalized zakharov equations[J]. Math. Comput., 1995, 64(210): 537-553.

- [7] W.Bao,D.Jaksch. 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.
- [8] A.Fannjiang,Shi Jin,and G.Papanicolaou. High frequency behaviour of the focusing nonlinear schrödinger equation with random inhomogeneities[J]. SIAM.J.Appl.Math, 2003, 63(4): 1328–1358.

SPLIT-STEP METHODS FOR THE NONLINEAR SCHRÖDINGER EQUATIONS AND THEIR APPLICATIONS IN SEMICLASSICAL CASE

XU Qiu-bin

(*School of Mathematics, Nanjing Audit University, Nanjing 211815, China*)

Abstract: In this paper,two split step Runge-Kutta methods and a split step spectral method for the nonlinear Schrödinger equations and their application in the semiclassical regimes are studied.The conservative properties of the schemes are obtained and the plane wave solution with $\beta = 0$ is analysed.The two Runge-Kutta schemes are conditionally stable by linearized analysis and the split step spectral method is unconditionally stable . The truncation error of the schemes are discussed.Furthermore, the computing results are compared with the two time-splitting spectral methods which are constructed in [1].The numerical experiments demonstrate that our algorithms are effective and reliable.

Keywords: Nonlinear Schrödinger equation(NLS); split step Runge-Kutta method; Split step spectral method; difference scheme

2010 MR Subject Classification: 65M06; 65M30