J. Math. Study
doi: 10.4208/jms.v48n1.15.03

Vol. **48**, No. 1, pp. 30-52
March 2015

Sixth-order Compact Extended Trapezoidal Rules for 2D Schrödinger Equation

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Received 30 November, 2014; Accepted (in revised version) 15 January, 2015

Abstract. Based on high-order linear multistep methods (LMMs), we use the class of extended trapezoidal rules (ETRs) to solve boundary value problems of ordinary differential equations (ODEs), whose numerical solutions can be approximated by boundary value methods (BVMs). Then we combine this technique with fourth-order Padé compact approximation to discrete 2D Schrödinger equation. We propose a scheme with sixth-order accuracy in time and fourth-order accuracy in space. It is unconditionally stable due to the favourable property of BVMs and ETRs. Furthermore, with Richardson extrapolation, we can increase the scheme to order 6 accuracy both in time and space. Numerical results are presented to illustrate the accuracy of our scheme.

AMS subject classifications: 65M06, 65M12, 65M15

Key words: Schrödinger equation, BVMs, ETRs, compact scheme, Richardson extrapolation.

1 Introduction

We concern ourselves with a high accurate numerical scheme for the following 2D Schrödinger equation with initial and Dirichlet boundary conditions:

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$$\begin{cases} -iu_t = u_{xx}+u_{yy}+\omega(x,y)u, & (x,y,t)\in[a,b]\times[a,b]\times[0,T], \\ u(x,y,0)=\varphi(x,y), \\ u(x,a,t)=\psi_1(x,t), \quad u(x,b,t)=\psi_2(x,t), & t\geq 0, \\ u(a,y,t)=\psi_3(y,t), \quad u(b,y,t)=\psi_4(y,t), & t\geq 0, \end{cases} \tag{1.1}$$

where $u(x,y,t)$ is the complex-valued wave function in continuous domain and $\omega(x,y)$ is an arbitrary potential function and $i=\sqrt{-1}$.

Early in 2006, an implicit semi-discrete compact scheme with convergence order $O(\tau^2 + h^4)$ was proposed by Kalita et. al. in [13]. However, there was no stability analysis of the scheme. Based on new type of discrete energy techniques for stability, Sun [21] and Liao et. al. [14] presented a fully discrete scheme with same order as the one in [13] in maximum norm, and raised the convergence order to $O(\tau^4+h^4)$ by Richardson extrapolation. Later, Liao et. al. [15] presented a stable compact ADI scheme resulting in a tri-diagonal linear system, which has advantages on the computational efficiency of multi-dimensional schemes over another high-order compact ADI (HOC-ADI) method proposed in [23]. In 2012, Xu et. al. [24] generalized this method to linear and nonlinear Schrödinger equations and unconditional stability could be obtained via Fourier analysis. Guo et. al. in [11] established a compact stable ADI scheme and considered also the stability by the discrete energy technique for both linear and nonlinear Schrödinger equations. The convergence order is only $O(\tau^2+h^4)$.

Another idea for the numerical approximation of Schrödinger equation is to use BVMs (boundary value methods) (See, e.g., in [1,3,4,6–9,19]). In 2003, Sun et. al. in [20] proposed a method by combining fourth-order BVMs with fourth-order compact difference scheme for solving one-dimensional heat equation. Then, Dehghan et. al. analogously developed methods by applying fourth-order compact scheme for space approximation and fourth-order BVMs for time integration [10,17]. By applying these methods to 2D Schrödinger equations, fourth-order schemes were obtained. Nevertheless, higher order BVMs and stability analysis could not be derived naturally from above work.

Based on high-order LMMs (linear multistep methods), a class of ETRs (extended trapezoidal rules) will be modified and employed to solve the ODEs in this paper. Actually we will develop a scheme with order $O(\tau^4+h^6)$. With the aid of Richardson extrapolation, the order will be increased to $O(\tau^6+h^6)$. By applying implicit Adams techniques to impose the initial and final conditions, we construct ETRs with various orders, and strengthen the stability of the ETRs approximations. In the meantime, we pointed out an unsuitable application of TOMs (top order methods) in [6].

The paper is organized as follows. In Section 2, the basic theory and applications with stability analysis of the methods such as LMMs, BVMs, and ETRs are reviewed. Especially, ETRs with various orders are constructed. In Section 3, combining sixth-order ETRs with fourth-order compact scheme, a highly accurate scheme for 2D Schrödinger equation is proposed. In addition, Richardson extrapolation is addressed to increase the order of accuracy. In Section 4, numerical experiments are given to test convergence order of various ETRs. Finally some concluding remarks are given in Section 5.

2 Application and stability analysis for ETRS

In this section, we describe the underlying idea of BVMs with (k_1,k_2)-boundary conditions, introduced by Brugnano et. al. in [6,8], which are based on high-order LMMs. The symmetric ETRs can be obtained from BVMs with special $(\nu,\nu-1)$-boundary conditions by a class of Adams-Moulton methods. We will construct various ETRs with fixed-value orders. With the notations of Kronecker product, the application of ETRs on ODEs is presented to solve liner systems of equations.

2.1 Linear multistep formula and (k_1,k_2)-boundary conditions

For a well-conditioned first-order continuous problem

$$y'=f(t,y), \qquad t\in[t_0,T], \qquad y(t_0)=y_0, \tag{2.1}$$

it can be approximated by the following $k-$step linear multistep formula [6–8,18,22]:

$$\sum_{i=0}^{k}\alpha_i y_{n+i}=\tau\sum_{i=0}^{k}\beta_i f_{n+i}, \quad n=k_1,\cdots,N-1, \tag{2.2}$$

with partition

$$t_i=t_0+i\tau, \quad i=0,\cdots,N+k_2-1, \quad \tau=\frac{T-t_0}{N+k_2-1},$$

where y_{n+i} is the discrete approximation to $y(t_{n+i})$ and $f_{n+i}=f(t_{n+i},y_{n+i})$. Coefficients α_i and β_i are chosen so that the equation (2.2) has an indicated order.

As for the two natural numbers k_1 and k_2, $k_1+k_2=k$ in (2.2), the (k_1,k_2)-boundary conditions are used with $y_0,\cdots,y_{k_1-1}$, being given at the initial points, and $y_N,\cdots,y_{N+k_2-1}$, being given at the final points.

However, only the first one y_0 of such k_1 values is available since it is provided in (2.1). In order to obtain other quantities independent of those provided by LMF (2.2), we need additional k_1-1 initial equations and k_2 final equations.

Here we give k_1-1 initial equations

$$\sum_{i=0}^{k}\alpha_i^r y_i=\tau\sum_{i=0}^{k}\beta_i^r f_i, \quad r=1,\cdots,k_1-1, \tag{2.3}$$

and k_2 final equations

$$\sum_{i=0}^{k}\alpha_i^r y_{N+k_2-1-i}=\tau\sum_{i=0}^{k}\beta_i^r f_{N+k_2-1-i}, \quad r=N,\cdots,N+k_2-1. \tag{2.4}$$

The step number of equation (2.3) and (2.4) is k. The coefficients $\{\alpha_i^r\}$ and $\{\beta_i^r\}$ should be chosen such that the truncation errors of these initial and final equations are of the same order as that in (2.2).

Remark 2.1. When $k_1 = k$, $k_2 = 0$, it reduces to the IVMs (initial value methods) (See, in [1,3,6–8]), which suffer from heavy theoretical limitations, and which are summarized by the two well-known Dahlquist barriers.

2.2 Modified ETRS

The explicit method *Adams-Bashforth* and the implicit method *Adams-Moulton* are two well-known forms of methods [18,19,22]. For instance, the Adams-Moulton formula is as follows:

$$y_n - y_{n-1} = \tau \sum_{i=0}^{k} \beta_i f_{n-i}, \qquad n = k, \cdots. \tag{2.5}$$

Along with reverse Adams methods [2], Amodio et al. [1] developed ETRs which are linear multistep methods with same numbers of initial and finial additional conditions. Combining with $(\nu,\nu-1)$-boundary conditions, we provide ETRs the initial and finial equations by using the reverse Adams implicit method and the Adams-Moulton respectively. Numerical solutions of (2.2) can be approximated by the following various forms of ETRs.

