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Optimal Error Estimates in Numerical Solution of Time Fractional Schrödinger Equations on Unbounded Domains

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Abstract. The artificial boundary method is used to reformulate the time fractional Schrödinger equation on the real line as a bounded problem with exact artificial boundary conditions. The problem appeared is solved by a numerical method employing the $L1$-formula for the Caputo derivative and finite differences for spatial derivatives. The convergence of the method studied and optimal error estimates in a special metric are obtained. The technique developed here can be also applied to study the convergence of approximation methods for standard Schrödinger equation.

AMS subject classifications: 65M06, 35B65

Key words: Time fractional Schrödinger equation, artificial boundary method, optimal error estimate, stability and convergence.

1. Introduction

Fractional partial differential equations (PDEs) attract a lot of attention because of wide applications in various fields of science and engineering. In particular, they help to address nonlocal phenomena in quantum physics and to explore the quantum behavior of long-range interactions or time-dependent processes with many scales. Thus fractional quantum models are described by fractional Schrödinger equations — cf. Refs. [5, 9, 11, 14, 17, 21–24, 29, 30]. Here we consider the numerical solutions of the time fractional Schrödinger equation

$$\mathrm{i}\,{}_0^C D_t^\alpha u(x,t) = -\partial_x^2 u(x,t) + V(x)u(x,t), \quad x\in\mathbb{R}, \quad 0<t\le T, \tag{1.1}$$

$$u(x,0)=\psi(x), \quad x\in\mathbb{R}, \tag{1.2}$$

$$u\to 0, \quad \text{as} \quad |x|\to\infty, \tag{1.3}$$

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on the unbounded domain $\mathbb{R}$. Note that $\mathrm{i}=\sqrt{-1}$, $u(x,t)$ represents a complex-valued wave function, the initial value $\psi(x)$ is a compactly supported function, $V(x)$ is the real-valued external potential function, and ${}_0^CD_t^\alpha u$, $0<\alpha<1$ refers to the Caputo fractional derivative

$$ {}_0^CD_t^\alpha u(x,t)=\frac{1}{\Gamma(1-\alpha)}\int_0^t \frac{\partial_s u(x,s)}{(t-s)^\alpha}ds. \tag{1.4}$$

There are many approximation methods for PDEs in unbounded domains with the artificial boundary method (ABM) being the one of most efficient [3, 6–8, 12, 13, 16]. The main idea of ABM is to introduce artificial boundaries and reduce the original problem to a problem on a bounded computational domain. Note that the design of artificial boundary conditions (ABCs) has an important impact on the overall performance and accuracy of the corresponding numerical schemes. The exact ABCs mean that the solution of the truncated domain problem is rendered exactly the same as in the unbounded domain problem. As was established in [19], the problem (1.1)-(1.3) can be reduced to the following initial-boundary value problem

$$\mathrm{i}\,{}_0^CD_t^\alpha u(x,t)+u_{xx}(x,t)+V(x)u(x,t)=0, \quad x\in(x_l,x_r), \quad t\in(0,T], \tag{1.5}$$

$$u_x(x_l,t)=\mathrm{e}^{-\pi\mathrm{i}/4}\,{}_0^CD_t^{\alpha/2}u(x_l,t), \quad t\in(0,T], \tag{1.6}$$

$$u_x(x_r,t)=-\mathrm{e}^{-\pi\mathrm{i}/4}\,{}_0^CD_t^{\alpha/2}u(x_r,t), \quad t\in(0,T], \tag{1.7}$$

$$u(x,0)=\psi(x), \quad x\in[x_l,x_r]. \tag{1.8}$$

It is worth mentioning that for the standard Schrödinger equation — i.e. in the case when $\alpha=1$, the development and analysis of unconditionally stable schemes for reduced problems in bounded domains requires substantial efforts. Thus Arnold and Ehrhard [2] derived exact discrete ABCs immediately from a fully discretised Schödinger equation. Schmidt and Yevick [26] proposed an efficient fully discrete scheme based on a finite element method for spatial discretisation. Mayfield [20], Baskakov and Popov [4], Antoine *et al.* [1], Han *et al.* [15] and Ducomet *et al.* [10] presented straightforward approaches to construct unconditionally stable discretisation schemes. However, although the stability of the methods is well studied, the optimal error estimates are less known. The main reason for this is that the temporal convolution arising in exact ABCs causes problems in convergence analysis. So far only the sub-optimal error estimate $\mathscr{O}(h^{3/2}+\tau^{3/2}h^{-1/2}+h^2+\tau^2)$ for the standard Schödinger equation has been established [15, 28]. Recently, Li *et al.* [18] proved an asymptotic optimal-order error estimate for a numerical scheme by including a constant damping term into the governing equation and modifying the standard Crank-Nicolson implicit scheme. For time fractional Schödinger equations with $0<\alpha\le 1$, the only existing sub-optimal estimate is $\mathscr{O}(h^{3/2}+\tau^{1/2+\alpha}h^{-1/2}+h^2+\tau^2)$ and it is obtained for L^2-norm errors.

The aim of this paper is to establish an optimal error estimate for the reduced problem with exact ABCs while discretising the Caputo derivative by the $L1$-formula and using finite differences for spatial derivatives. In particular, we evaluate spatial-related errors in H^1-norm and time-related ones in L^2-norm, denoting the resulting measure as $L^2(H^1)$. This is because in contrast to anomalous diffusion equations [12], the imaginary part of the inner