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On the numerical solution of the eigenvalue problem in fractional quantum mechanics ☆

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ABSTRACT

In this work we propose a Control Volume Function Approximation (CVFA) method to solve equations involving the fractional Laplacian. The function approximation part is carried out with Radial Basis Function (RBF) interpolation. The physical application of interest is the eigenvalue problem for the time independent fractional Schrödinger equation. Fractional derivatives are considered in the Riesz potentials sense.

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1. Introduction

In recent years, fractional calculus has become a topic of great research activity. This is due to the fact that generalizations of integer to fractional derivatives in connection with physical systems, have found applications in most fields. See for instance the historical survey presented in Machado et al. [1].

The application of interest in this work is to fractional quantum mechanics. Here, the Schrödinger equation is generalized by considering fractional powers of the Laplacian, the *fractional Laplacian*, in the Hamiltonian. A physically sound generalization is that of Laskin [2–4]. Therein a derivation of the fractional Schrödinger equation is developed based on Feynman path integrals over Levy trajectories. Following these works, there has been an explosion on research regarding fractional Schrödinger equations. For instance, in Wang and Xu [5] a fractional Schrödinger equation with space–time fractional derivatives is considered. A solution is proposed by the method of integral transforms. Application to the free particle and square well potential is presented. Of related interest is Tarasov [6], where a fractional generalization of Heisenberg equation is developed, yielding a generalization to quantum Hamiltonian systems. An alternative approach, the D-deformed calculus, to model fractional-dimension systems is introduced in Matos-Abigue [7]. The free particle and the harmonic oscillator are considered as systems in the so called framework of D-deformed quantum mechanics, the process resembles to the classical case. Finally, on the theoretical side, Ionescu and Pusateri [8] carry out a well-posedness analysis for a nonlinear fractional Schrödinger equation in one dimension.

This work is from a numerical perspective. Our purpose is to introduce a numerical method to solve the time independent Schrödinger equation, namely,

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$$\left[D_\alpha\left(-\hbar^2\Delta\right)^{\alpha/2}+V(r)\right]\psi(r)=E\psi(r),\quad 1<\alpha\leqslant 2.$$

Here D_α is a generalized diffusion coefficient, and the fractional Laplacian is defined in terms of the Fourier Transform, namely

$$\left(-\hbar^2\Delta\right)^{\alpha/2}\psi(r)=\frac{1}{(2\pi)^3}\int d^3p\,\exp\left(i\frac{p\cdot r}{\hbar}\right)|p|^\alpha\psi(p).$$

Numerical methods to solve this eigenvalue problem are scarce at best. For the one dimensional case, a collocation method is presented in Amore et al. [9]. Within the method, sampling functions, sampling points and interval of definition of the wave functions, are to be determined according to the prescribed boundary conditions. There is no apparent extension to higher dimensions. In Zoia et al. [10], a matrix representation of the fractional Laplacian is introduced. The eigenvalues and eigenfunctions of such a matrix, converge to the eigenvalues and eigenfunctions of the fractional Laplacian when the size of the matrix tends to infinity. Apparently, the method requires large matrix sizes. For instance, in Kwaśnicki [11], the method is used to approximate the eigenvalues associated to the infinite well potential. Therein, a matrix of size $O(10^3)$ is required.

A difficulty on approximating the Fractional Laplacian, or any fractional derivative for that matter, is its non local property. Consequently, one is led to full and large matrix systems. Moreover, on bounded domains boundary conditions need to be dealt carefully. To address these issues, we propose a method based on the Control Volume Function Approximation method (CVFA), see Li et al. [12]. After integrating on control volumes, function approximation is carried out on the boundaries by local interpolation. Our proposal is to use Radial Basis Function (RBF) for global interpolation. It is well known that RBF approximations lead to ill-posed full matrix systems, but give satisfactory results on coarse discretizations. As we shall see, the latter, and the global feature of RBF are well suited to approximate the fractional Laplacian in the eigenvalue problem. We provide numerical results for the one dimensional cases in the works above. We remark that in all examples it suffices to solve $O(10^2)$ matrix problems. The matrix eigenvalue problem is solved simply by the inverse power method and deflation.

The outline is as follows.

In Section 2 we introduce the classical definition of the fractional Laplacian in terms of Riesz potentials and the Fourier Transform. The restriction to bounded domains is as in Musina and Nazarov [13]. In Section 3 we introduce a Control Volume Radial Basis Function (CVRBF) Method for the eigenvalue problem, in any dimension. We use the simplest radial function, $\phi(r)=r$, for approximation. The matrix problem for the one dimensional case is constructed in Section 4. Numerical results are presented in Section 5. We solve the eigenvalue problem for the infinite well potential, the harmonic potential and the quartic anharmonic potential. In Section 6 we draw conclusions and comment of future work.

2. The fractional Laplacian

2.1. Riesz potentials and the fractional Laplacian

The results in this section are well known, proofs are found for instance in Helgason [14].

We shall use the definition of Fourier Transform as follows

$$\widehat{f}(\mathbf{k})\equiv\mathcal{F}(f)(\mathbf{k})=\int_{\mathbb{R}^d}\exp\left(-i\mathbf{k}\cdot\mathbf{x}\right)f(\mathbf{x})d\mathbf{x}$$

with inverse

$$\mathcal{F}^{-1}(F)(\mathbf{x})=\frac{1}{(2\pi)^d}\int_{\mathbb{R}^d}\exp\left(i\mathbf{k}\cdot\mathbf{x}\right)F(\mathbf{k})d\mathbf{k}.$$

For $s\geqslant 0$ the Sobolev space $H^s(\mathbb{R}^d)\equiv H^s$ is defined as customary by

$$H^s=\left\{f\in L^2:\int_{\mathbb{R}^d}\left(1+|\,\mathbf{k}|^2\right)^s|\,\widehat{f}(\mathbf{k}|^2d\mathbf{k}<+\infty\right\}.$$

Let $\mathcal{S}$ and $\mathcal{S}'$ the spaces of tempered functions and tempered distributions respectively. For the case $s<0$, the Sobolev space is defined as follows

$$H^s=\left\{f\in\mathcal{S}':\int_{\mathbb{R}^d}\left(1+|\,\mathbf{k}|^2\right)^s|\,\widehat{f}(\mathbf{k}|^2d\mathbf{k}<+\infty\right\}.$$

By means of the Fourier Transform, the fractional Laplacian operator, $(-\Delta)^s$ is defined for $f\in H^s$ by

$$(-\Delta)^s f=\mathcal{F}^{-1}\left[|\mathbf{k}|^{2s}\mathcal{F}(f)\right].$$

Let us recall the *Riesz potential*

$$I^\gamma(f)(\mathbf{x})=\frac{1}{H_d(\gamma)}\int f(\mathbf{y})|\mathbf{x}-\mathbf{y}|^{\gamma-d}d\mathbf{y}$$

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