ETR1s: $\kappa = 0$ or 1. Different initial and final equations are used.

$$\begin{cases} y_n - y_{n-1} = \tau \sum\limits_{i=-\nu}^{\nu-1} \beta_{i+\nu} f_{n+i}, & n = \nu, \cdots, N-1, \\ y_r - y_{r-1} = \tau \sum\limits_{i=0}^{2\nu-2+\kappa} \beta_i^r f_i, & r = 1, \cdots, \nu-1, \\ y_r - y_{r-1} = \tau \sum\limits_{i=N-(\nu+\kappa)}^{N+\nu-2} \beta_{i-N+\nu+\kappa}^r f_i, & r = N, \cdots, N+\nu-2. \end{cases} \tag{2.6}$$

ETR2s: They are from [9] but modified. Initial and final conditions are provided by Adams-Moulton.

$$\begin{cases} \sum\limits_{i=-\nu}^{\nu-1} \alpha_{i+\nu} y_{n+i} = \dfrac{\tau}{2}(f_n + f_{n-1}), & n = \nu, \cdots, N-1, \\ \sum\limits_{i=0}^{2\nu-1} \alpha_i^r y_i = \dfrac{\tau}{2}(f_r + f_{r-1}), & r = 1, \cdots, \nu-1, \\ \sum\limits_{i=N-\nu-1}^{N+\nu-2} \alpha_{i-N+\nu+1}^r y_i = \dfrac{\tau}{2}(f_r + f_{r-1}), & r = N, \cdots, N+\nu-2, \end{cases} \tag{2.7}$$

TOMs: They are from [6,8] but modified. Initial and final conditions are provided by Adams-Moulton combining with $(\nu,\nu-1)$-boundary conditions.

$$\begin{cases} \sum_{i=-\nu}^{\nu-1} \alpha_{i+\nu} y_{n+i} = \tau \sum_{i=-\nu}^{\nu-1} \beta_{i+\nu} f_{n+i}, & n=\nu,\cdots,N-1. \\ y_r - y_{r-1} = \tau \sum_{i=0}^{2k-2} \beta_i^r f_i, & r=1,\cdots,\nu-1, \\ y_r - y_{r-1} = \tau \sum_{i=0}^{2k-2} \beta_i^r f_{N+\nu-2-i}, & r=N,\cdots,N+\nu-2. \end{cases} \tag{2.8}$$

The coefficients in ETR1s, ETR2s and TOMs are given in accordance with the following requirements.

- $\{\beta_i\},\{\alpha_i\}$ are determined such that the maximum order of ETRs is $O(\tau^{k+1})$, and that of TOMs is $O(\tau^{2k})$.
- $\{\beta_i^r\},\{\alpha_i^r\}$ in ETRs are determined such that the truncation error of the imposing initial and final equations are $O(\tau^{k+1})$.
- $\{\beta_i^r\}$ in TOMs are determined such that the truncation error of the imposing initial and final equations are at least $O(\tau^{2k-1})$.

In addtion, Tables 1 and 2 show the values of coefficients $\{\beta_i\},\{\alpha_i\}$. For convenience, we take $\beta_i=\beta_i/\eta_k,\alpha_i=\alpha_i/\eta_k$.

Remark 2.2. The above ETRs and TOMs methods with $(\nu,\nu-1)$-boundary conditions have the following properties [1,8].

(1) When $\nu=1$, they reduce to the trapezoidal rule.

(2) When $\nu\geq 1$, the number of steps is odd, $k=2\nu-1$.

(3) Coefficients $\{\beta_i\}$ are symmetric, i.e., $\beta_i=\beta_{k-i}, \quad i=0,\cdots,k$.

(4) Coefficients $\{\alpha_i\}$ are skew-symmetric, i.e., $\alpha_i=-\alpha_{k-i}, \quad i=0,\cdots,k$.

2.3 Stability

For relevant stability analysis of LMMs, we consider the following definitions. Quinney basically gave in [19] the notions of zero stability or Dahlquist-stability, relative stability, and A-stability. Amodio et. al. in [1–3, 16] used with BVMs the notions of BV zero-stability, BV-stability, and ABV-stability. Brugnano et. al. in [6–8] gave different explanations of zero-stability and A-stability generalized from the notions of Schur and von Neumann polynomials.

Table 1: Coefficients of ETR1s ([1,8]).

k	ν	η_k	β_0	β_1	β_2	β_3	β_4
1	1	2	1				
3	2	24	-1	13			
5	3	1440	11	-93	802		
7	4	120960	-191	1879	-9531	68323	
9	5	7257600	2479	-28939	162680	-641776	4134338

Table 2: Coefficients of ETR2s ([8]).

k	ν	η_k	α_0	α_1	α_2	α_3	α_4
1	1	1	-1				
3	2	12	-1	-9			
5	3	120	1	-15	-80		
7	4	840	-1	14	-126	-525	
9	5	5040	1	-15	120	-840	-3024

The stability analysis of ETRs used with $(\nu,\nu-1)$-boundary conditions reads as follows.

Theorem 2.1. ([1]) *The $(2\nu-1)-$step ETRs are BV-zero stable and BV-A-stable. The BV-stability domain of the methods is the negative complex half-plane.*

As for TOMs with $(\nu,\nu-1)$-boundary conditions mentioned above, we point out one catastrophic instability examples of order 6, i.e., $k=3$ and $\nu=2$. From (2.8), the corresponding coefficients can be obtained by Taylor expansion with truncation error at least 5,

$$11y_{n+1}+27y_n+27y_{n-1}-11y_{n-2}=3\tau[f_{n+1}+9f_n+9f_{n-1}+f_{n-2}].$$

Please see [19] for details of instability. In fact, the 3-step method is always unstable. There is a restriction on the accuracy which can be obtained for any value of k.

Theorem 2.2. ([19]) *The order of a stable odd $k-$step method is at most $k+1$.*

Theorem 2.3. ([19]) *The order of a stable even $k-$step method is at most $k+2$.*

Theorem 2.2 implies that the order of the above example is less than or equal to 4 for being stable.

Remark 2.3. Brugnano et. al. gave in [6,8] numerical examples approximated by fourth-order ETR1 and sixth-order TOM. Due to above theorems, we know that the sixth-order TOM is catastrophically unstable except that the order is less than or equal to 4. So it is clear that there may be some unsuitable applications of TOMs in [6].

2.4 Special ETRs

Five specific forms of ETRs with fixed orders are constructed from the general form of ETRs in Section 2.2. They are listed here in order to be used for implementation in Section 4.

Fourth-order ETR1 ($\nu=2$, $k=3$ and $\kappa=1$). Derived from (2.6):

$$\begin{cases} y_n-y_{n-1}=\dfrac{\tau}{24}(-f_{n-2}+13f_{n-1}+13f_n-f_{n-1}), \quad n=2,\cdots,N-1, \\ y_1-y_0=\dfrac{\tau}{24}(9f_0+19f_1-5f_2+f_3), \\ y_N-y_{N-1}=\dfrac{\tau}{24}(f_{N-3}-5f_{N-2}+19f_{N-1}+9f_N). \end{cases} \tag{2.9}$$

Another form of fourth-order ETR1 ($\kappa=0$). Derived form (2.6):

$$\begin{cases} y_n-y_{n-1}=\dfrac{\tau}{24}(-f_{n-2}+13f_{n-1}+13f_n-f_{n-1}), \quad n=2,\cdots,N-1, \\ y_1-y_0=\dfrac{\tau}{12}(5f_0+8f_1-f_2), \\ y_N-y_{N-1}=\dfrac{\tau}{24}(-f_{N-2}+8f_{N-1}+5f_N). \end{cases} \tag{2.10}$$

Sixth-order ETR1 ($\nu=3$, $k=5$ and $\kappa=1$). Derived form (2.6) with 4 additional equations:

$$\begin{cases} y_n-y_{n-1}=\dfrac{\tau}{1440}(11f_{n-3}-93f_{n-2}+802f_{n-1}+802f_n-93f_{n+1}+11f_{n+2}), \\ \qquad\qquad\qquad\qquad\qquad\qquad n=3,\cdots,N-1, \\ y_1-y_0=\dfrac{\tau}{720}(251f_0+646f_1-264f_2+106f_3-19f_4), \\ y_2-y_1=\dfrac{\tau}{720}(-19f_0+346f_1+456f_2-74f_3+11f_4), \\ y_N-y_{N-1}=\dfrac{\tau}{720}(11f_{N-3}-74f_{N-2}+456f_{N-1}+346f_N-19f_{N+1}), \\ y_{N+1}-y_N=\dfrac{\tau}{720}(-19f_{N-3}+106f_{N-2}-264f_{N-1}+646f_N+251f_{N+1}). \end{cases} \tag{2.11}$$

