

# Compact Extrapolation Schemes for a Linear Schrödinger Equation

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## Abstract

This paper proposes a kind of compact extrapolation schemes for a linear Schrödinger equation. The schemes are convergent with fourth-order accuracy both in space and time. Especially, a specific scheme of sixth-order accuracy in space is given. The stability and discrete invariants of the schemes are analyzed. The schemes satisfy discrete conservation laws of original Schrödinger equation. The numerical example indicates the efficiency of the new schemes.

## Keywords

Schrödinger Equation, Compact Scheme, Stability, Discrete Invariant, Extrapolation

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## 1. Introduction

Partial differential equations (PDEs) describe many physical phenomena. They are an important research topic in many scientific fields, such as hydrodynamics, plasma physics, nonlinear optics, molecular dynamics, celestial mechanics. The numerical investigations of PDEs can be found in [1]-[3] and references therein. To meet the demands of massive computation with high accuracy, many compact schemes have been presented recently in fluid dynamics, optics and plasma [4]-[6]. The schemes are high-order accurate with small stencil and little cost.

Schrödinger equations are important mathematical physical models [7]. They satisfy some conservation laws related to some physical quantities. Numerical preservation of these conservation laws is as important as high accuracy of numerical solutions [8]-[10]. So in this paper, we apply compact schemes to Schrödinger equations and analyze the discrete invariants of the schemes.

Consider the initial-boundary problems of the linear Schrödinger equation

$$iu_t + u_{x^4} + 2\rho u = 0, u(x, 0) = u_0(x), u(0, t) = u(2\pi, t), x \in [0, 2\pi], t \in [0, T], \quad (1)$$

where  $i^2 = -1$  and  $u_0(x)$  is a known differential function. For an integer  $m$ ,  $u_{x^m}$  and  $u_{t^m}$  means the  $m$ -order partial derivatives of  $u$  with respect to  $x$  and  $t$ , respectively.

**Proposition 1.** Under the periodic boundary condition, the solution of (1) satisfies the following conservation laws: (1) Norm conservation

$$Q(t) = \int_0^{2\pi} |u(x,t)|^2 dx = Q(0), \quad (2)$$

(2) Energy conservation

$$E(t) = \int_0^{2\pi} |u_{xx}|^2 + \rho|u|^2 dx = E(0), \quad (3)$$

## 2. Compact Extrapolation Schemes

Introduce the following uniform mesh grids

$$\{(x_k, t_n) = (kh, n\tau) | k = 0, 1, \dots, N, n = 0, 1, \dots, M\},$$

Denote the numerical values of  $u(x_k, t_n)$  by  $u_k^n$ . The symbols  $u_k$  and  $u^n$  means the numerical solution vectors at  $x = x_k$  and  $t = t^n$  with components  $u_k^n$ , respectively. Furthermore, we will denote

$$u_k^{n+\frac{1}{2}} = \frac{1}{2}(u_k^n + u_k^{n+1}).$$

### 2.1. Spatial Discretization

By introducing the following linear operators

$$\delta_x^4 u_k = A^{-1} B u_k, \quad A u_k = \alpha u_{k-1} + u_{k-1} + \alpha u_{k+1}, \quad (4)$$

$$B u_k = \frac{b}{6h^4} (u_{k+3} - 9u_{k+1} + 16u_k - 9u_{k-1} + u_{k-3}) + \frac{a}{h^4} (u_{k+2} - 4u_{k+1} + 6u_k - 4u_{k-1} + u_{k-2}),$$

we adopt the formula (4) to approximate  $u_{x^4}$ . A family of fourth-order schemes is derived with

$a = 2(1-\alpha)$ ,  $b = 4\alpha - 1$ . The leading term of the truncation error of the method is  $\frac{7-26\alpha}{240} (u_{x^6})_k h^4$ . We are also

interested in a sixth-order scheme with  $\alpha = \frac{7}{26}$ ,  $a = \frac{19}{13}$ ,  $b = \frac{1}{13}$ . The dominant term of the truncation error is

