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

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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

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

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