Fourth-order ETR2 ($\nu=2$, $k=3$). Derived from (2.7) with 2 additional equations:

$$\begin{cases} \dfrac{1}{12}(-y_{n-2}-9y_{n-1}+9y_n+y_{n+1})=\dfrac{\tau}{2}(f_{n-1}+f_n), \quad n=2,\cdots,N-1, \\ \dfrac{1}{12}(-13y_0+15y_1-3y_2+y_3)=\dfrac{\tau}{2}(f_0+f_1), \\ \dfrac{1}{12}(-y_{N-3}+3y_{N-2}-15y_{N-1}+13y_N)=\dfrac{\tau}{2}(f_{N-1}+f_N). \end{cases} \tag{2.12}$$

Sixth-order ETR2 ($\nu = 3$, $k = 5$). Derived from (2.7) with 4 additional equations:

$$\begin{cases} \frac{1}{120}(y_{n-3}-15y_{n-2}-80y_{n-1}+80y_n+15y_{n+1}-y_{n+2})=\frac{\tau}{2}(f_{n-1}+f_n), \; n=3,\dots,N-1, \\ \frac{1}{120}(-149y_0+235y_1-180y_2+140y_3-55y_4+9y_5)=\frac{\tau}{2}(f_0+f_1), \\ \frac{1}{120}(-9y_0-95y_1+100y_2+0y_3+5y_4-1y_5)=\frac{\tau}{2}(f_1+f_2), \\ \frac{1}{120}(1y_{N-4}-5y_{N-3}+0y_{N-2}-100y_{N-1}+95y_N+9y_{N+1})=\frac{\tau}{2}(f_N+f_{N-1}), \\ \frac{1}{120}(-9y_{N-4}+55y_{N-3}-140y_{N-2}+180y_{N-1}-235y_N+149y_{N+1})=\frac{\tau}{2}(f_{N+1}+f_N). \end{cases} \tag{2.13}$$

Remark 2.4. The following is the fourth-order ETR2 ($\nu = 2$, $k = 3$)used in [10,17,20] which is different from our fourth-order ETR2 (2.12).

$$\begin{cases} \frac{1}{12}(-y_{n-2}-9y_{n-1}+9y_n+y_{n+1})=\frac{\tau}{2}(f_{n-1}+f_n), \quad n=2,\cdots,N-1, \\ \frac{1}{24}(-17y_0+9y_1+9y_2-y_3)=\frac{\tau}{4}(f_0+3f_1), \\ \frac{1}{24}(y_{N-3}-9y_{N-2}-9y_{N-1}+17y_N)=\frac{\tau}{4}(3f_{N-1}+f_N). \end{cases} \tag{2.14}$$

2.5 Applications to ODEs

The basic ODE of (2.1) can be numerically approximated by ETRs. See, for example, in [10,17,20], the fourth-order ETR2 (2.14) applies.

Now, let us apply the sixth-order ETR1 (2.11) to solve ODE (2.1). We approximate (2.1) with $N+1$ equations in form $A_e y_e = \tau B_e f_e(t_e, y_e)$, where $t_e, y_e \in \mathbb{R}^{N+1}$, $A_e, B_e \in \mathbb{R}^{(N+1)\times(N+2)}$, and $f_e = (f_0, f_1, \cdots, f_N, f_{N+1})^T$. Using partitions $A_e = [a_0, A]$ and $B_e = [b_0, B]$, where a_0 is the first column of A_e, and b_0 is the first column of B_e, we get a linear system for unknowns $y \in \mathbb{R}^{N+1}$,

$$\begin{cases} Ay = \tau B f(t,y) + \bar{g}_0, \\ \bar{g}_0 = -a_0 y_0 + \tau b_0 f(t_0, y_0), \end{cases}$$

where $\bar{g}_0$ contains the initial information. From sixth-order ETR1 (2.11), the matrices A, B, a_0 and b_0 can be explicitly given as follows:

$$A=\begin{pmatrix} 1 & & & & & \\ -1 & 1 & & & & \\ & -1 & \ddots & & & \\ & & \ddots & \ddots & & \\ & & & \ddots & \ddots & \\ & & & & -1 & 1 \end{pmatrix}_{(N+1)\times(N+1)}$$

$$B=\begin{pmatrix} \frac{646}{720} & \frac{-264}{720} & \frac{106}{720} & \frac{-19}{720} & & & & \\ \frac{346}{720} & \frac{456}{720} & \frac{-74}{720} & \frac{11}{720} & & & & \\ \frac{-93}{1440} & \frac{802}{1440} & \frac{802}{1440} & \frac{-93}{1440} & \frac{11}{1440} & & & \\ \frac{11}{1440} & \frac{-93}{1440} & \frac{802}{1440} & \frac{802}{1440} & \frac{-93}{1440} & \frac{11}{1440} & & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & & \frac{11}{1440} & \frac{-93}{1440} & \frac{802}{1440} & \frac{802}{1440} & \frac{-93}{1440} & \frac{11}{1440} \\ & & & \frac{11}{720} & \frac{-74}{720} & \frac{456}{720} & \frac{346}{720} & \frac{-19}{720} \\ & & & \frac{-19}{720} & \frac{106}{720} & \frac{-264}{720} & \frac{646}{720} & \frac{251}{720} \end{pmatrix}_{(N+1)\times(N+1)}$$

$a_0=[-1,0,\ldots,0]^T_{1\times(N+1)}, \quad b_0=\left[\frac{251}{720},\frac{-19}{720},\frac{11}{1440},0,\ldots,0\right]^T_{1\times(N+1)}.$

As for a linear system of ODEs, i.e.,

$$\dot{y}(t)=B_x y(t)+g(t), \qquad y(0)=y_0, \qquad t\geq 0, \tag{2.15}$$

where $y(t)=[y_1(t),\ldots,y_n(t)]^T$, $g(t)=[g_1(t),\ldots,g_n(t)]^T$, and B_x is an $n\times n$ matrix. Then the sixth-order ETR1 for (2.15) can be written as

$$(A\otimes I_n-\tau B\otimes B_x)y=\tau(B\otimes I_n)g+\tau(b_0\otimes(B_x y_0+g_0))-a_0\otimes y_0, \tag{2.16}$$

where $\otimes$ indicates Kronecker product, I_n is an $n\times n$ identity, $g_0=g(t_0)$, and

$$y\approx[y_1(t_1),\ldots,y_n(t_1),y_1(t_2),\ldots,y_n(t_2),\ldots,y_1(t_{N+1}),\ldots,y_n(t_{N+1})]^T,$$

$$g=[g_1(t_1),\ldots,g_n(t_1),g_1(t_2),\ldots,g_n(t_2),\ldots,g_1(t_{N+1}),\ldots,g_n(t_{N+1})]^T.$$

If we rewrite problem (2.15) into a more complicated form, i.e.,

$$A_x\dot{y}(t)=B_x y(t)+g(t), \qquad y(0)=y_0, \qquad t\geq 0, \tag{2.17}$$

where A_x is an $n\times n$ nonsingular matrix, then the relevant linear system of equations with Kronecker product matrix [9,12] should be

$$(A\otimes A_x-\tau B\otimes B_x)y=\tau(B\otimes I_n)g+\tau(b_0\otimes(B_x y_0+g_0))-a_0\otimes A_x y_0. \tag{2.18}$$

In special 2D case of (2.17), we have

$$A_{xy}\dot{y}(t)=B_{xy}y(t)+g(t), \qquad y(0)=y_0, \qquad t\geq 0, \tag{2.19}$$

$$(A\otimes A_{xy}-\tau B\otimes B_{xy})y=\tau(B\otimes I_{n^2})g+\tau(b_0\otimes(B_{xy}y_0+g_0))-a_0\otimes A_{xy}y_0, \tag{2.20}$$

where A_{xy}, B_{xy} are $n^2\times n^2$ nonsingular matrices, and I_{n^2} is an $n^2\times n^2$ identity.