$\frac{193}{393120} (u_{x^{10}})_k h^6$ . Here, we consider periodic boundary condition. Applying the approximation (4) to Schrödinger Equation (1), we obtain the following semi-discretization system

$$i(u_t)_k = -\delta_x^4 u_k - 2\rho u_k, \quad k = 1, 2, \dots, N. \quad (5)$$

### 2.2. Temporal Discretization

We use the central difference operator

$$\delta_t u_k^n = \frac{u_k^{n+1} - u_k^n}{\tau} \quad (6)$$

to approximate the temporal derivative  $u_t(x_k, t_{n+\frac{1}{2}})$ . The resulting dominant truncation error is  $\frac{\tau^2}{24} (u_{tt})_k^{n+\frac{1}{2}}$ .

Substituting the Formula (6) to (5) results in the full discretization

$$i\delta_t u_k^n = -\delta_x^4 u_k^{n+\frac{1}{2}} - 2\rho u_k^{n+\frac{1}{2}}, \quad k = 1, 2, \dots, N. \quad (7)$$

The resulting dominant truncation error is  $R_k^n = \frac{\tau^2}{24}u_{ttt} + \frac{h^4}{240}(7 - 26\alpha)u_{x^8}$ . The Richardson extrapolation

method can be used to improve the scheme (7). We adopt the following formula

$$U_k^n = a_1 u_k^{nj_1} + a_2 \bar{u}_k^{nj_2} + a_3 \tilde{u}_k^{nj_3}, \tag{8}$$

where  $u_k^{nj_1}, \bar{u}_k^{nj_2}, \tilde{u}_k^{nj_3}$  are the solutions of (7) with temporal step-sizes  $\tau/j_1, \tau/j_2, \tau/j_3$ , respectively. To approximate (1) with fourth order in both time and space, the parameters should satisfy the constraints

$$\sum_{m=1}^3 a_m = 1, \sum_{m=1}^3 a_m j_m^{-2} = \sum_{m=1}^3 a_m j_m^{-3} = 0.$$

Clearly, if the scheme (7) has the discrete invariants, the extrapolations (8) are numerical stable. In our numerical example, we use two kinds of parameters:

$$j_n = n, a_1 = 1/12, a_2 = -4/3, a_3 = 9/4; j_n = 2^{n-1}, a_1 = 1/21, a_2 = -4/7, a_3 = 32/21.$$

### 2.3. Stability Analysis

Now we consider the stability of (8), which comes from that of (7). According to the Fourier analysis, assume the formal wave solution of (7) is  $u_k^n = v^n e^{ik\beta h}$  with wave number  $\beta$  and stability factor  $v$ . First we can derive

$$\delta_x^4 u_k = \mu u_k, \quad \mu = \frac{4(w-1)^2(3a+2b+bw)}{3h^4(1+2\alpha w)}, \quad w = \cos \beta h. \tag{9}$$

Next, with (7) and (9), we obtain

$$|v| = \left| \frac{2i - \mu\tau - 2\rho\tau}{2i + \mu\tau + 2\rho\tau} \right| = 1, \quad \forall \tau, h.$$

Therefore, the scheme (7) is unconditionally stable. Moreover, by its symmetry, it is non-dissipative.

### 3. Invariants Analysis

**Theorem 1.** Let  $\|u^n\|_2^2 = h \sum_k |u_k^n|^2$ . Then  $\|u^n\|_2^2$  is the discrete norm invariant of the scheme (7), which implies the discrete norm conservation law of (1).

