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Computing the Ground and First Excited States of the Fractional Schrödinger Equation in an Infinite Potential Well

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Abstract. In this paper, we numerically study the ground and first excited states of the fractional Schrödinger equation in an infinite potential well. Due to the nonlocality of the fractional Laplacian, it is challenging to find the eigenvalues and eigenfunctions of the fractional Schrödinger equation analytically. We first introduce a normalized fractional gradient flow and then discretize it by a quadrature rule method in space and the semi-implicit Euler method in time. Our numerical results suggest that the eigenfunctions of the fractional Schrödinger equation in an infinite potential well differ from those of the standard (non-fractional) Schrödinger equation. We find that the strong nonlocal interactions represented by the fractional Laplacian can lead to a large scattering of particles inside of the potential well. Compared to the ground states, the scattering of particles in the first excited states is larger. Furthermore, boundary layers emerge in the ground states and additionally inner layers exist in the first excited states of the fractional nonlinear Schrödinger equation. Our simulated eigenvalues are consistent with the lower and upper bound estimates in the literature.

AMS subject classifications: 35Q40, 45C05, 65M06, 81Q05, 82D05

Key words: Fractional Schrödinger equation, Riesz fractional Laplacian, infinite potential well, ground states, first excited states, quadrature rule.

1 Introduction

The fractional Schrödinger equation, a fundamental model of fractional quantum mechanics, was first introduced by Laskin as the path integral of the Lévy trajectories [29,30]. It is a nonlocal integro-differential equation that is expected to reveal some novel phenomena of the quantum mechanics. Recently, the fractional Schrödinger equation in an

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infinite potential well has attracted massive attention from both physicists and mathematicians, and numerous studies have been devoted to finding its eigenvalues and eigenfunctions; see [6, 12, 19, 20, 23, 26, 30, 31, 36] and references therein. However, one continuing debate in the literature is whether the fractional linear Schrödinger equation in an infinite potential well has the same eigenfunctions as those of its standard (non-fractional) counterpart [6, 12, 19, 23, 31]. The main goal of this paper is to numerically study the ground and first excited states of the fractional Schrödinger equation in an infinite potential well so as to advance the understanding of this problem.

We consider the one-dimensional (1D) fractional Schrödinger equation of the following form [6,19,20,23,24,30,31]:

$$i\partial_t\psi(x,t)=(-\Delta)^{\alpha/2}\psi+V(x)\psi+\beta|\psi|^2\psi, \qquad x\in\mathbb{R}, \quad t>0, \tag{1.1}$$

where $\psi(x,t)$ is a complex-valued wave function, and $i=\sqrt{-1}$ is the imaginary unit. The constant $\beta\in\mathbb{R}$ describes the strength of local (or short-range) interactions between particles (positive for repulsive interactions and negative for attractive interactions), and $V(x)$ represents an external trapping potential. In this paper, we are interested in the case that $\beta\geq 0$ and $V(x)$ is an infinite potential well (also known as box potential), i.e.,

$$V(x)=\begin{cases} 0, & \text{if } |x|<L, \\ \infty, & \text{otherwise}, \end{cases} \qquad x\in\mathbb{R}, \tag{1.2}$$

with the constant $L>0$. The Riesz fractional Laplacian $(-\Delta)^{\alpha/2}$ is defined as [11, 13, 31, 32, 34]:

$$(-\Delta)^{\alpha/2}u(x)=C_{1,\alpha}\,\text{P.V.}\int_{\mathbb{R}}\frac{u(x)-u(y)}{|x-y|^{1+\alpha}}dy, \qquad \alpha\in(0,2), \tag{1.3}$$

where P.V. stands for principal value, and $C_{1,\alpha}$ is a normalization constant given by

$$C_{1,\alpha}=\frac{2^{\alpha-1}\alpha\Gamma((1+\alpha)/2)}{\sqrt{\pi}\Gamma(1-\alpha/2)}=\frac{\Gamma(1+\alpha)\sin(\alpha\pi/2)}{\pi}, \qquad \alpha\in(0,2).$$

The fractional Laplacian in (1.3) can be obtained from the inverse of the Riesz potential [28, 32]. It is discussed in [11, 13, 35] as a special case of nonlocal operators with the kernel function proportional to $\mathcal{K}(x,y)=1/|x-y|^{1+\alpha}$. In the literature, the Riesz fractional Laplacian $(-\Delta)^{\alpha/2}$ is also defined via a pseudo-differential operator with the symbol $|\kappa|^\alpha$ [24,30,32,41]:

$$(-\Delta)^{\alpha/2}u(x)=\mathcal{F}^{-1}(|\kappa|^\alpha\mathcal{F}(u)), \tag{1.4}$$

where $\mathcal{F}(u)$ represents the Fourier transform of $u(x)$, and $\mathcal{F}^{-1}$ denotes the inverse Fourier transform. We remark that if the function $u(x)$ belongs to the Schwartz space, the integral representation of the fractional Laplacian $(-\Delta)^{\alpha/2}$ in (1.3) is equivalent to its pseudo-differential representation in (1.4) [32,34,37]. For more discussion on the equivalence of (1.3) and (1.4), we refer the readers to [22,27,28,34] and references therein.