Remark 2.5. If we consider to use the fourth-order ETRs to approximate ODE, then it will be simpler. As a matter of fact, we will get a linear system for unknowns $y\in\mathbb{R}^N$.

3 Compact difference scheme combined with ETRs

In this section we need the fourth-order Padé approximation for space discretization of Shrödinger equation (1.1). The sixth-order ETR1 (2.11) on the compact scheme is implemented and a scheme with sixth-order accuracy in time and fourth-order accuracy in space is constructed. Richardson extrapolation will be incorporated with the scheme to get it with sixth-order accuracy in space and in time.

3.1 Compact difference scheme

Let n and N be two positive integers and $h=\frac{b-a}{n}$, $\tau=\frac{T}{N+1}$. Denote

$$x_r=a+rh,\ y_j=a+jh, \quad r,j=0,1,\dots,n,$$
$$t_k=k\tau, \quad k=0,1,\dots,N+1.$$

Shrödinger equation (1.1) can be rewritten as

$$-i\frac{\partial u}{\partial t}(x,y,t)-\omega(x,y)u(x,y,t)=\frac{\partial^2 u}{\partial x^2}(x,y,t)+\frac{\partial^2 u}{\partial y^2}(x,y,t). \tag{3.1}$$

Let us denote

$$Q(x,y,t)=\frac{\partial^2 u}{\partial x^2}(x,y,t)+\frac{\partial^2 u}{\partial y^2}(x,y,t), \tag{3.2}$$

and introduce the second-order central difference operators,

$$\delta_x^2 u_{r,j}=\frac{u_{r+1,j}-2u_{r,j}+u_{r-1,j}}{h^2}, \qquad \delta_y^2 u_{r,j}=\frac{u_{r,j+1}-2u_{r,j}+u_{r,j-1}}{h^2}.$$

At any point (x_r,y_j,t), the space discretization with respect to x and y leads to

$$\delta_x^2 u_{r,j}(t)+\delta_y^2 u_{r,j}(t)-R_{r,j}(t)=Q_{r,j}(t), \tag{3.3}$$

where $u_{r,j}(t)\approx u(x_r,y_j,t)$, $Q_{r,j}(t)=Q(x_r,y_j,t)$, and the truncation error $R_{r,j}(t)$ is

$$R_{r,j}(t)=\frac{h^2}{12}\left(\frac{\partial^4 u}{\partial x^4}+\frac{\partial^4 u}{\partial y^4}\right)_{r,j}+\frac{h^4}{360}\left(\frac{\partial^6 u}{\partial x^6}+\frac{\partial^6 u}{\partial y^6}\right)_{r,j}+O(h^6). \tag{3.4}$$

According to the approximation in [10, 17], the fourth-order partial derivatives of u are as follows:

$$\left(\frac{\partial^4 u}{\partial x^4}\right)_{r,j}=\left(\frac{\partial^2 Q}{\partial x^2}-\frac{\partial^4 u}{\partial x^2\partial y^2}\right)_{r,j},\quad \left(\frac{\partial^4 u}{\partial y^4}\right)_{r,j}=\left(\frac{\partial^2 Q}{\partial y^2}-\frac{\partial^4 u}{\partial y^2\partial x^2}\right)_{r,j}. \tag{3.5}$$

If we replace the fourth-order partial derivatives of u in (3.4) with (3.5), and go back to (3.3), then we have

$$\left[\delta_x^2+\delta_y^2+\frac{h^2}{6}\delta_x^2\delta_y^2\right]u_{r,j}(t)=\left[1+\frac{h^2}{12}(\delta_x^2+\delta_y^2)\right]Q_{r,j}(t)+O(h^4)+O(h^6). \tag{3.6}$$

Thus, we obtain a fourth-order compact scheme in space for problem (3.1),

$$\begin{aligned}&\left[\delta_x^2+\delta_y^2+\frac{h^2}{6}\delta_x^2\delta_y^2\right]u_{r,j}(t) \\ =&-\left[1+\frac{h^2}{12}(\delta_x^2+\delta_y^2)\right](iu'_{r,j}(t)+\omega_{r,j}u_{r,j}(t))+O(h^4)+O(h^6),\end{aligned} \tag{3.7}$$

where $\omega_{r,j}=\omega(x_r,y_j)$ and $u'_{r,j}(t)=\frac{\partial u}{\partial t}(x_r,y_j,t)$.

Instead of using the approximation of $\delta_x^2(\omega_{r,j}u_{r,j})$,

$$\delta_x^2(\omega_{r,j}u_{r,j})=(\delta_x^2\omega_{r,j})u_{r,j}+2(\delta_x w_{r,j})(\delta_x u_{r,j})+\omega_{r,j}(\delta_x^2 u_{r,j}), \tag{3.8}$$

given in [10,13,17,23], we prefer to utilizing the approximation of $\delta_x^2(\omega_{r,j}u_{r,j})$

$$\delta_x^2(\omega_{r,j}u_{r,j})=(\omega_{r+1,j}u_{r+1,j}-2\omega_{r,j}u_{r,j}+\omega_{r-1,j}u_{r-1,j})/h^2,$$

which was provided by Tian et. al. in [23].

In a same way, the approximation of $\delta_y^2(\omega_{r,j}u_{r,j})$ can be derived, too.

3.2 Implementing ETRs on compact scheme

By cutting off the truncation errors, we obtain the fourth-order compact difference scheme (3.7) onto grid points.

$$\begin{aligned}&-i\left(4u'_{r,j}(t)+\frac{1}{2}u'_{r+1,j}(t)+\frac{1}{2}u'_{r-1,j}(t)+\frac{1}{2}u'_{r,j+1}(t)+\frac{1}{2}u'_{r,j-1}(t)\right)\\ =&\frac{1}{h^2}\big(4\left[u_{r+1,j}(t)+u_{r,j+1}(t)+u_{r-1,j}(t)+u_{r,j-1}(t)\right]\\ &\quad+\left[u_{r+1,j+1}(t)+u_{r-1,j+1}(t)+u_{r+1,j-1}(t)+u_{r-1,j-1}(t)\right]-20u_{r,j}(t)\big)+4\omega_{r,j}u_{r,j}(t)\\ &\quad+\frac{1}{2}\left[\omega_{r+1,j}(t)u_{r+1,j}(t)+\omega_{r-1,j}(t)u_{r-1,j}(t)+\omega_{r,j+1}(t)u_{r,j+1}(t)+\omega_{r,j-1}(t)u_{r,j-1}(t)\right].\end{aligned}$$

This scheme is essentially a linear system of ordinary differential equations,

$$\big(A_{xy}u(t)+c_1(t)\big)'=B_{xy}u(t)+c_2(t), \tag{3.9}$$

where $u(t),c_1(t),c_2(t)$ are vectors, and A_{xy},B_{xy} are matrices. Especially,

$$u(t)=[u_{1,1}(t),\dots,u_{1,n-1}(t),u_{2,1}(t),\dots,u_{2,n-1}(t),\dots,u_{n-1,1}(t),\dots,u_{n-1,n-1}(t)]^T_{1\times(n-1)^2},$$
$$A_{xy}=tri[A_1,A_2,A_3]_{(n-1)^2}, B_{xy}=tri[B_1,B_2,B_3]_{(n-1)^2}.$$

Here $tri[a_1,a_2,a_3]_{n-1}$ denotes an $(n-1)\times(n-1)$ tridiagonal matrix. Each row of this matrix contains the values a_1,a_2,a_3 on its subdiagonal, diagonal, superdiagonal respectively. Matrix I_{n-1} is an $(n-1)\times(n-1)$ identity. So,

$$\begin{aligned}
&A_1=-\frac{i}{2}I_{n-1},\quad A_2=-tri\left[\frac{i}{2},4i,\frac{i}{2}\right]_{n-1},\quad A_3=-\frac{i}{2}I_{n-1},\\
&B_1=\left[\frac{1}{h^2},\frac{4}{h^2}+\frac{1}{2}\omega_{r-1,j},\frac{1}{h^2}\right]_{n-1},\\
&B_2=\left[\frac{4}{h^2}+\frac{1}{2}\omega_{r,j-1},\frac{-20}{h^2}+4\omega_{r,j},\frac{4}{h^2}+\frac{1}{2}\omega_{r,j+1}\right]_{n-1},\\
&B_3=\left[\frac{1}{h^2},\frac{4}{h^2}+\frac{1}{2}\omega_{r+1,j},\frac{1}{h^2}\right]_{n-1}.
\end{aligned}$$