**Proof.** Let  $c_0 = 16b + 36a$ ,  $c_1 = -9b - 24a$ . Denote two symmetric and cyclic matrices by

$$A = \begin{pmatrix} 1 & \alpha & 0 & \dots & \dots & 0 & \alpha \\ \alpha & 1 & \alpha & 0 & \dots & \vdots & 0 \\ 0 & \alpha & 1 & \alpha & 0 & \vdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \dots & \ddots & \alpha & 1 & \alpha & 0 \\ 0 & \dots & \dots & 0 & \alpha & 1 & \alpha \\ \alpha & 0 & \dots & \dots & 0 & \alpha & 1 \end{pmatrix}, \quad B = \begin{pmatrix} c_0 & c_1 & 6a & b & 0 & \dots & \dots & 0 & b & 6a & c_1 \\ c_1 & c_0 & c_1 & 6a & b & 0 & \dots & \dots & 0 & b & 6a \\ 6a & c_1 & c_0 & c_1 & 6a & b & 0 & \dots & \dots & 0 & b \\ b & 6a & c_1 & c_0 & c_1 & 6a & b & 0 & \dots & \dots & 0 \\ 0 & b & 6a & c_1 & c_0 & c_1 & 6a & b & 0 & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & 0 & b & 6a & c_1 & c_0 & c_1 & 6a & b & 0 \\ 0 & \dots & \dots & 0 & b & 6a & c_1 & c_0 & c_1 & 6a & b \\ b & 0 & \dots & \dots & 0 & b & 6a & c_1 & c_0 & c_1 & 6a \\ 6a & b & 0 & \dots & \dots & 0 & b & 6a & c_1 & c_0 & c_1 \\ c_1 & 6a & b & 0 & \dots & \dots & 0 & b & 6a & c_1 & c_0 \end{pmatrix}.$$

Then the matrix form of (4) is

$$\delta_x^4 u^n = A^{-1} B u^n. \tag{10}$$

Correspondingly, (7) can be written as

$$u^{n+1} = H_1^{-1} H_2 u^n, \quad H_1 = (1 - i\tau\rho)I_N - \frac{i\tau}{2}A^{-1}B, \quad H_2 = (1 + i\tau\rho)I_N + \frac{i\tau}{2}A^{-1}B. \quad (11)$$

The Equation (11) implies  $\|u^{n+1}\|_2 \leq \|H_1^{-1}H_2\|_2 \|u^n\|_2$ . According to the properties of  $A$  and  $B$ , we can see that  $H_1$  and  $H_2$  are symmetric and their eigenvalues are  $\lambda(H_1) = 1 - i\tau\rho - \frac{i\tau}{2}\lambda(A^{-1}B)$ ,  $\lambda(H_2) = 1 + i\tau\rho + \frac{i\tau}{2}\lambda(A^{-1}B)$ , respectively. Therefore This implies that  $\lambda(H_1^{-1}H_2) = 1$ ,  $\|H_1^{-1}H_2\|_2 = 1$ . Similarly, from  $u^n = H_2^{-1}H_1 u^{n+1}$ , we can also get  $\|u^n\|_2 \leq \|u^{n+1}\|_2$ . This completes the proof.

In fact, we have another proof. Multiplying (7) by  $\overline{u_k^{n+1}}$  and summing over  $k$ , we obtain

$$0 = i \sum_k \left[ |u_k^{n+1}|^2 - |u_k^n|^2 \right] + \sum_k \left[ \overline{u_k^n} u_k^{n+1} + \overline{u_k^{n+1}} u_k^n + (c + 2\rho\tau) u_k^{n+1/2} \overline{u_k^{n+1/2}} \right], \quad (12)$$

where  $c = \tau A^{-1}B$ . By the symmetry of  $c$ , the second summation term of (12) is real, while the first term is purely imaginary, which implies  $\|u^n\|_2 = \|u^{n+1}\|_2$ .

**Theorem 2.** Denote

$$Cu^n = \frac{1}{2}(a_1 u_{k+1}^n + a_2 u_k^n), \quad a_1 = \sqrt{1+2\alpha} + \sqrt{1-2\alpha}, \quad a_2 = \sqrt{1+2\alpha} - \sqrt{1-2\alpha},$$

$$v_k^n = \frac{b}{3h^2}(u_{k+3}^n - u_k^n) + \frac{3b}{2h^2}(u_{k+1}^n - u_k^n) + \frac{a}{h^2}(u_{k+2}^n - 3u_{k+1}^n + 3u_k^n - u_{k-1}^n).$$

Then under the periodic boundary condition,  $E^n = \|v^n\|^2 + \rho \|Cu^n\|^2$  is discrete energy invariant of the scheme (7), which implies the discrete energy conservation law of (1).

**Proof.** Multiplying (7) by  $A$ , we get

$$A(u_k^{n+1} - u_k^n) = i\tau B u_k^{n+1/2} + i2\tau\rho A u_k^{n+1/2}. \quad (13)$$

Multiplying (13) by  $\overline{u_k^{n+1}} - \overline{u_k^n}$  and summing over  $k$ , we obtain

$$\begin{aligned} & \frac{i\tau}{2} \sum_k \left[ \overline{B u_k^{n+1}} u_k^{n+1} - \overline{B u_k^n} u_k^n \right] + i\tau\rho \sum_k \left[ \overline{A u_k^{n+1}} u_k^{n+1} - \overline{A u_k^n} u_k^n \right] \\ & + \frac{i\tau}{2} \sum_k \left[ \overline{B u_k^{n+1}} u_k^n - \overline{B u_k^n} u_k^{n+1} \right] + i\tau\rho \sum_k \left[ \overline{A u_k^{n+1}} u_k^n - \overline{A u_k^n} u_k^{n+1} \right] = \sum_k \left[ A(u_k^{n+1} - u_k^n) (\overline{u_k^{n+1}} - \overline{u_k^n}) \right]. \end{aligned} \quad (14)$$

The first two summation terms in above equality are purely imaginary, while the last three summation terms are real. Moreover,

$$\sum_k \left[ \overline{A u_k^n} u_k^n \right] = \sum_k \left[ \overline{C u_k^n} C u_k^n \right], \quad \sum_k \left[ \overline{B u_k^n} u_k^n \right] = - \sum_k \left[ \overline{v_k^n} v_k^n \right].$$

Therefore, taking the imaginary parts of (14) we can get  $E^n = E^{n+1}$ .

## 4. Numerical Result

Denote the schemes (7) with sixth-order and fourth-order in space by CT6 and CT4, respectively. Denote the extrapolation schemes (8) with  $j_n = n$  and  $j_n = 2^{n-1}$  by RE1 and RE2, respectively. By applying fixed  $h$  and different  $\tau$ , we verify the temporal accuracy of the schemes. While the spacial accuracy can be verified by fixed  $\tau$  and different  $h$ . We also investigate the two discrete invariants of the schemes.

We use the above schemes to solve the linear Schrödinger equation with periodic boundary condition

$$iu_t + u_{x^4} + u = 0, u(x, 0) = 4(\sin x + \cos x), x \in [0, 2\pi], t > 0.$$

Its exact solution is  $u(x, t) = 4e^{2it}(\sin x + \cos x)$ .

**Table 1** lists the numerical results of scheme RE1 combined with CT6 at  $t = 3$ . It conforms that the scheme is convergent with fourth-order in time. **Table 2** lists the numerical results of scheme CT6 at  $t = 1$ . We can see that scheme CT6 is convergent with sixth-order in space with respect to the  $l^2$  norm and  $l^\infty$  norm.

**Table 3** lists the numerical results of scheme CT4 at  $t = 1$ . We can see that scheme CT4 is convergent with fourth-order in space. **Table 4** lists the numerical results of scheme RE2 combined with CT4 at  $t = 1.5$ . It conforms that the scheme is convergent with fourth-order in time.