Vectors $c_1(t)$ and $c_2(t)$ can be obtained from the boundary values of u. For example,

$$\begin{aligned}
c_1(t)=\Big[&\frac{-i}{2}(\psi_3(y_1,t)+\psi_1(x_1,t)),\frac{-i}{2}\psi_3(y_2,t),\dots,\frac{-i}{2}\psi_3(y_{n-2},t),\\
&\frac{-i}{2}\Big(\psi_3(y_{n-1},t)+\psi_2(x_1,t)\Big),\frac{-i}{2}\psi_1(x_2,t),0,\dots,0,\frac{-i}{2}\psi_2(x_2,t),\dots,\\
&\frac{-i}{2}\psi_1(x_{n-2},t),0,\dots,0,\frac{-i}{2}\psi_2(x_{n-2},t),\frac{-i}{2}(\psi_4(y_1,t)+\psi_1(x_{n-1},t)),\\
&\frac{-i}{2}\psi_4(y_2,t),\dots,\frac{-i}{2}\psi_4(y_{n-2},t),\frac{-i}{2}\Big(\psi_4(y_{n-1},t)+\psi_2(x_{n-1},t)\Big)\Big].
\end{aligned}$$

The basic form of $c_2(t)$ is similar to $c_1(t)$. It depends on coefficients from matrix B_{xy}. For the sake of simplicity, we omit it.

By (2.19) and (2.20), we obtain the sixth-order ETR1 solver for (3.9).

$$\begin{aligned}
(A\otimes A_{xy}-\tau B\otimes B_{xy})u=&-(A\otimes I_{(n-1)^2})c_1+\tau(B\otimes I_{(n-1)^2})c_2-a_0\otimes A_{xy}u_0\\
&+\tau(b_0\otimes\Big(B_{xy}u_0)\Big)-a_0\otimes c_1(0)+\tau\Big(b_0\otimes I_{(n-1)^2}c_2(0)\Big),
\end{aligned}\tag{3.10}$$

where matrices A,B and vectors a_0,b_0 are those given in Section 2.5, and

$$\begin{aligned}
&u\approx[u_{1,1}(t_1),\dots,u_{1,n-1}(t_1),\dots,u_{n-1,1}(t_1),\dots,u_{n-1,n-1}(t_1),\dots,\\
&u_{1,1}(t_{N+1}),\dots,u_{1,n-1}(t_{N+1}),\dots,u_{n-1,1}(t_{N+1}),\dots,u_{n-1,n-1}(t_{N+1})]^T,
\end{aligned}$$

$$c_1=\left[c_1(t_1)^T,\ldots,c_1(t_{N+1})^T\right]^T,\quad c_2=\left[c_2(t_1)^T,\ldots,c_2(t_{N+1})^T\right]^T,$$
$$u_0=[\phi(x_1,y_1),\ldots,\phi(x_1,y_{n-1}),\ldots,\phi(x_{n-1},y_1),\ldots,\phi(x_{n-1},y_{n-1})]^T,$$

The linear system of (3.10) has a sparse coefficient matrix. We use GMRES iterative method to solve it. For more details, please see [5] and references therein.

Remark 3.1. If ETRs with various orders are used to obtain systems (3.10), then the convergence order in time of numerical solutions will be alternatively changed, say, from four to six.

Remark 3.2. By the stability analysis in Section 2.3, we know that the sixth-order ETR1 solver to (3.10) is unconditionally stable. The solution of (3.10) is indeed approximate solution of (3.9). Error accumulation will not really impact the accuracy of approximation.

3.3 Richardson extrapolation

To our knowledge, the convergence order of (3.10) will reach $O(\tau^6+h^4)$. Let us denote $u_{r,j}^k \approx u(x_r,y_j,t_k)$. According to (3.6), we have

$$u_{r,j}^k(\tau,h)=u(x_r,y_j,t_k)+O(h^4)+O(h^6)+O(\tau^6), \tag{3.11}$$
$$u_{2r,2j}^k(\tau,\frac{h}{2})=u(x_r,y_j,t_k)+O(\frac{h^4}{16})+O(h^6)+O(\tau^6). \tag{3.12}$$

Multiplying (3.11) and (3.12) by $-\frac{1}{15}$ and $\frac{16}{15}$ respectively, and adding the two products together, we will obtain a sum without $O(h^4)$. Actually we obtain a new approximate solution $(u_E)_{r,j}^k$ with convergence order $O(\tau^6+h^6)$.

$$\begin{cases} \frac{16}{15}u_{2r,2j}^k(\tau,\frac{h}{2})-\frac{1}{15}u_{r,j}^k(\tau,h)=u(x_r,y_j,t_k)+O(\tau^6+h^6). \\ (u_E)_{r,j}^k=\frac{16}{15}u_{2r,2j}^k(\tau,\frac{h}{2})-\frac{1}{15}u_{r,j}^k(\tau,h). \end{cases} \tag{3.13}$$

Remark 3.3. Richardson extrapolation is a widely used technique to increase the convergence order. Zhou et. al. in [25] provided an extrapolation method to increase the convergence order to $O(\tau^6+h^6)$ for parabolic equations. More applications of Richardson extrapolation for two-dimensional linear Schrödinger equation, please refer to [11,15,23,24].

Remark 3.4. Our method associated with Richardson extrapolation for solving Schrödinger equation is compact sixth-order extended trapezoidal rules both in space and time. This method is also feasible and useful to unsteady convection-diffusion problems instead of the fourth-order compact boundary method in [10].

4 Numerical experiments

For frequently used linear Shrödinger equations [11, 13, 17, 23, 24], we compute four test examples by using ETRs with various orders. With different steps h,τ, we perform our methods on AMD Phenom (tm) II X4 830 CPU 2.79 GHZ with 3 GB RAM. All codes are written in Python on Linux system. Notice that the CBBVM in [10,17,20] is not employed here to require the save of computational cost. But instead, the basic GMRES iterative method is used to produce satisfactory results.

All the numerical results in following tables are maximum errors on which our comparison depends.

4.1 Test example 1

Consider (1.1) with $a=0$, $b=1$, $\omega(x,y)=0$. Provide the following initial function $\varphi(x,y)=(\sin(x)+\sin(y))$. The exact solution is thus

$$u(x,y,t)=e^{-it}(\sin(x)+\sin(y)). \tag{4.1}$$

Table 3: Ex. 1 by ETR1.

h,τ	fourth-order ETR1		sixth-order ETR1		E sixth-order	
	Real part	Imag part	Real part	Imag part	Real part	Imag part
(1/8,1/8)	1.3540e-06	8.8259e-07	3.4690e-08	7.5288e-08	8.4125e-08	2.1036e-07
(1/12,1/12)	1.0545e-07	2.5040e-07	7.3539e-09	4.9541e-09	2.3273e-09	7.0549e-09
(1/16,1/16)	7.0706e-08	9.4122e-08	1.3887e-09	1.7045e-09	1.0927e-09	0.6540e-09
(1/20,1/20)	3.0634e-08	2.3440e-08	5.9386e-10	4.1091e-10	2.9704e-10	3.7602e-10
(1/24,1/24)	1.0131e-08	9.3758e-09	1.3333e-10	1.1091e-10	*	*
(1/28,1/28)	5.9374e-09	4.9877e-09	1.3041e-10	9.9124e-11	*	*
(1/32,1/32)	3.1493e-09	2.0664e-09	1.6033e-10	1.4815e-10	*	*
(1/40,1/40)	1.0670e-09	1.1926e-09	1.6118e-10	1.1070e-10	*	*

Table 4: Ex. 1 by ETR2.

h,τ	fourth-order ETR2		fourth-order ETR2 [17]		sixth-order ETR2		E sixth-order	
	Real part	Imag part	Real part	Imag part	Real part	Imag part	Real part	Imag part
(1/8,1/8)	1.3148e-05	5.2298e-06	7.6846e-07	6.3543e-07	2.0807e-07	2.1801e-07	2.9299e-07	3.3033e-07
(1/12,1/12)	2.1100e-06	8.5024e-06	1.0500e-07	2.3244e-07	6.7764e-09	6.6343e-09	1.1011e-08	1.4451e-08
(1/16,1/16)	1.5537e-06	1.5067e-06	6.3209e-08	6.1597e-08	9.2613e-10	2.1092e-09	6.8127e-10	3.8448e-09
(1/20,1/20)	3.4172e-07	3.2150e-07	2.0116e-08	1.6998e-08	5.1817e-10	2.3474e-10	4.9722e-10	8.6423e-10
(1/24,1/24)	1.4377e-07	2.5205e-07	7.7260e-09	9.1422e-09	2.0071e-10	1.7681e-10	*	*
(1/28,1/28)	9.7861e-08	7.1996e-08	4.5811e-09	3.8960e-09	1.2913e-10	1.9966e-10	*	*
(1/32,1/32)	5.8910e-08	3.8071e-08	1.8049e-09	2.1598e-09	2.3721e-10	8.5120e-11	*	*
(1/40,1/40)	1.9583e-08	4.6734e-08	6.8149e-10	4.5188e-10	7.8032e-11	2.5671e-10	*	*

4.2 Test example 2

Consider (1.1) with $a=0,b=1,\omega(x,y)=3-2\tanh^2(x)-2\tanh^2(y)$. Provide the following initial function $\varphi(x,y)=\frac{i}{\cosh(x)\cosh(y)}$. The exact solution is thus

$$u(x,y,t)=\frac{i\exp(it)}{\cosh(x)\cosh(y)}. \tag{4.2}$$

Boundary conditions can be naturally derived from (4.2).

Table 5: Ex. 2 by ETR1.

h,τ	fourth-order ETR1		sixth-order ETR1		E sixth-order	
	Real part	Imag part	Real part	Imag part	Real part	Imag part
(1/8,1/8)	2.5222e-06	2.4376e-06	1.5391e-06	3.4223e-06	8.4125e-08	2.1036e-07
(1/12,1/12)	1.8556e-07	6.2470e-07	7.9454e-08	1.7105e-07	2.3273e-09	7.0549e-09
(1/16,1/16)	7.5293e-08	1.8440e-07	3.7134e-08	2.6676e-08	1.0927e-09	0.6540e-09
(1/20,1/20)	6.1375e-08	3.7746e-08	2.3561e-08	4.5981e-08	2.9704e-10	3.7602e-10
(1/24,1/24)	1.0764e-08	2.2840e-08	1.2933e-08	1.1936e-08	*	*
(1/28,1/28)	9.9627e-09	1.0448e-08	1.2755e-08	6.1271e-09	*	*
(1/32,1/32)	9.7173e-09	3.8983e-09	6.1118e-09	5.4980e-09	*	*
(1/40,1/40)	3.3095e-09	2.6256e-09	*	*	*	*

Table 6: Ex. 2 by ETR2.

h,τ	fourth-order ETR2		fourth-order ETR2 [17]		sixth-order ETR2		E sixth-order	
	Real part	Imag part	Real part	Imag part	Real part	Imag part	Real part	Imag part
(1/8,1/8)	1.5524e-05	8.2397e-06	2.2938e-06	3.0451e-06	3.1526e-06	3.0019e-06	1.9322e-07	2.9219e-07
(1/12,1/12)	4.2587e-07	7.0620e-06	1.2353e-07	4.9920e-07	1.4857e-07	2.6754e-07	4.8235e-09	1.6058e-08
(1/16,1/16)	5.1793e-07	1.4646e-06	5.4540e-08	1.1617e-07	3.4205e-08	3.4464e-08	1.3352e-09	2.1394e-09
(1/20,1/20)	2.5559e-07	4.4610e-07	5.2634e-08	5.6841e-08	1.8918e-08	4.2241e-08	5.2749e-10	3.7849e-10
(1/24,1/24)	1.6608e-07	2.0237e-07	9.0371e-09	1.9222e-08	1.7633e-08	1.1129e-08	*	*
(1/28,1/28)	8.9307e-08	7.2697e-08	1.3044e-08	9.3083e-09	1.2201e-08	9.4687e-09	*	*
(1/32,1/32)	5.2799e-08	3.9565e-08	8.8403e-09	4.7043e-09	4.7484e-09	6.0042e-09	*	*
(1/40,1/40)	1.8341e-08	3.0571e-08	2.6740e-09	3.2745e-09	1.8541e-09	2.6080e-09	*	*

4.3 Test example 3

Consider (1.1) with an open domain problem, where $a=-2.5,b=2.5,\omega(x,y)=0$. Provide the following initial function $\varphi(x,y)=e^{-ik_0x-(x^2+y^2)}$, which generates the transient Gaussian distribution

$$u(x,y,t)=\frac{i}{i-4t}e^{\left(-i((x^2+y^2+ik_0x+k_0^2it)/(i-4t))\right)}. \tag{4.3}$$

The function $u(x,y,t)$ is initially centered at $(0,0)$ and then moving along the negative x-direction as time evolves. The wave number k_0 is here tested with $k_0=2.5$ and $k_0=0.5$. Boundary conditions can also be derived from (4.3).

Case k_0=2.5

Table 7: Ex. 3 by ETR1 with k_0=2.5.

space step	time step	fourth-order ETR1		sixth-order ETR2	
		Real part	Imag part	Real part	Imag part
40	40	0.000213346	0.000214359	0.000213205	0.000214225
50	50	8.59215e-05	8.80028e-05	8.58587e-05	8.79400e-05
55	55	5.90311e-05	6.00736e-05	5.89912e-05	6.00341e-05
60	60	4.08308e-05	4.29534e-05	4.08055e-05	4.29232e-05
65	65	3.0153e-05	3.0830e-05	*	*

Table 8: Ex. 3 by ETR2 with k_0=2.5.

space step	time step	fourth-order ETR2		sixth-order ETR2	
		Real part	Imag part	Real part	Imag part
40	40	0.000213320	0.000214334	0.000213205	0.000214225
50	50	8.59058e-05	8.79875e-05	8.58584e-05	8.79401e-05
55	55	5.90204e-05	6.00629e-05	5.89911e-05	6.00342e-05
60	60	4.08239e-05	4.29544e-05	4.08054e-05	4.29232e-05
65	65	3.01534e-05	3.08300e-05	3.01378e-05	3.08138e-05

Table 9: Ex. 3 by E sixth-order with k_0=2.5.

space step	time step	E sixth-order ETR1		E sixth-order ETR2	
		Real part	Imag part	Real part	Imag part
10	10	0.001127727	0.000571239	0.001124961	0.000572365
20	20	1.25567e-05	1.25337e-05	1.25598e-05	1.25362e-05
25	25	3.24548e-06	3.25194e-06	3.25454e-06	3.25911e-06
30	30	*	*	1.12320e-06	1.09956e-06

Case $k_0=0.5$

Table 10: Ex. 3 by ETR1 with k_0=0.5.

space step	time step	fourth-order ETR1		sixth-order ETR1	
		Real part	Imag part	Real part	Imag part
40	40	1.44238e-05	9.57133e-06	1.44191e-05	9.56810e-06
50	50	5.93460e-06	3.91038e-06	5.93270e-06	3.90917e-06
55	55	4.01793e-06	2.66899e-06	4.01676e-06	2.66804e-06
60	60	2.86247e-06	1.88233e-06	2.86154e-06	1.88174e-06
65	65	2.05508e-06	1.36505e-06	*	*

Table 11: Ex. 3 by ETR2 with k_0=0.5.

space step	time step	fourth-order ETR2		sixth-order ETR2	
		Real part	Imag part	Real part	Imag part
40	40	1.44229e-05	9.57078e-06	1.44191e-05	9.56809e-06
50	50	5.93417e-06	3.91009e-06	5.93270e-06	3.90921e-06
55	55	4.01765e-06	2.66874e-06	4.01676e-06	2.66805e-06
60	60	2.86222e-06	1.88215e-06	2.86154e-06	1.88178e-06
65	65	2.05493e-06	1.36490e-06	2.05451e-06	1.36454e-06