**Figure 1** and **Figure 2** plot the residuals of discrete invariants of scheme CT6 and scheme CT4, respectively.

In the two figures, we depict the residuals of norm and energy of numerical solutions with  $h = \pi/10$  and  $\tau = 0.01$ , respectively. From the figures, we can see that the two schemes preserve two discrete conservation laws. **Figure 3** and **Figure 4** plot the residuals of discrete invariants of scheme RE1 combined with scheme CT6 and scheme RE2 combined with scheme CT4, respectively. In the two figures, we depict the residuals of norm and energy of numerical solutions with  $h = \pi/10$  and  $\tau = 0.003$ , respectively.

The figures tell us that the two methods preserve two discrete conservation laws too.

The compact extrapolation schemes established in this paper have some advantages such as compactness,

**Table 1.** Temporal order test of scheme RE1 combined with scheme CT6 with  $h = \pi/50$ .

$\tau$	$\ e\ _\infty$	order	$\ e\ _2$	order
0.06	8.69301e-7	-	2.0904e-6	-
0.03	5.4126e-8	4.0055	1.3108e-7	3.9953
0.015	3.3449e-9	4.0163	7.9238e-9	4.0481

**Table 2.** Spatial order test of scheme CT6 with  $\tau = 1/10000$ .

$h$	$\ e\ _\infty$	order	$\ e\ _2$	order
$\pi/5$	2.7893e-6	-	5.1073e-6	-
$\pi/10$	4.2397e-8	6.0389	7.7631e-8	6.0389
$\pi/20$	6.7532e-10	5.9722	1.2214e-9	5.9900

**Table 3.** Spatial order test of scheme CT4 with  $\tau = 1/10000$ .

$h$	$\ e\ _\infty$	order	$\ e\ _2$	order
$\pi/5$	3.0164e-4	-	5.9528e-4	-
$\pi/10$	1.7599e-5	4.0993	3.4732e-5	4.0992
$\pi/20$	1.1023e-6	3.9969	2.1487e-6	4.0147

**Table 4.** Temporal order test of scheme RE2 combined with scheme CT4 with  $h = \pi/100$ .

$\tau$	$\ e\ _\infty$	order	$\ e\ _2$	order
0.06	2.1526e-7	-	4.4798e-7	-
0.03	1.1942e-8	4.1720	2.5879e-8	4.1136
0.015	6.9185e-10	4.1094	1.1823e-9	4.2521

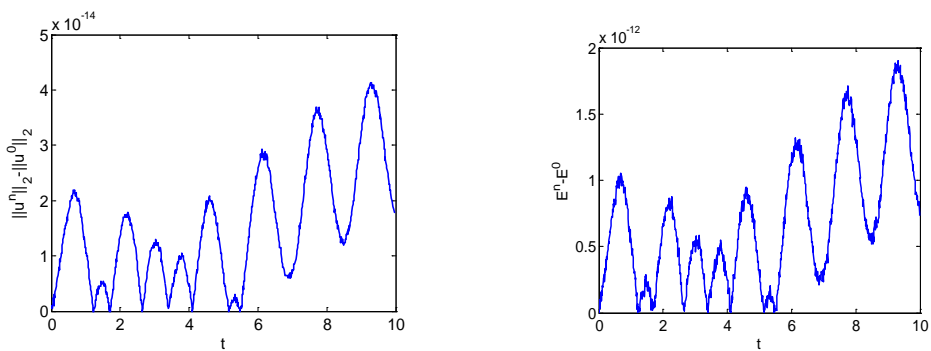


Figure 1. Residuals of norm and energy by scheme CT6 with  $h = \pi/10, \tau = 0.01$ .