Table 12: Ex. 3 by E sixth-order with k_0=0.5.

space step	time step	E sixth-order ETR1		E sixth-order ETR2	
		Real part	Imag part	Real part	Imag part
10	10	4.68075e-05	2.28108e-05	4.68103e-05	2.28387e-05
20	20	5.62901e-07	3.84382e-07	5.62130e-07	3.85044e-07
25	25	1.51025e-07	9.94895e-08	1.50925e-07	9.96516e-08
30	30	5.20329e-08	3.29773e-08	5.20190e-08	3.31157e-08

4.4 Test example 4

Consider (1.1) with

$$a=0,b=1,\omega(x,y)=-\frac{4x^2+4y^2-4x-4y+\beta^2-4\beta+2}{\beta^2}.$$

Provide the following initial function $\varphi(x,y)=e^{-\frac{(x-0.5)^2}{\beta}-\frac{(y-0.5)^2}{\beta}}$, which generates the transient Gaussian distribution

$$u(x,y,t)=e^{-\frac{(x-0.5)^2}{\beta}-\frac{(y-0.5)^2}{\beta}-it} \tag{4.4}$$

Table 13: Ex. 4 by ETR1 with β=0.5.

h,τ	fourth-order ETR1		sixth-order ETR1		E sixth-order	
	Real part	Imag part	Real part	Imag part	Real part	Imag part
(1/8,1/8)	2.8923e-05	5.4086e-05	4.1791e-06	1.1666e-05	1.4463e-08	6.8715e-09
(1/12,1/12)	1.0391e-06	5.7207e-07	4.0181e-06	1.6374e-06	9.3227e-09	3.5786e-09
(1/16,1/16)	6.0380e-07	4.5665e-07	7.1341e-07	4.0877e-07	1.4679e-09	1.1960e-09
(1/20,1/20)	2.3410e-07	1.4718e-07	5.0302e-07	2.0591e-07	2.4981e-10	2.6100e-10
(1/24,1/24)	1.3021e-07	9.5952e-08	2.7930e-07	9.2733e-08	*	*
(1/28,1/28)	7.5273e-08	5.1069e-08	1.4236e-07	4.6678e-08	*	*
(1/32,1/32)	4.4995e-08	2.1869e-08	8.2092e-08	2.9901e-08	*	*
(1/40,1/40)	2.7763e-08	1.5645e-08	*	*	*	*

Table 14: Ex. 4 by ETR2 with β=0.5.

h,τ	fourth-order ETR2		sixth-order ETR2		E sixth-order	
	Real part	Imag part	Real part	Imag part	Real part	Imag part
(1/8,1/8)	4.5767e-05	0.00011081	1.1424e-05	1.4378e-05	2.5206e-08	3.3978e-08
(1/12,1/12)	2.7952e-06	2.1359e-06	3.5067e-06	2.1118e-06	1.4313e-08	6.9036e-09
(1/16,1/16)	2.2082e-07	3.8459e-07	1.0870e-06	5.1952e-07	1.3022e-09	1.7616e-09
(1/20,1/20)	2.7006e-07	2.3705e-07	4.5702e-07	2.4896e-07	4.4629e-10	1.1144e-10
(1/24,1/24)	2.3529e-07	1.2006e-07	2.6795e-07	9.1002e-08	*	*
(1/28,1/28)	1.5812e-07	7.5954e-08	1.2414e-07	5.5799e-08	*	*
(1/32,1/32)	7.3039e-08	4.6183e-08	6.9837e-08	4.0550e-08	*	*
(1/40,1/40)	2.6131e-08	1.2273e-08	2.1414e-08	1.4899e-08	*	*

Boundary conditions can be easily derived from (4.4). We set $\beta=0.5$ and the initial condition is a Gaussian pulse with unit height centered at $x=0.5$ and $y=0.5$.

For test examples (4.1) and (4.2), we show the comparison of numerical results by conducting fixed-order ETRs in coarse steps in time and space. Results in Tables 3, 4, 5 and 6 show the high accuracy of fourth-order ETRs and sixth-order ETRs. The sixth-order extrapolation results are also illustrated. However, due to the truncation errors produced by E sixth-order ETRs, there is no information being definitely positive for sixth-order ETRs and E sixth-order ETRs. Here we actually do not claim the priority of ETR1 and ETR2, even though the numerical results and computational cost show the advantage of ETR2. In addition, the numerical results of test examples (4.3) and (4.4) are quite affected by the different values of parameters k_0 and β. The reason for this phenomenon seems to be another topic to be studied in the future. At the same time, for problem (4.3) in case $k_0=2.5$ or case $k_0=0.5$, there is small difference between the results of fourth-order and sixth-order ETR1. If we compare the results of ETR1 and ETR2, the same phenomenon occurs. For test example (4.4), we draw six pictures about surface plot of error with different steps corresponding to Table 14.

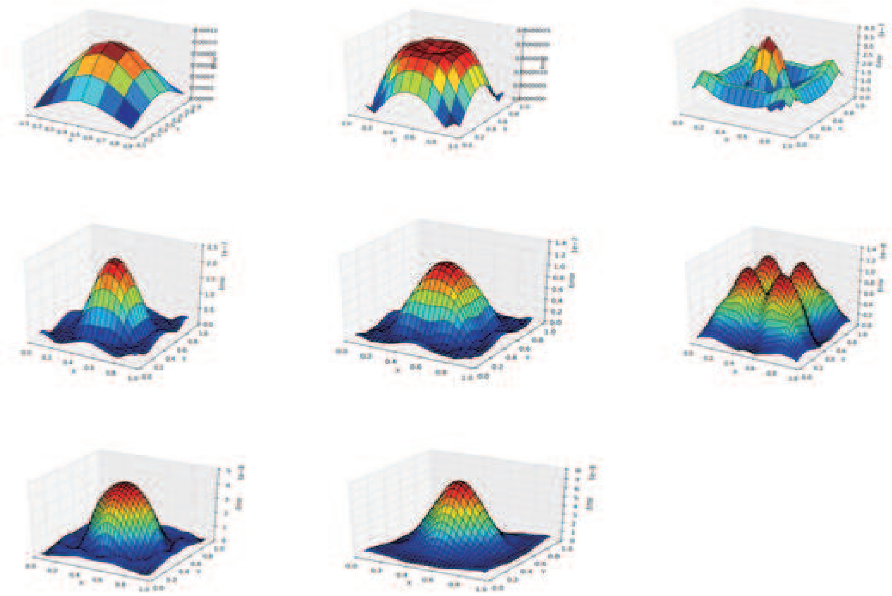

Figure 1: Imag part of Fourth-order ETR2, error surface vs steps.

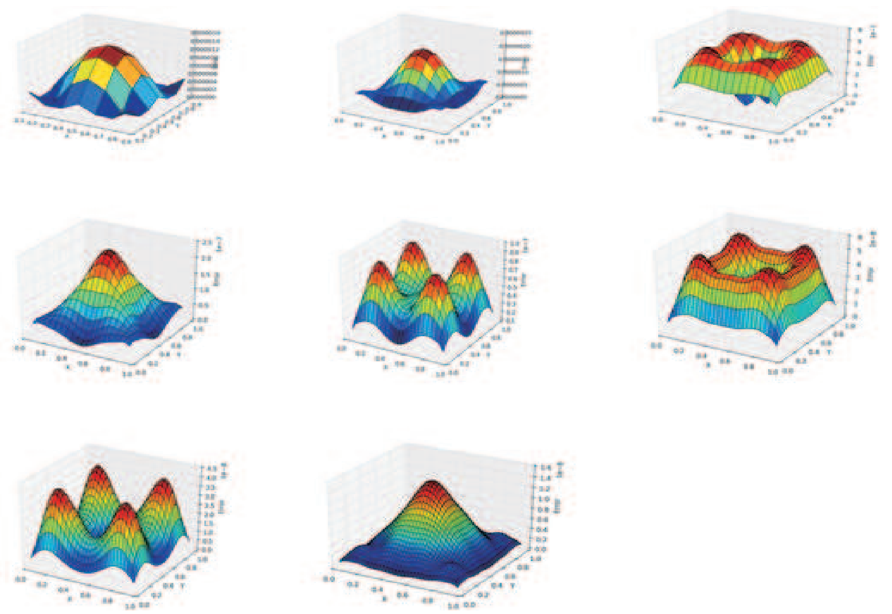

Figure 2: Imag part of Sixth-order ETR2, error surface vs steps.

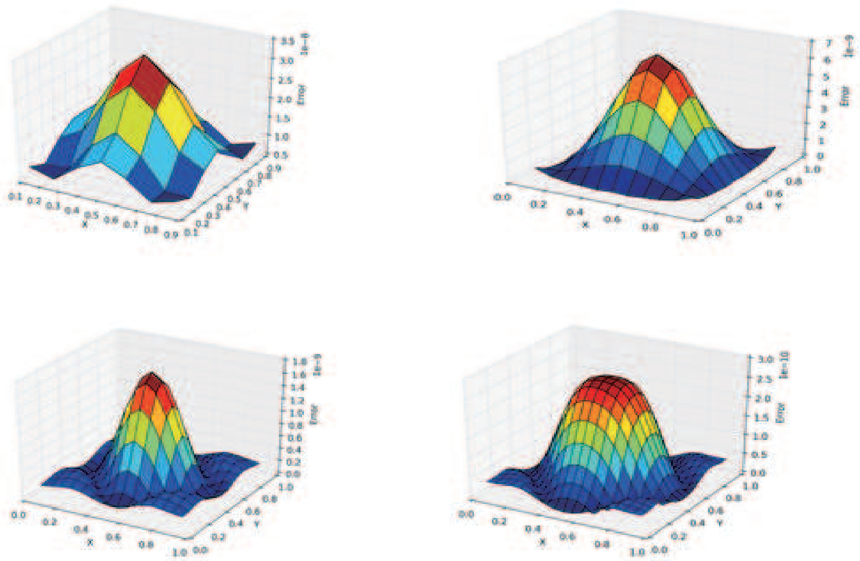

Figure 3: Imag part of E Sixth-order ETR2, error surface vs steps.

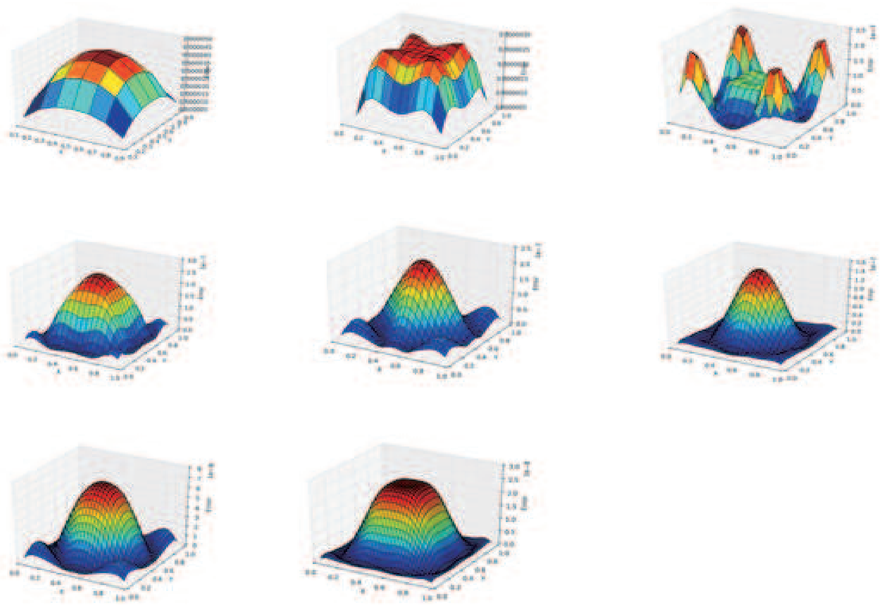

Figure 4: Real part of Fourth-order ETR2, error surface vs steps.

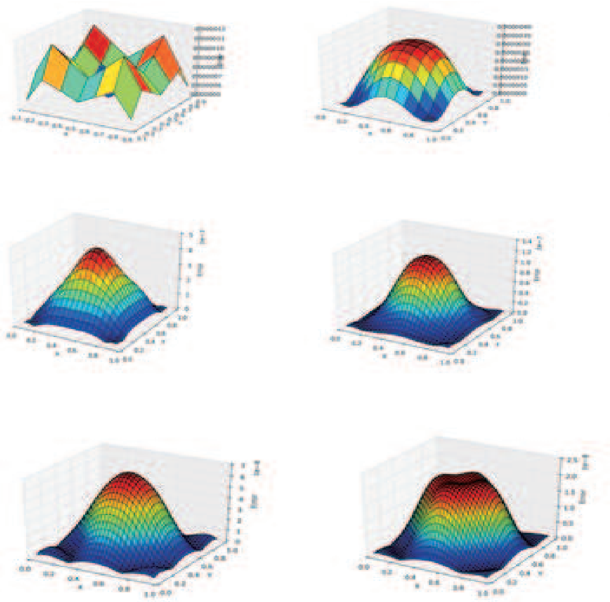

Figure 5: Real part of Sixth-order ETR2, error surface vs steps.

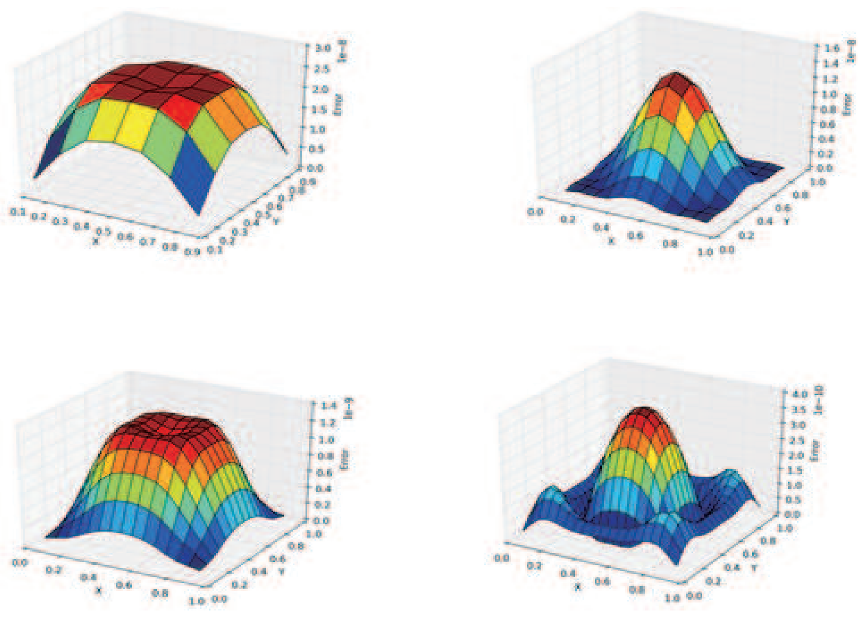

Figure 6: Real part of E Sixth-order ETR2, error surface vs steps.

Numerical experiments performed give illustration that the fourth-order ETR1, sixth-order ETR1, E sixth-order ETR1 and fourth-order ETR2, sixth-order ETR2, E sixth-order ETR2 combined with the fourth-order Padé compact technique are in high accuracy for solving Shrödinger equation.

5 Conclusion

Combining BVMs with $(\nu,\nu-1)$-boundary conditions, we modify symmetric ETRs with same numbers of initial and finial equations, which can be obtained by a class of Adams-Moulton. Making use of the Kronecker products, we extend the application of ETRs with various orders to ODEs. Instead of using compact ADI schemes from [11, 13–15, 23, 24] for Schrödinger equation, we apply the sixth-order ETRs to the fourth-order Padé compact scheme. Then a stable scheme with order $O(\tau^6+h^4)$ is presented. Furthermore the convergence order in time can be changed alternatively by using various ETRs. By virtue of Richardson extrapolation, the convergence order will be raised to $O(\tau^6+h^6)$. This is a good method with high accuracy. Finally, numerical tests of four examples are carried out to confirm the stability and the high convergence of our methods.

Acknowledgments

This work was supported by NSFC (No.11471150 and 11401281), National Basic Research (No.973), Program of China under Grant (No.2011CB706903), and the CAPES and CNPq in Brazil. We are indebted to two anonymous responsible referees for valuable comments on an earlier version of the article.

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