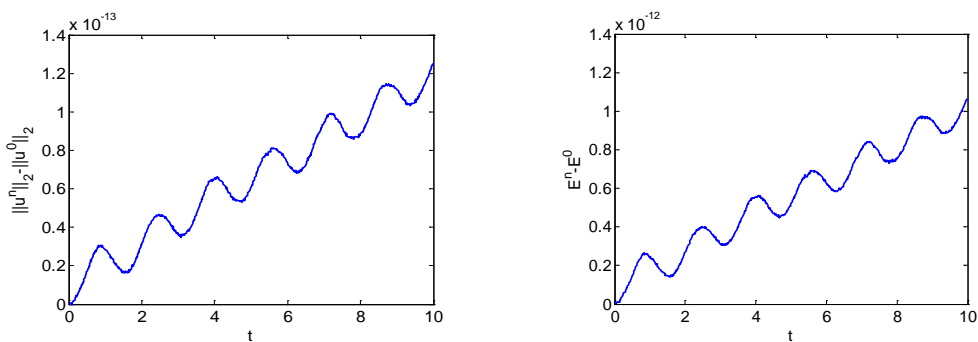


Figure 2. Residuals of norm and energy by scheme CT4 with  $h = \pi/10, \tau = 0.01$ .

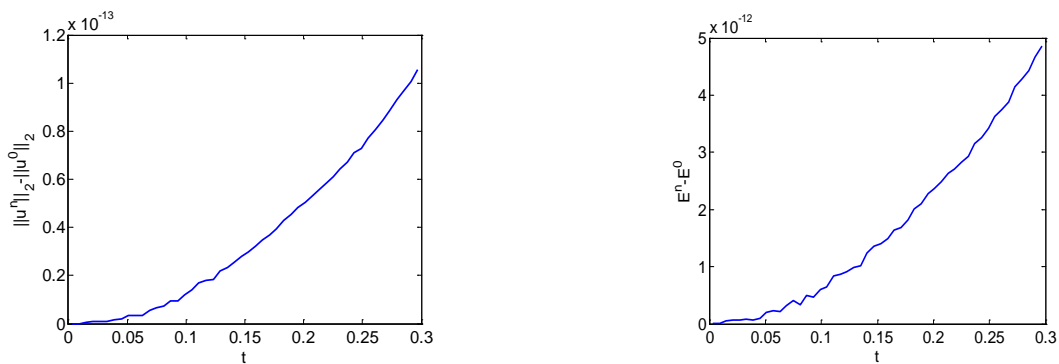


Figure 3. Residuals of norm and energy by scheme RE1 combined with scheme CT6 with  $h = \pi/10, \tau = 0.003$ .

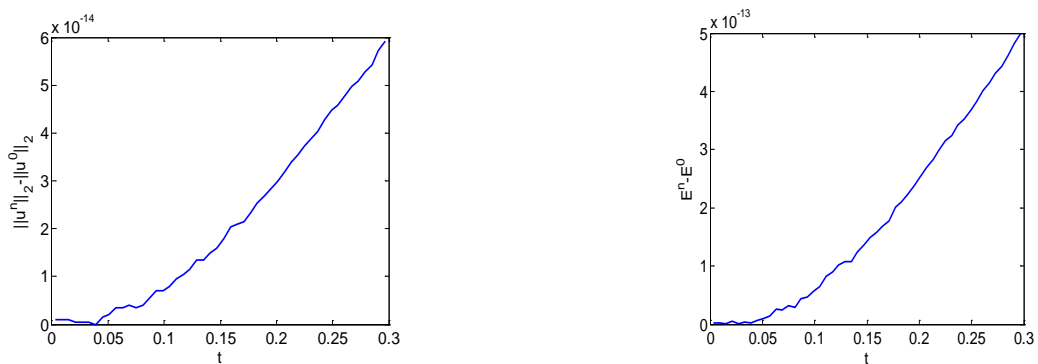


Figure 4. Residuals of norm and energy by scheme RE2 combined with scheme CT4 with  $h = \pi/10, \tau = 0.003$ .

high accuracy, less memory and less computational cost. The schemes are also stable, non-dissipative and conservative with respect to the charge and energy conservation laws. We can generalize the methods to other kind of PDEs.

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